



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:24 AM UTC

PDB ID : 4CR2 / pdb\_00004cr2  
EMDB ID : EMD-2594  
Title : Deep classification of a large cryo-EM dataset defines the conformational landscape of the 26S proteasome  
Authors : Unverdorben, P.; Beck, F.; Sledz, P.; Schweitzer, A.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Foerster, F.  
Deposited on : 2014-02-25  
Resolution : 7.70 Å(reported)

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:

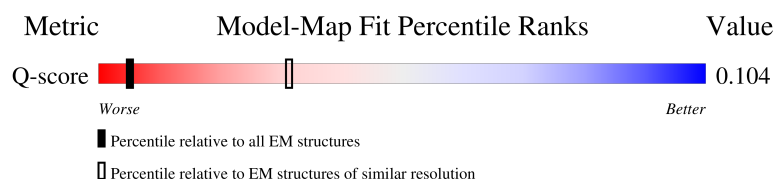
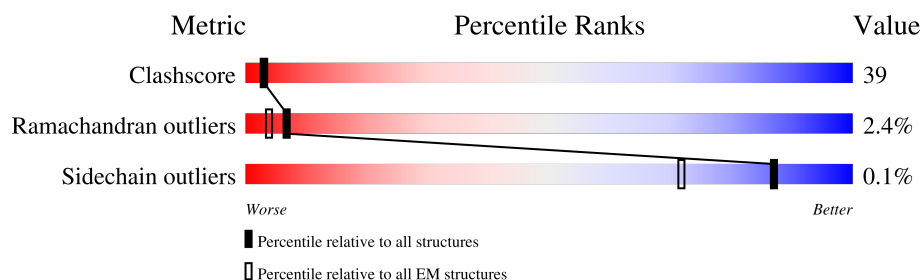
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 7.70 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                       | 384 ( 7.20 - 8.20 )                                      |

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   | 1     | 215    |                  |
| 2   | 2     | 261    |                  |
| 3   | 3     | 205    |                  |
| 4   | 4     | 198    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | 5     | 287    |                  |
| 6   | 6     | 241    |                  |
| 7   | 7     | 266    |                  |
| 8   | A     | 252    |                  |
| 9   | B     | 250    |                  |
| 10  | C     | 258    |                  |
| 11  | D     | 254    |                  |
| 12  | E     | 260    |                  |
| 13  | F     | 234    |                  |
| 14  | G     | 288    |                  |
| 15  | H     | 467    |                  |
| 16  | I     | 437    |                  |
| 17  | J     | 405    |                  |
| 18  | K     | 428    |                  |
| 19  | L     | 437    |                  |
| 20  | M     | 434    |                  |
| 21  | N     | 945    |                  |
| 22  | O     | 393    |                  |
| 23  | P     | 445    |                  |
| 24  | Q     | 434    |                  |
| 25  | R     | 429    |                  |
| 26  | S     | 523    |                  |
| 27  | T     | 274    |                  |
| 28  | U     | 338    |                  |
| 29  | V     | 306    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                         |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------|
| 30  | W     | 268    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>32%24%33%15%•26%</div></div> |
| 31  | X     | 156    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>33%22%39%19%•19%</div></div> |
| 32  | Y     | 89     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>•7%11%•79%</div></div>       |
| 33  | Z     | 993    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>30%25%38%18%•18%</div></div> |

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 80139 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 PROTEASOME COMPONENT PRE3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1576  | 996 | 261 | 312 | 7 |         |       |

- Molecule 2 is a protein called PROTEASOME COMPONENT PUP1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 2     | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1692  | 1067 | 294 | 324 | 7 |         |       |

- Molecule 3 is a protein called PROTEASOME COMPONENT PUP3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 3     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |       |

- Molecule 4 is a protein called PROTEASOME COMPONENT C11.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | 4     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1585  | 1005 | 269 | 305 | 6 |         |       |

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | 5     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1646  | 1045 | 282 | 312 | 7 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 5     | 33      | ARG      | LYS    | SEE REMARK 999 | UNP P30656 |

- Molecule 6 is a protein called PROTEASOME COMPONENT C5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | 6     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |       |

- Molecule 7 is a protein called PROTEASOME COMPONENT PRE4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | 7     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |       |

- Molecule 8 is a protein called PROTEASOME COMPONENT C7-ALPHA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | A     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1921  | 1221 | 322 | 370 | 8 |         |       |

- Molecule 9 is a protein called PROTEASOME COMPONENT Y7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | B     | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |       |

- Molecule 10 is a protein called PROTEASOME COMPONENT Y13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | C     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1913  | 1207 | 323 | 380 | 3 |         |       |

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | D     | 242      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1899  | 1186 | 333 | 376 | 4 |         |       |

- Molecule 12 is a protein called PROTEASOME COMPONENT PUP2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | E     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1165 | 315 | 380 | 7 |         |       |

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | F     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1795  | 1129 | 312 | 350 | 4 |         |       |

- Molecule 14 is a protein called PROTEASOME COMPONENT C1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | G     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1207 | 331 | 358 | 4 |         |       |

- Molecule 15 is a protein called 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | H     | 359      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2792  | 1755 | 499 | 523 | 15 |         |       |

- Molecule 16 is a protein called 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | I     | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2822  | 1773 | 471 | 563 | 15 |         |       |

- Molecule 17 is a protein called 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | J     | 373      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2928  | 1837 | 527 | 547 | 17 |         |       |

- Molecule 18 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | K     | 381      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3019  | 1898 | 530 | 581 | 10 |         |       |

- Molecule 19 is a protein called 26S PROTEASE SUBUNIT RPT4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | L     | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2853  | 1798 | 507 | 536 | 12 |         |       |

- Molecule 20 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | M     | 367      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2866  | 1799 | 503 | 553 | 11 |         |       |

- Molecule 21 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 21  | N     | 849      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6562  | 4174 | 1099 | 1261 | 28 |         |       |

- Molecule 22 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | O     | 387      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3182  | 2047 | 520 | 606 | 9 |         |       |

- Molecule 23 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | P     | 415      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3401  | 2166 | 571 | 655 | 9 |         |       |

- Molecule 24 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | Q     | 431      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3471  | 2205 | 574 | 676 | 16 |         |       |

- Molecule 25 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | R     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3218  | 2051 | 527 | 630 | 10 |         |       |

- Molecule 26 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | S     | 353      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2893  | 1857 | 482 | 541 | 13 |         |       |

- Molecule 27 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN12.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | T     | 272      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2235  | 1432 | 355 | 441 | 7 |         |       |

- Molecule 28 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | U     | 255      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2061  | 1312 | 352 | 391 | 6 |         |       |

- Molecule 29 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | V     | 247      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1942  | 1225 | 328 | 376 | 13 |         |       |

- Molecule 30 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | W     | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1534  | 962 | 269 | 300 | 3 |         |       |

- Molecule 31 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | X     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 664 | 169 | 195 | 4 |         |       |

- Molecule 32 is a protein called 26S PROTEASOME COMPLEX SUBUNIT SEM1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 32  | Y     | 19       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 168   | 101 | 30 | 37 |         |       |

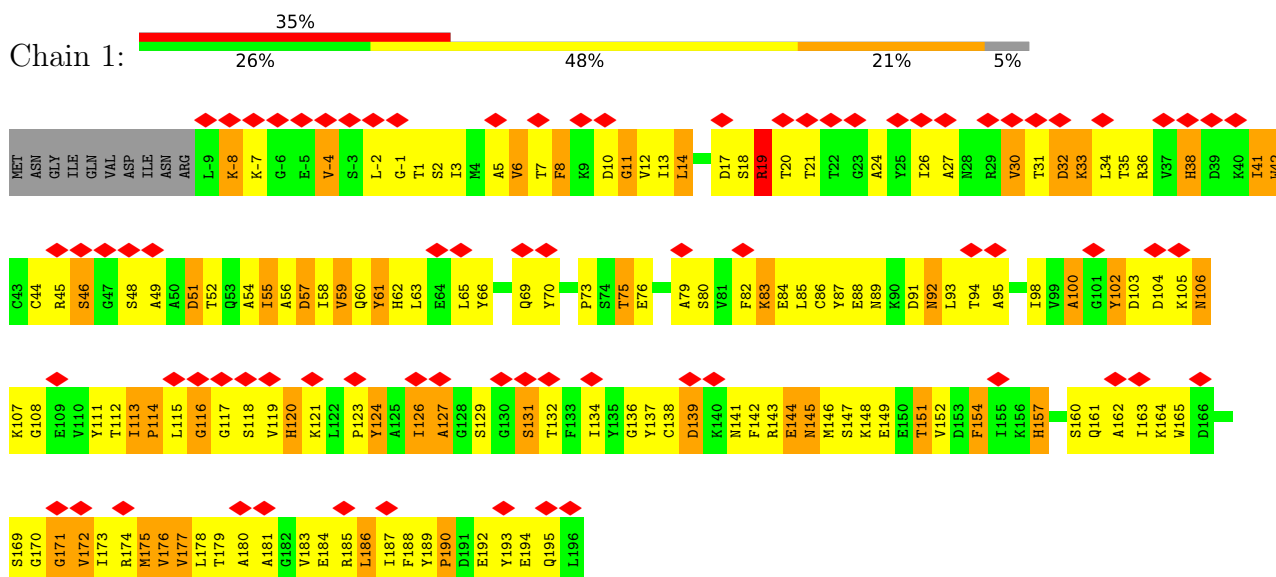
- Molecule 33 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 33  | Z     | 813      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6289  | 3995 | 1029 | 1236 | 29 |         |       |

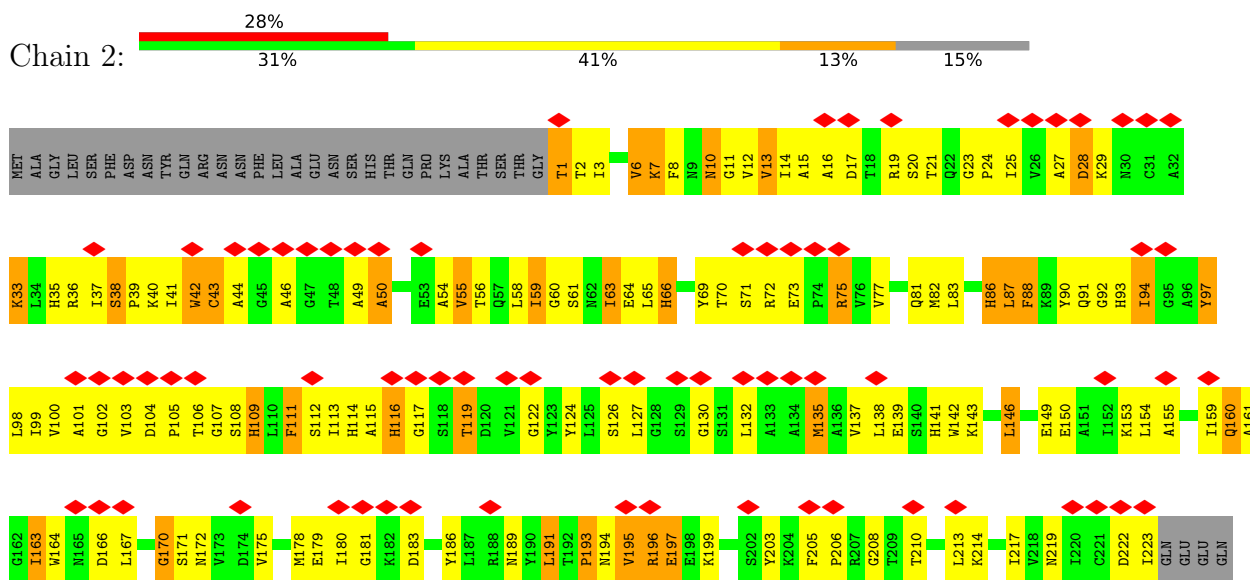
### 3 Residue-property plots

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: PROTEASOME COMPONENT PRE3

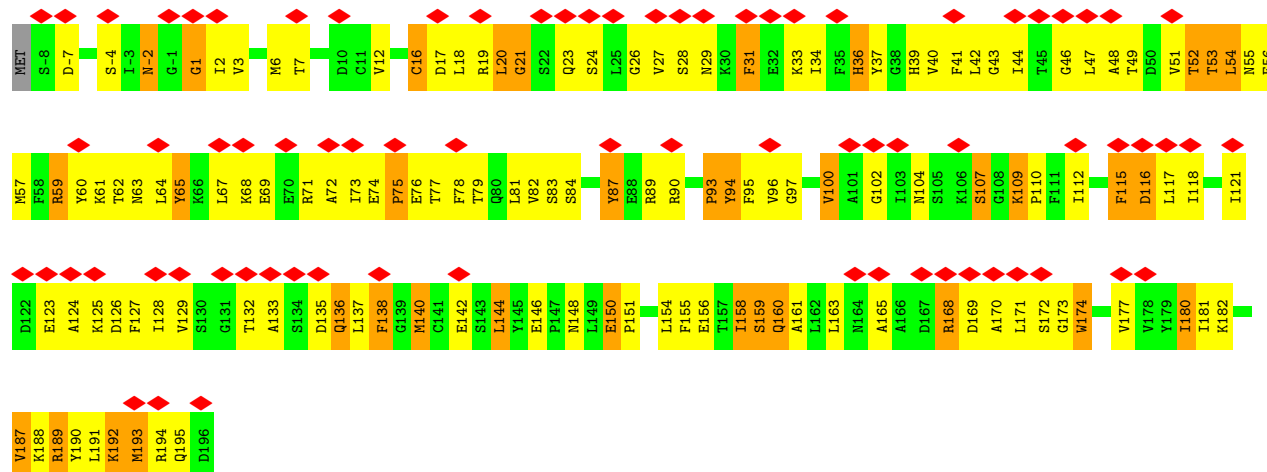


#### • Molecule 2: PROTEASOME COMPONENT PUP1



VAL  
ASP  
ILE  
THR  
ALA

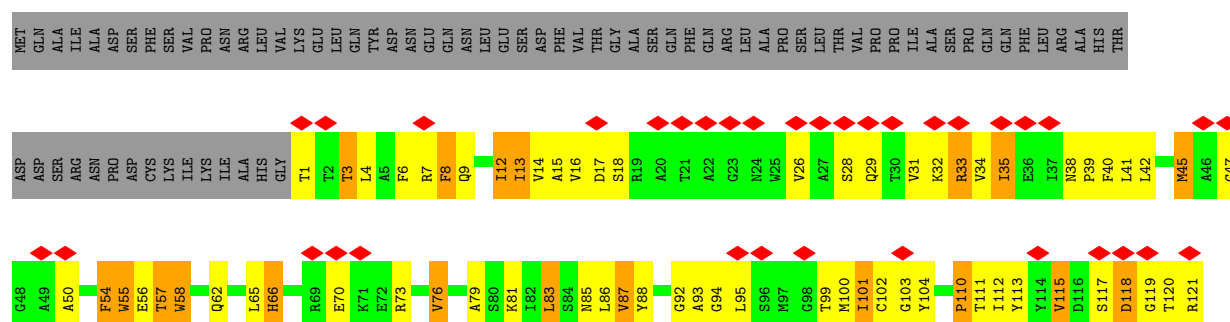
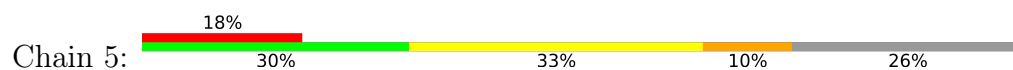
• Molecule 3: PROTEASOME COMPONENT PUP3

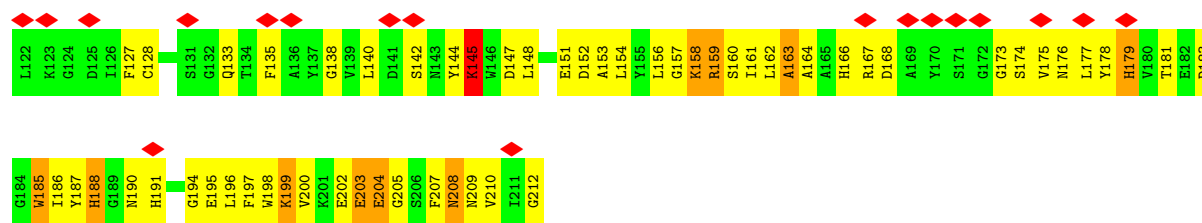


• Molecule 4: PROTEASOME COMPONENT C11

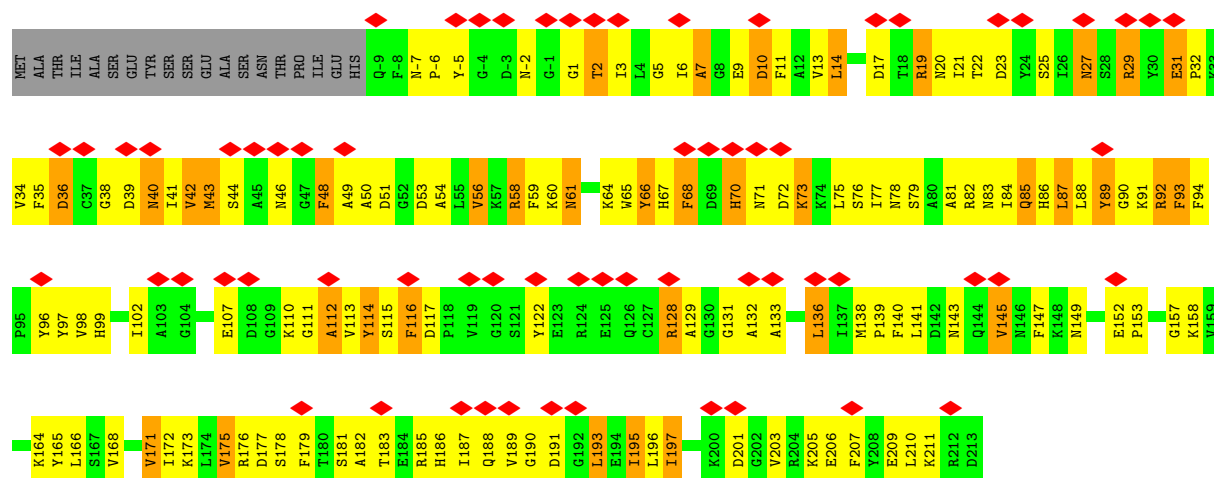


• Molecule 5: PROTEASOME COMPONENT PRE2

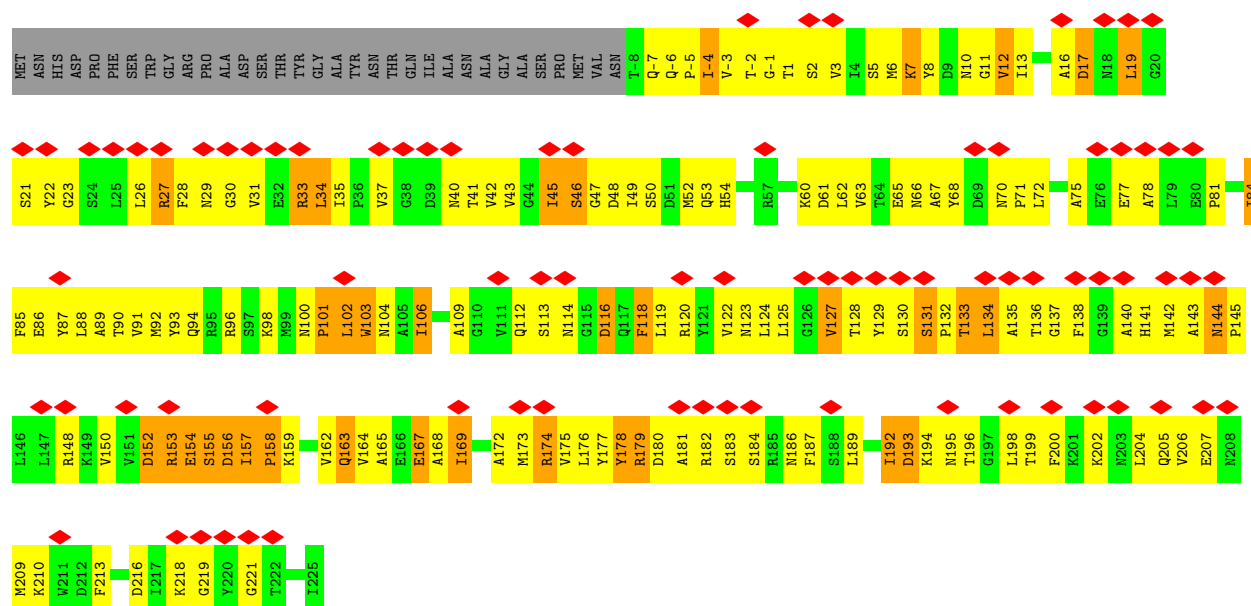




• Molecule 6: PROTEASOME COMPONENT C5

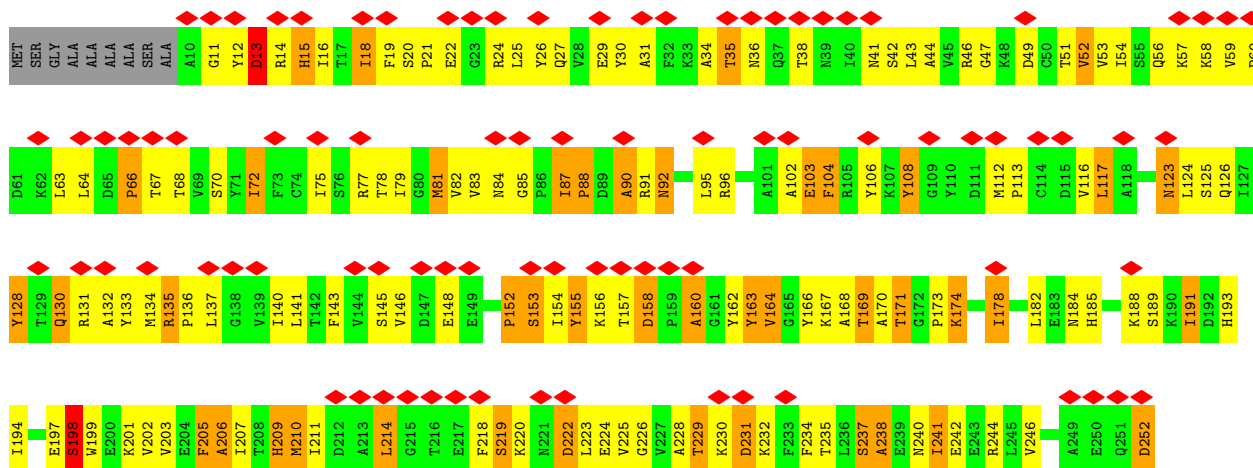


• Molecule 7: PROTEASOME COMPONENT PRE4

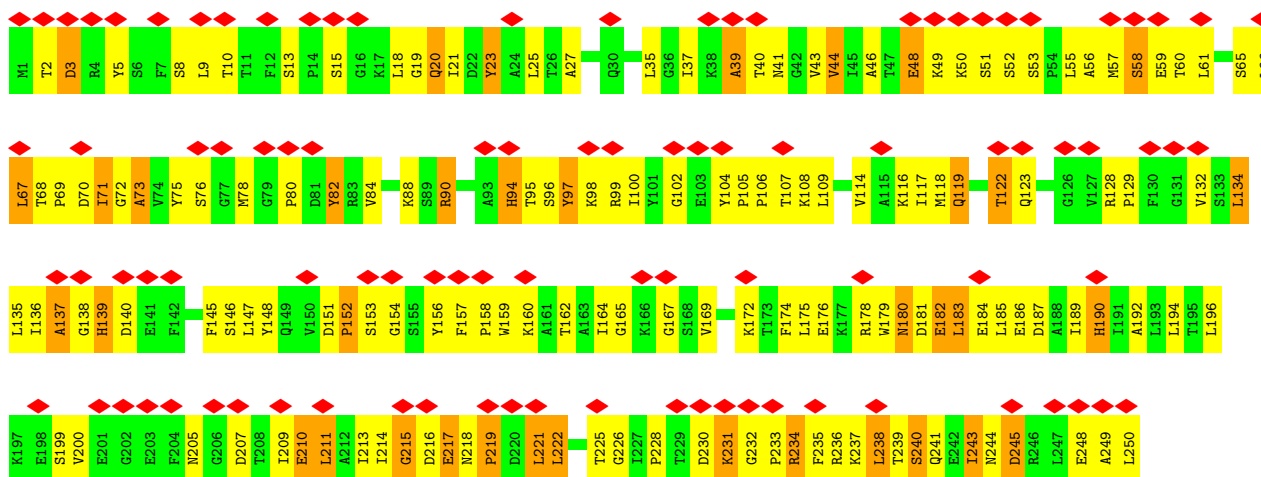


• Molecule 8: PROTEASOME COMPONENT C7-ALPHA

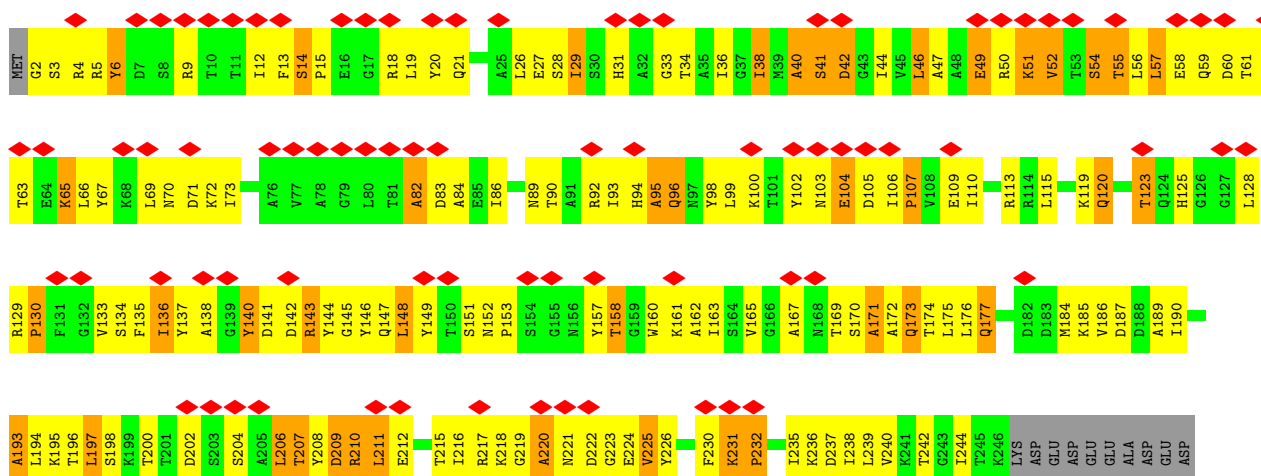




• Molecule 9: PROTEASOME COMPONENT Y7

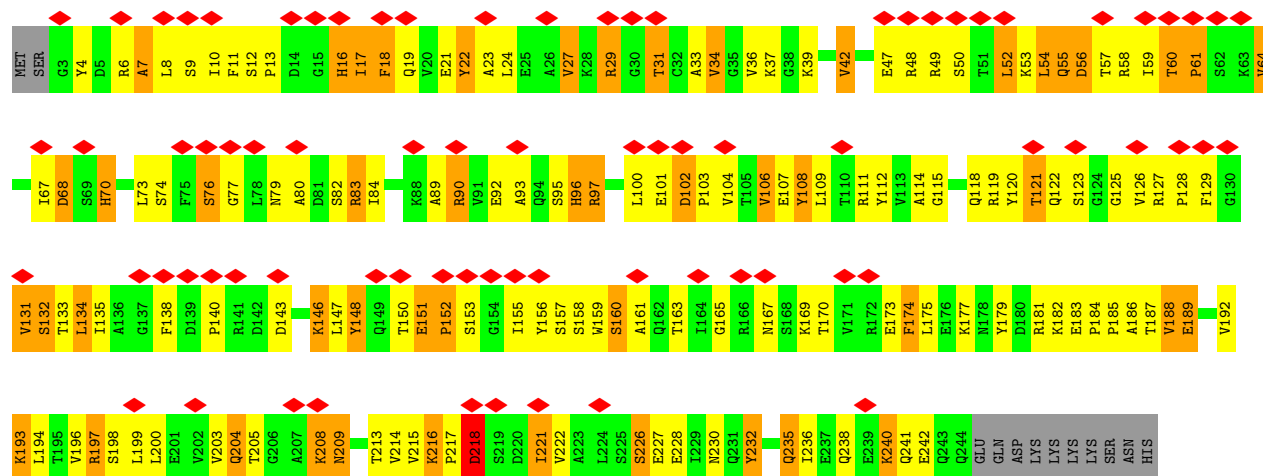


• Molecule 10: PROTEASOME COMPONENT Y13

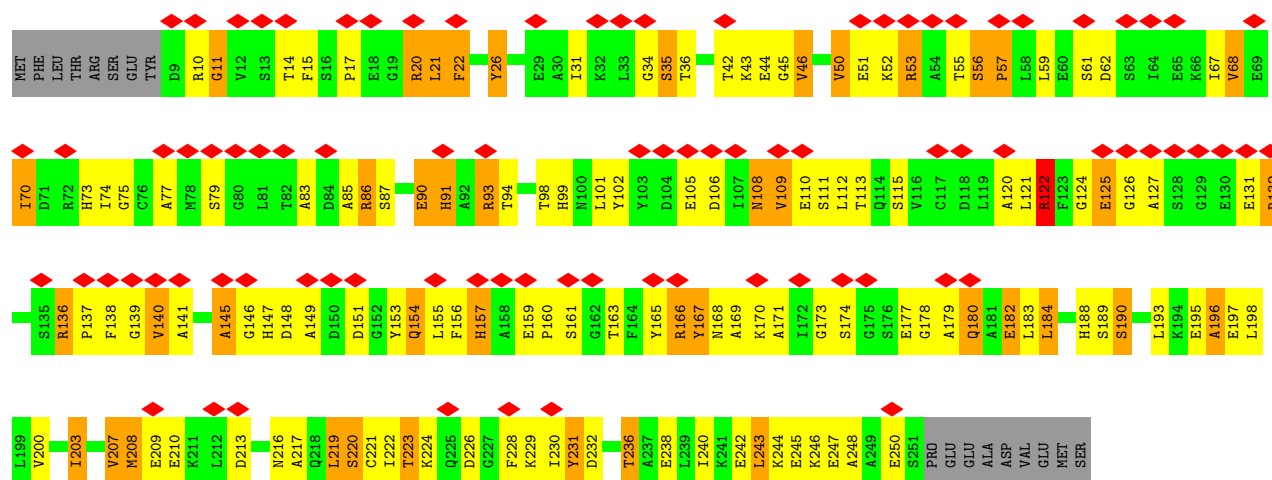


MET  
LYS

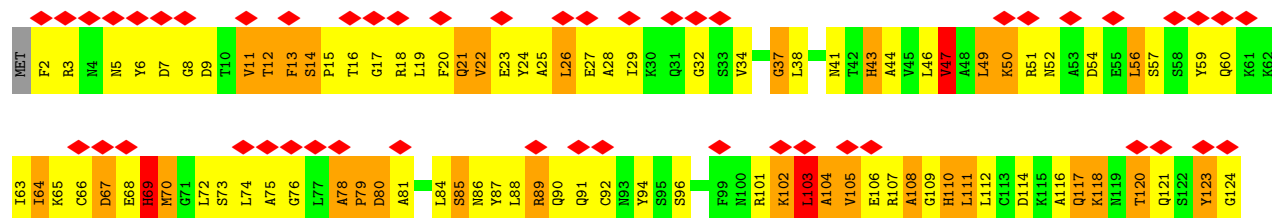
- Molecule 11: PROTEASOME COMPONENT PRE6



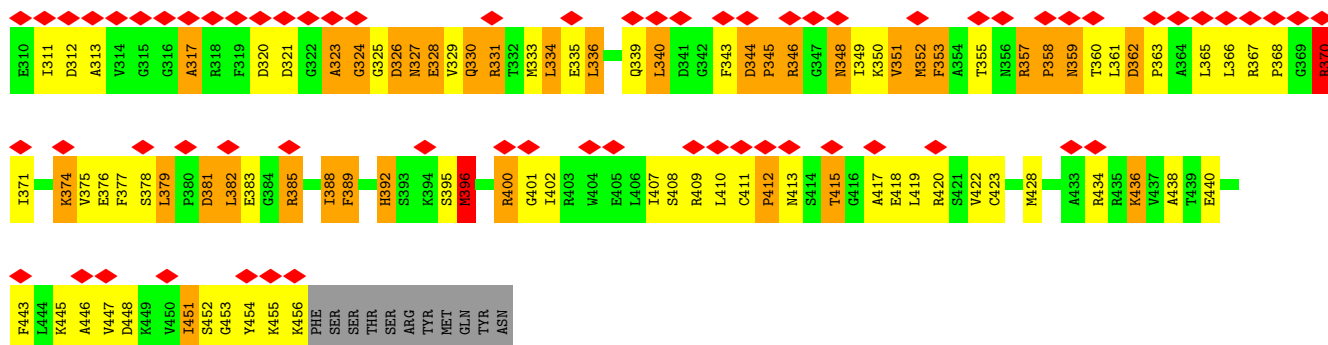
- Molecule 12: PROTEASOME COMPONENT PUP2



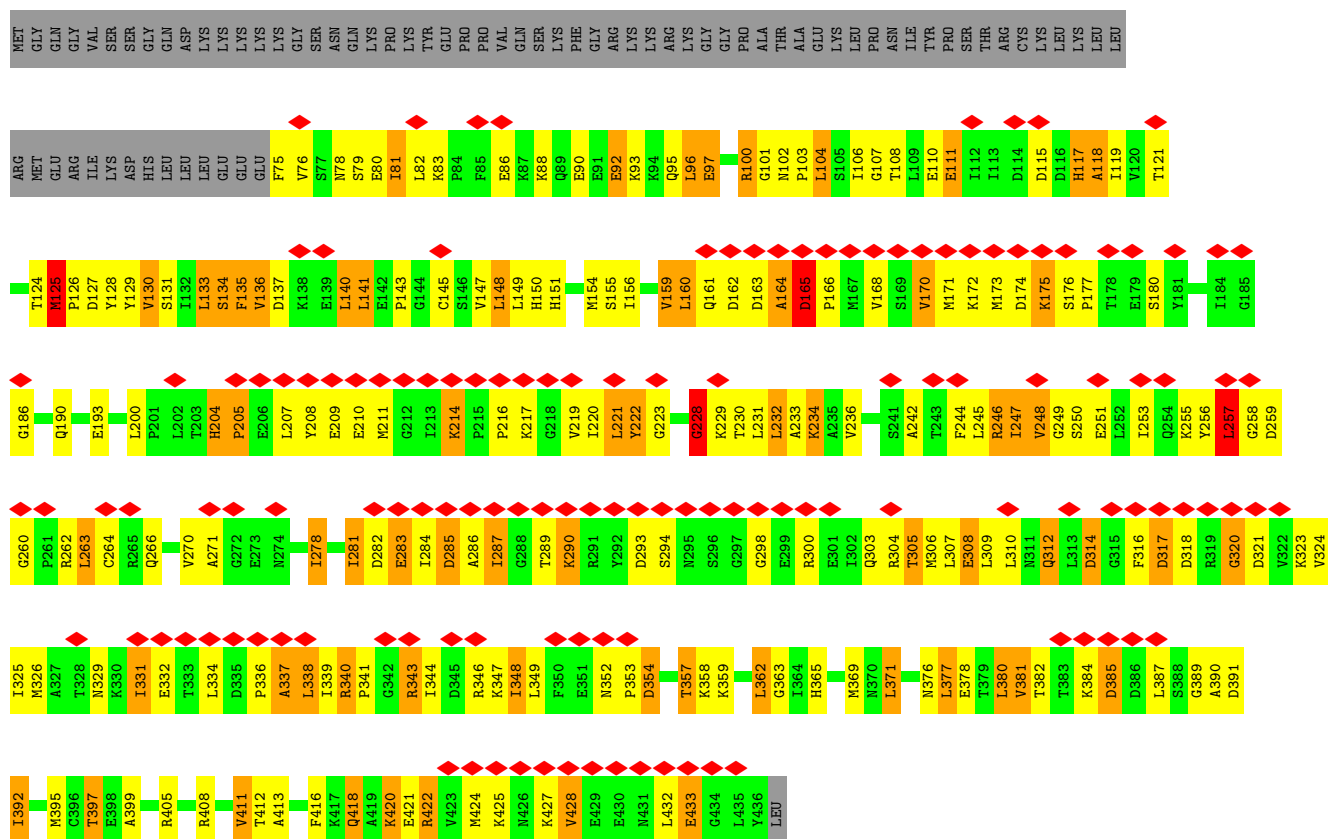
- Molecule 13: PROTEASOME COMPONENT PRE5



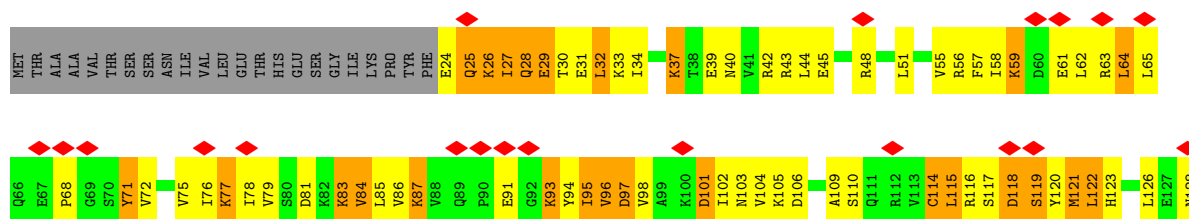


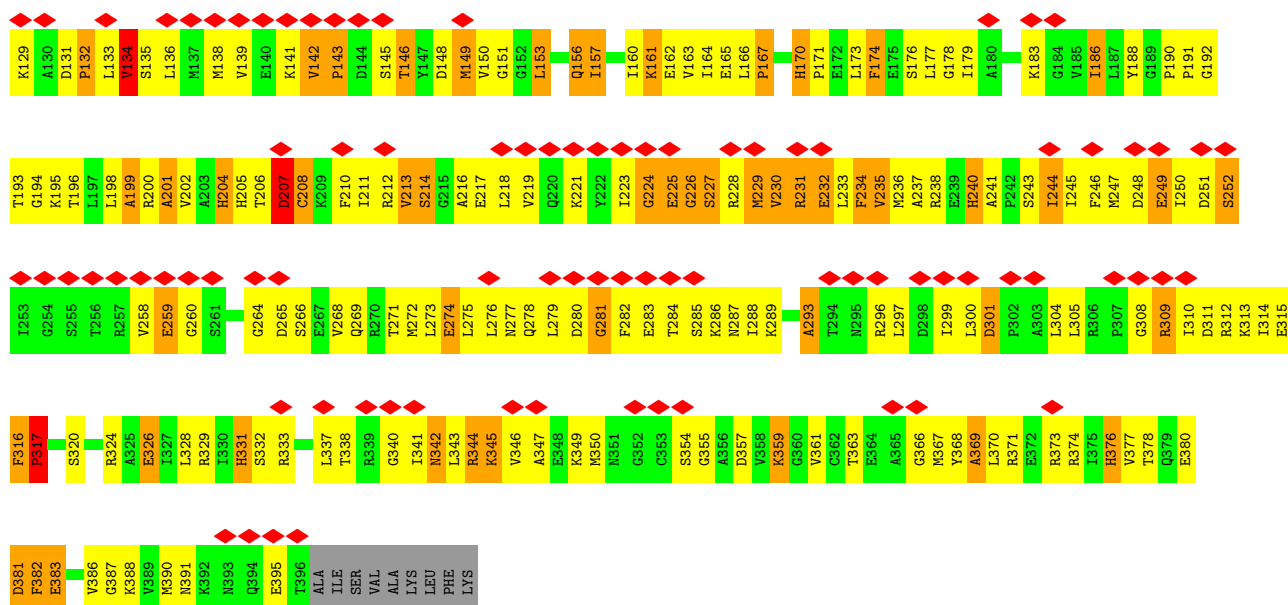


• Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

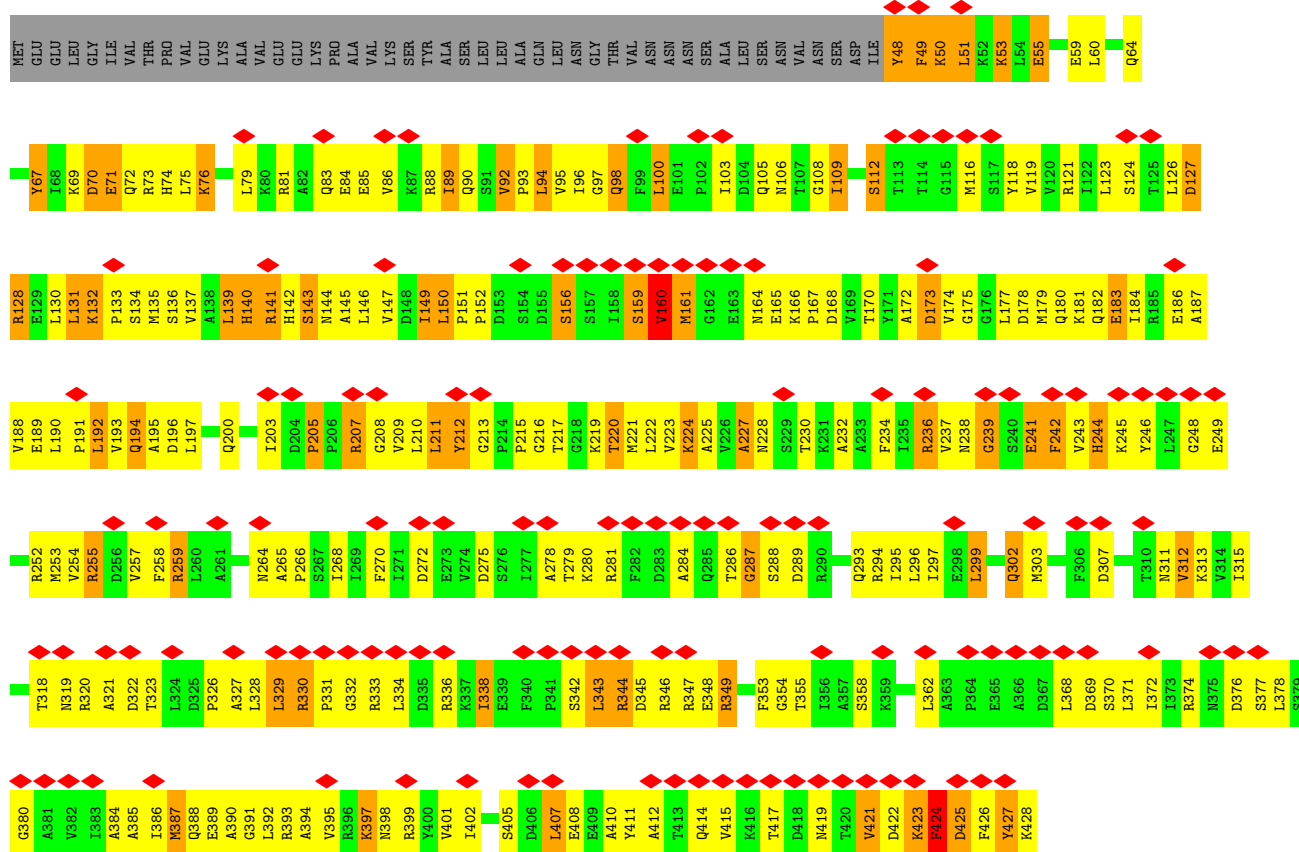


• Molecule 17: 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG

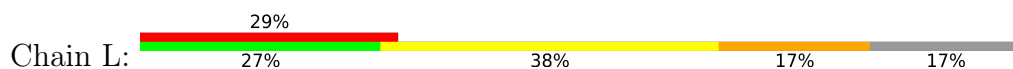


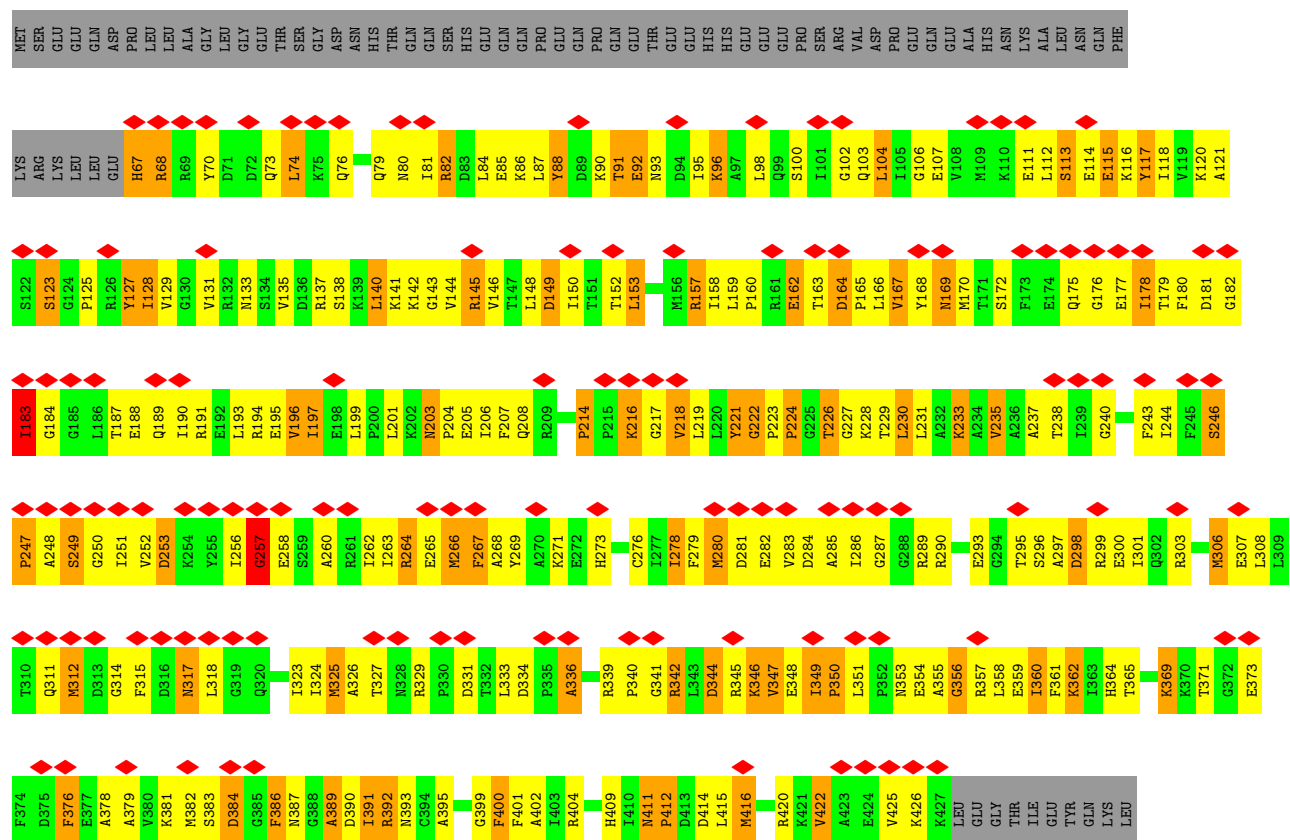


• Molecule 18: 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG

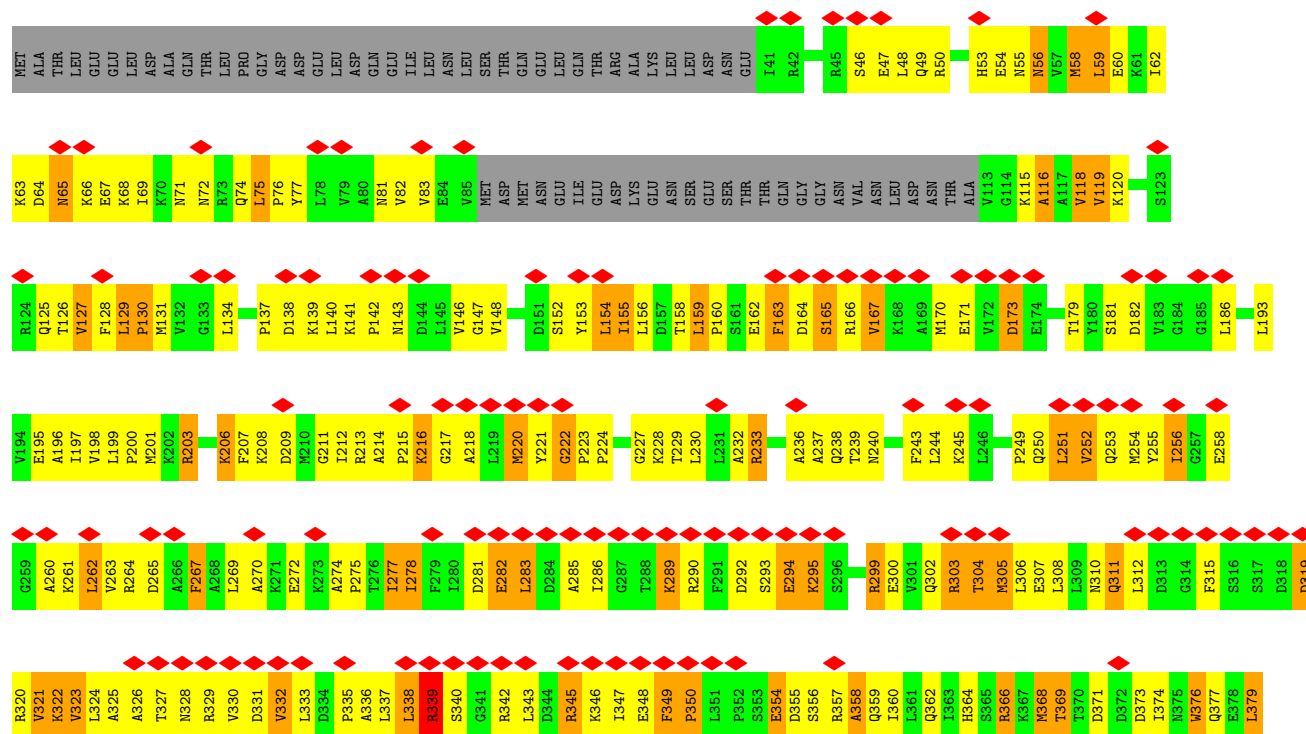


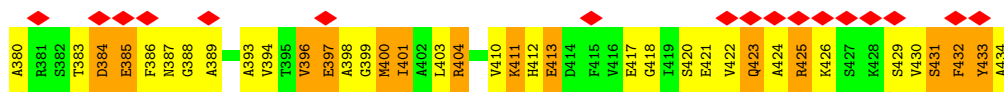
• Molecule 19: 26S PROTEASE SUBUNIT RPT4



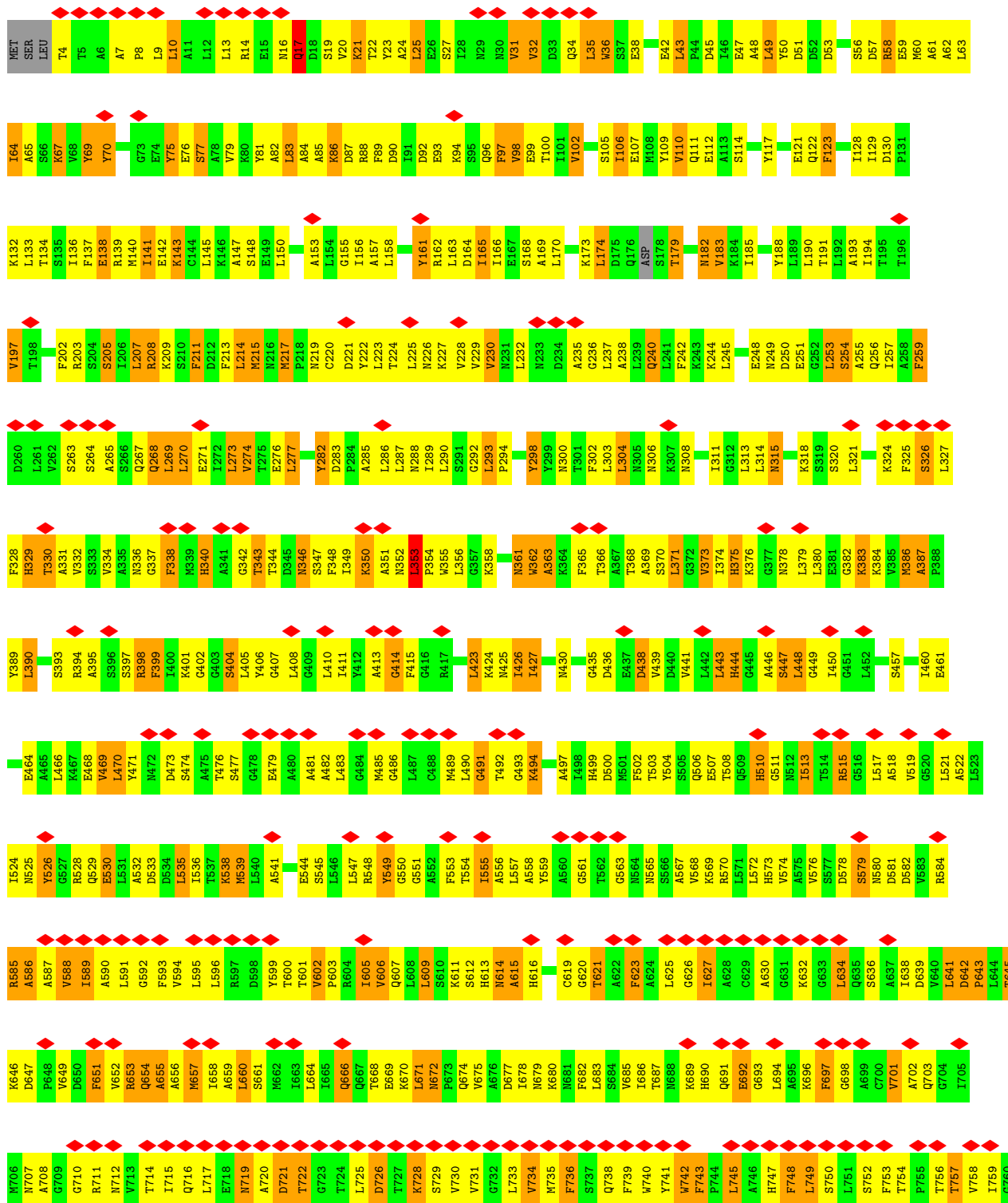
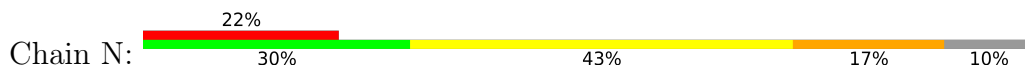


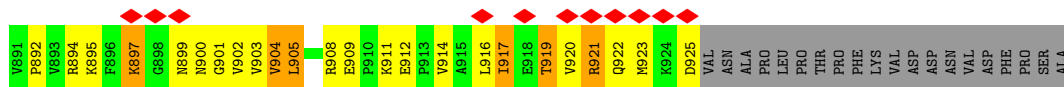
• Molecule 20: 26S PROTEASE REGULATORY SUBUNIT 6A

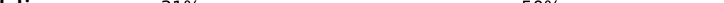


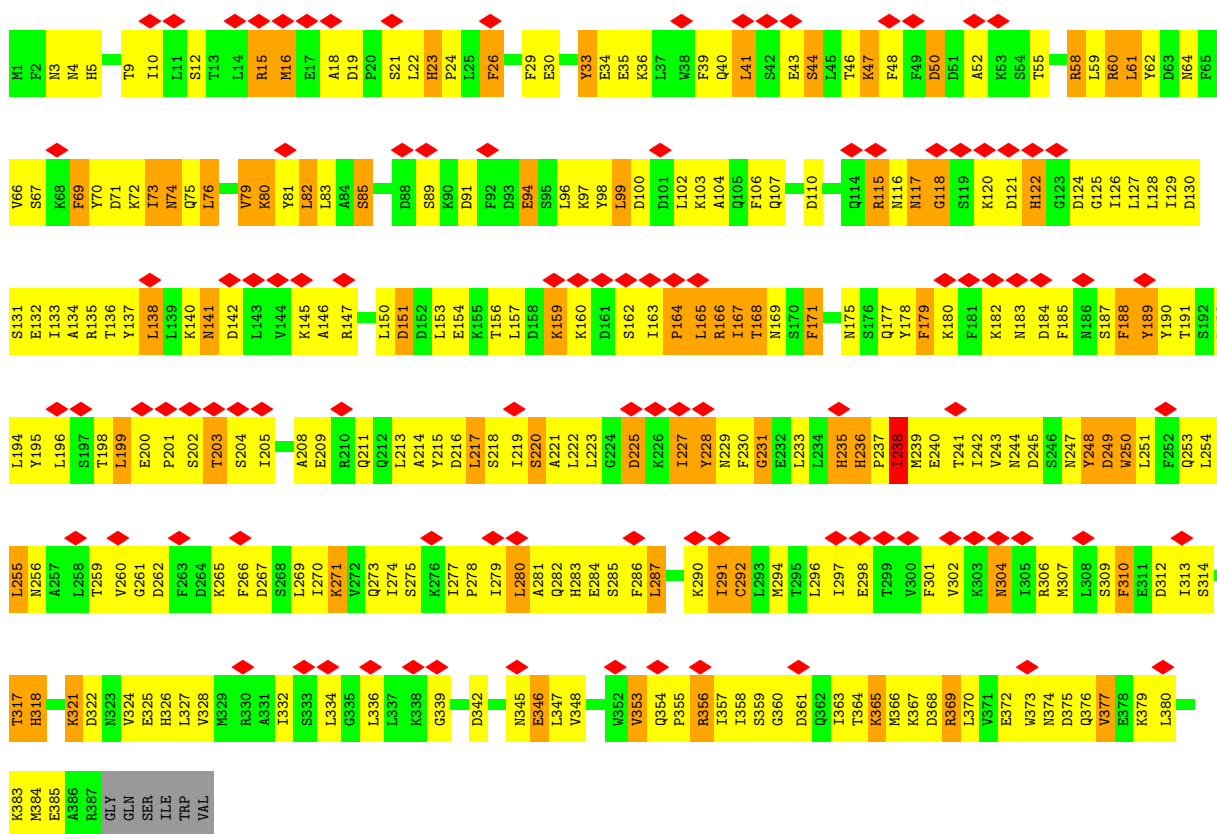


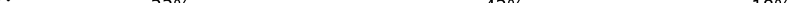
• Molecule 21: 26S PROTEASOME REGULATORY SUBUNIT RPN2

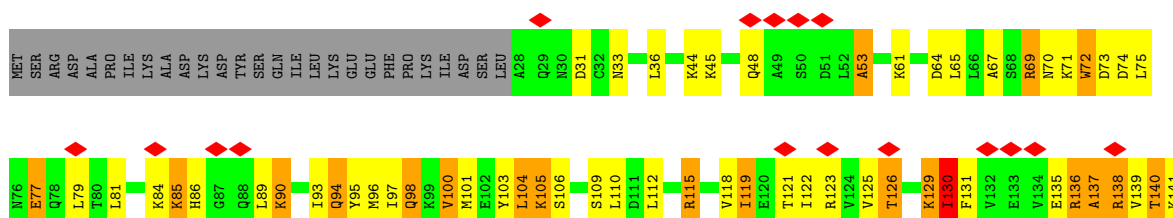


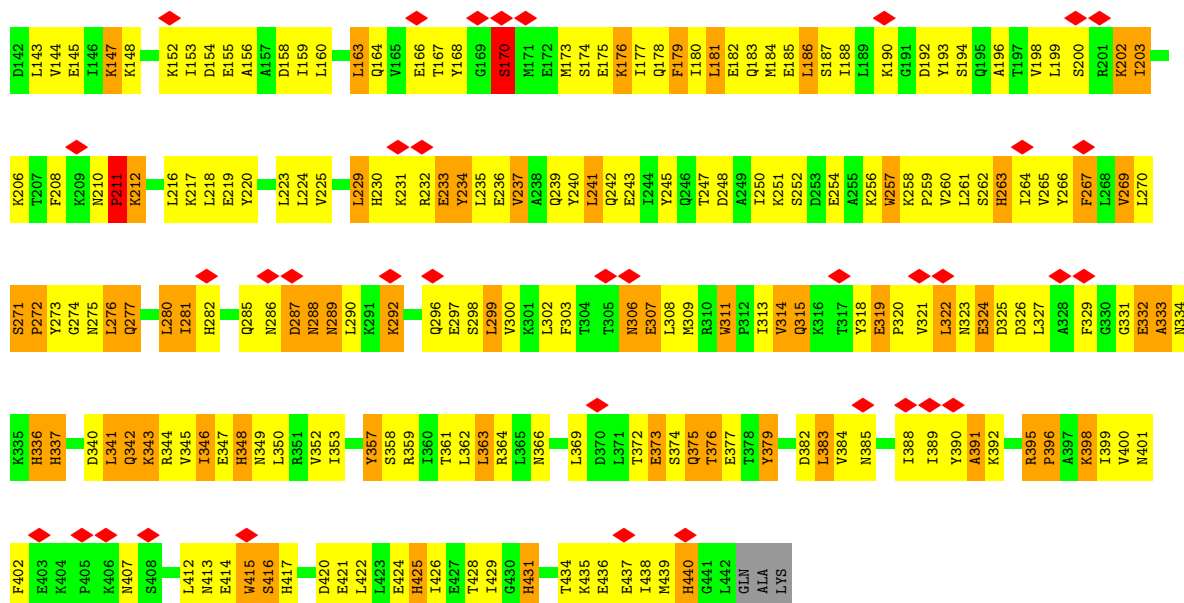


Chain O: 

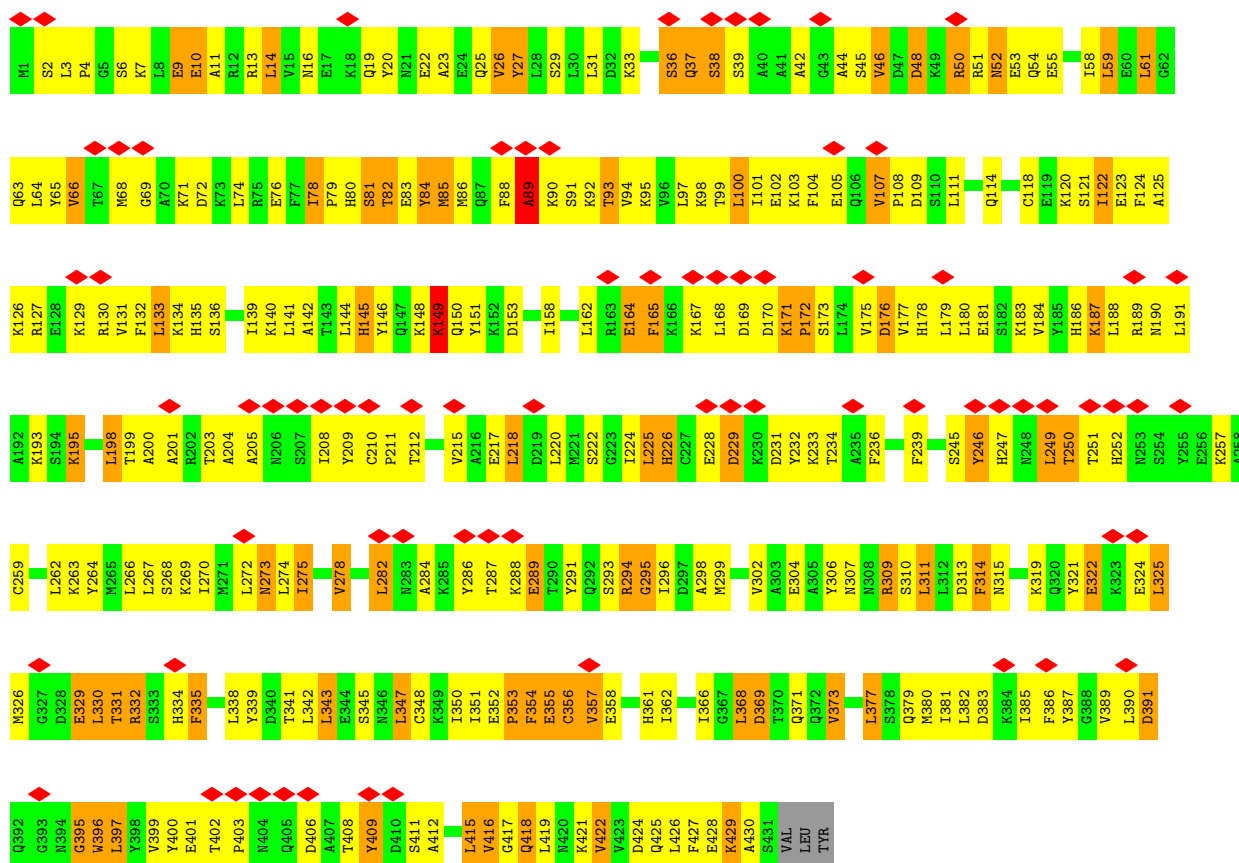


Chain P: 

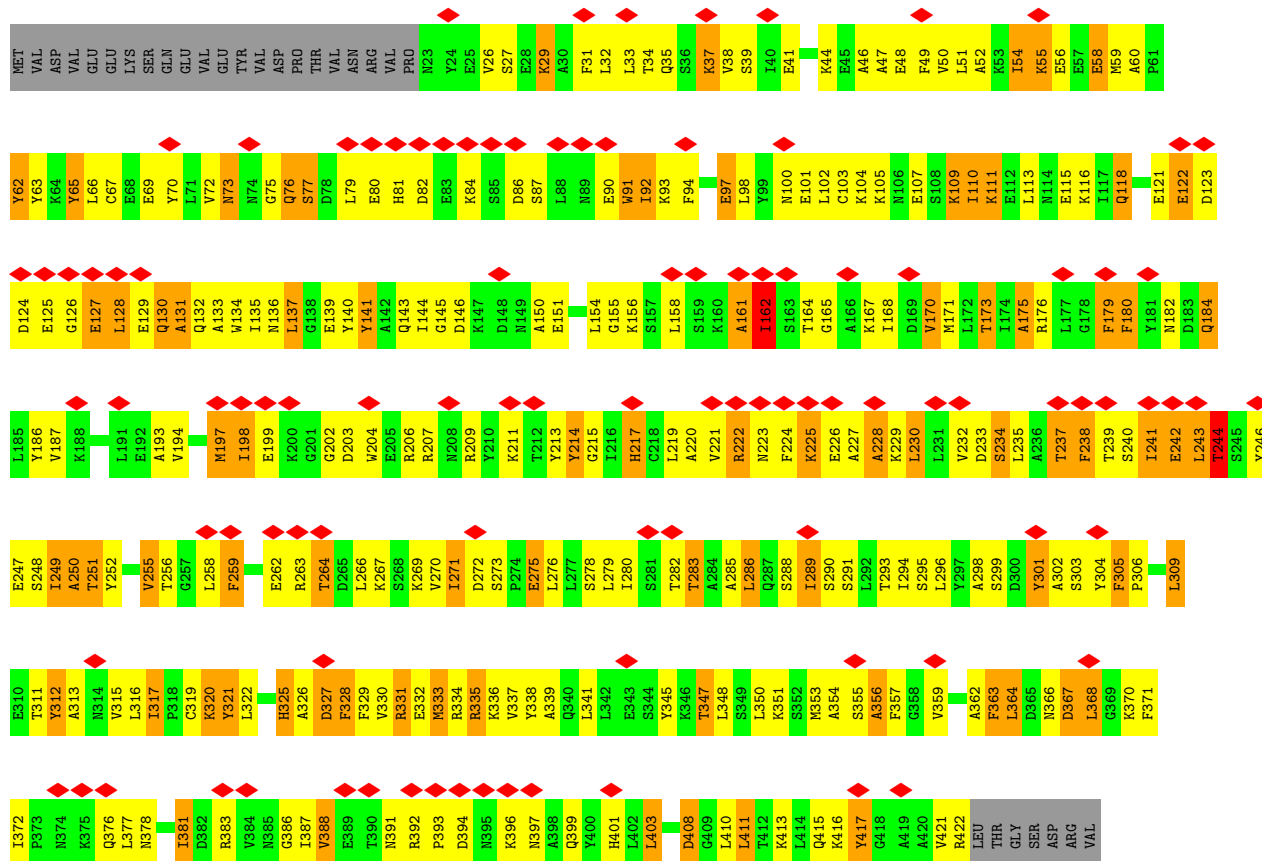




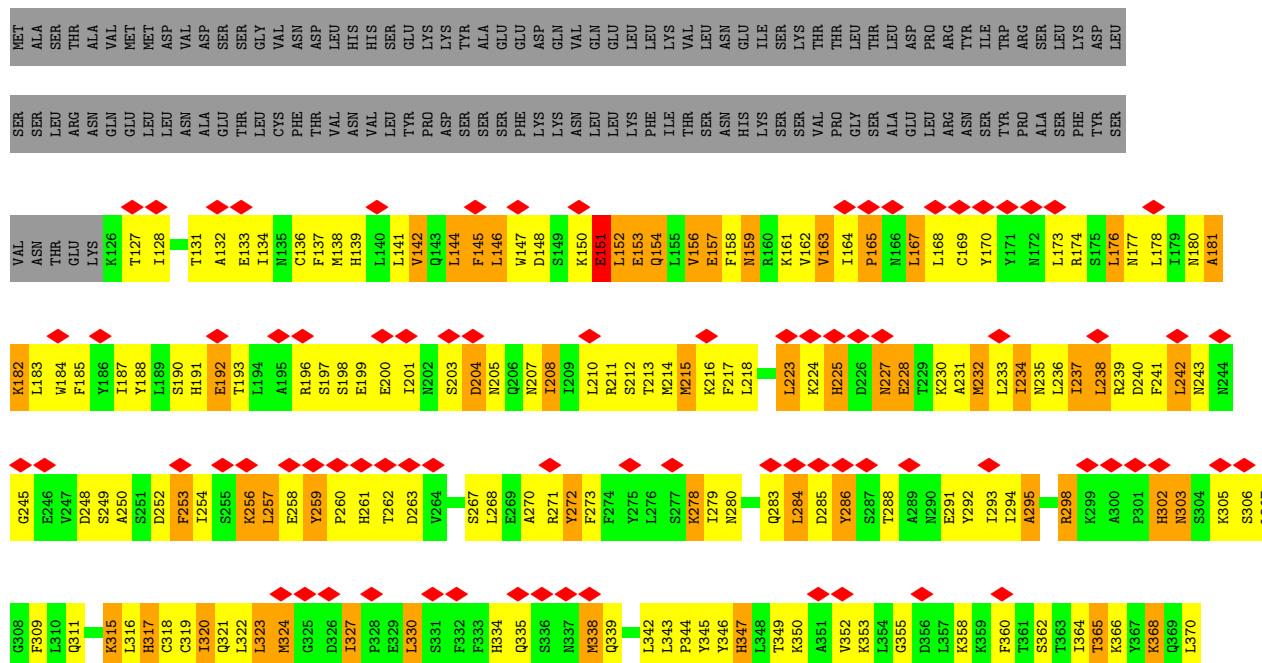
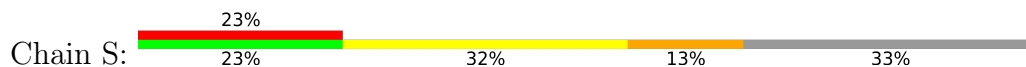
• Molecule 24: 26S PROTEASOME REGULATORY SUBUNIT RPN6

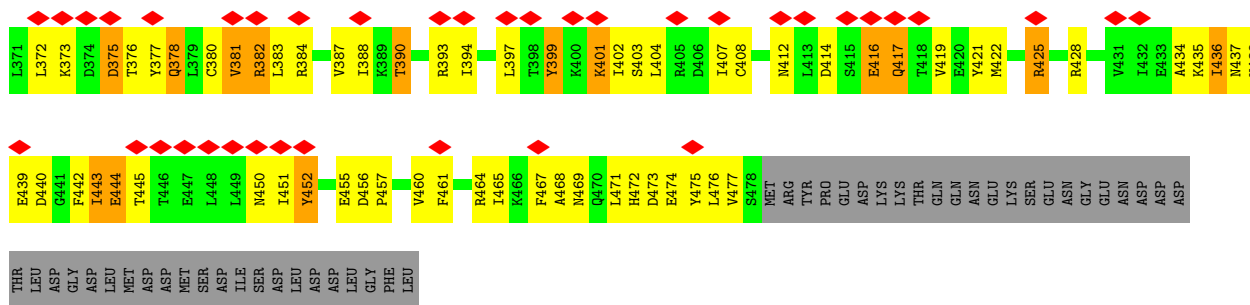


• Molecule 25: 26S PROTEASOME REGULATORY SUBUNIT RPN7

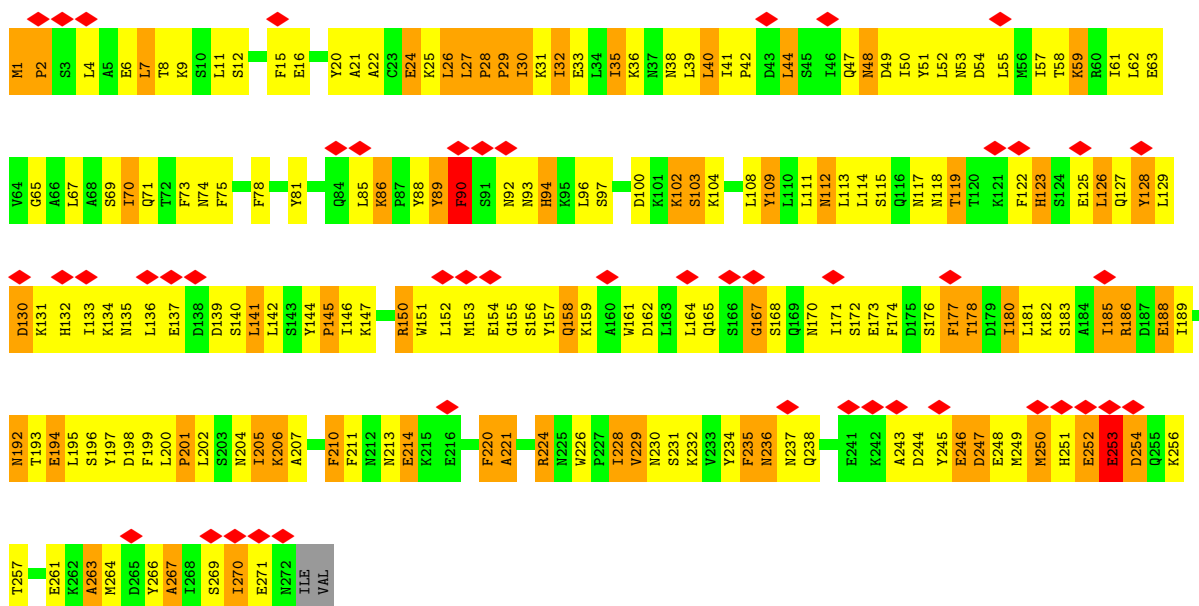


• Molecule 26: 26S PROTEASOME REGULATORY SUBUNIT RPN3

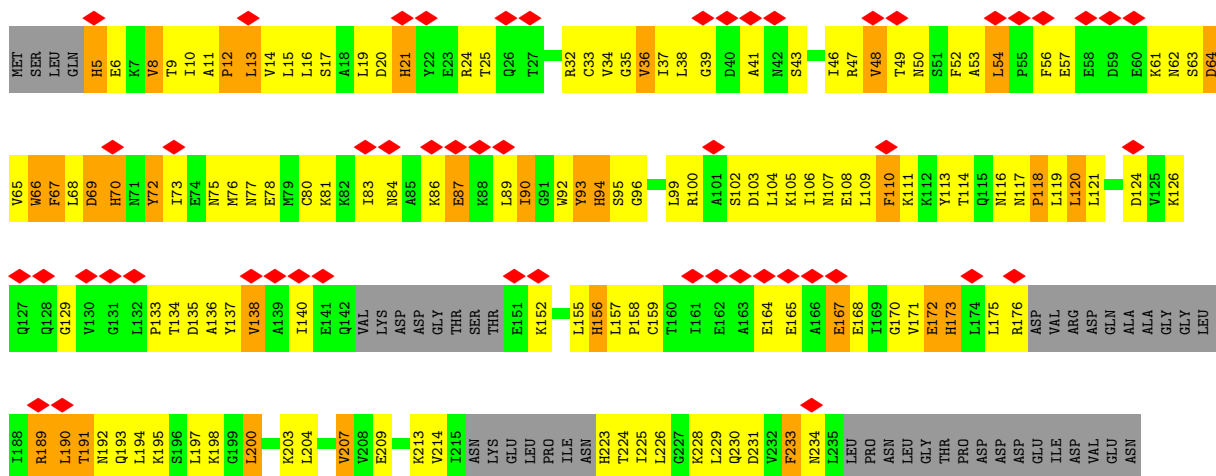
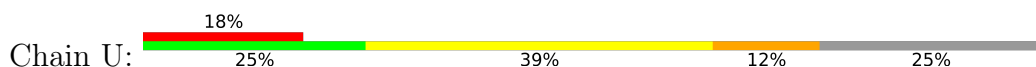




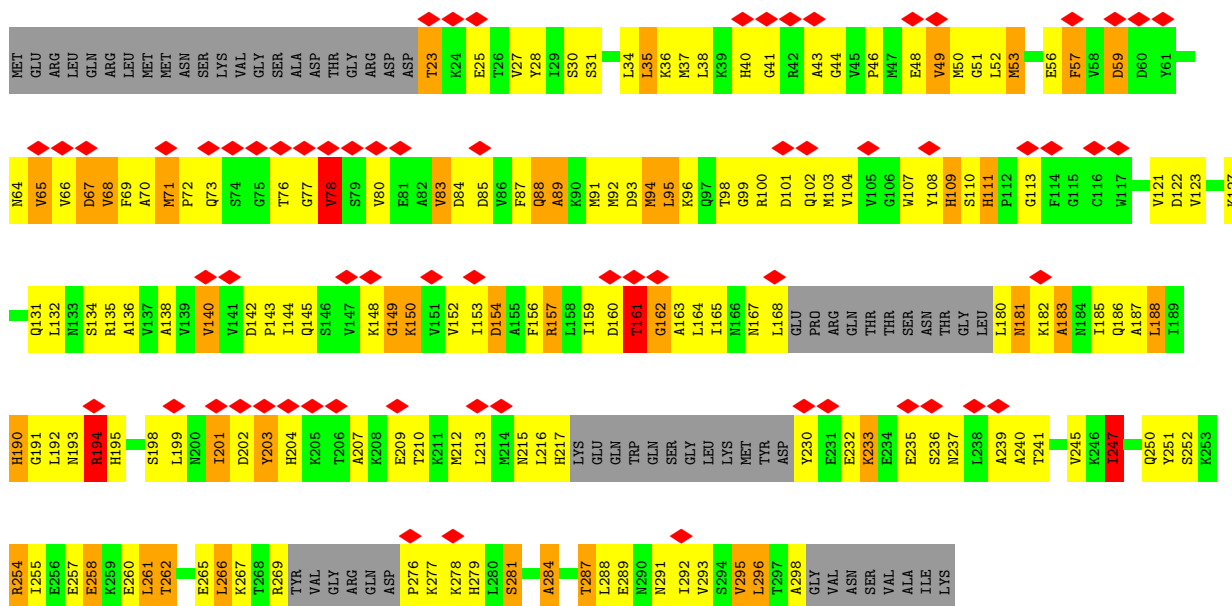
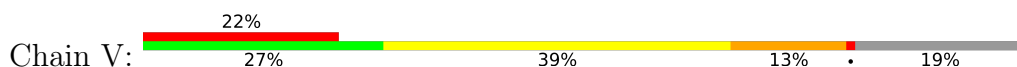
• Molecule 27: 26S PROTEASOME REGULATORY SUBUNIT RPN12



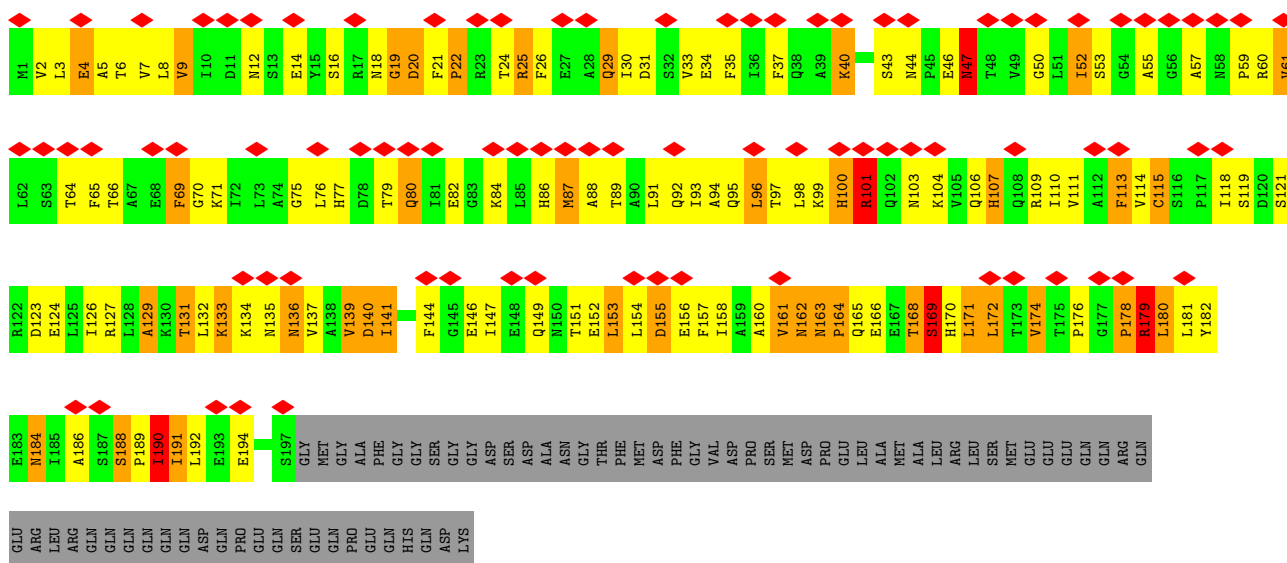
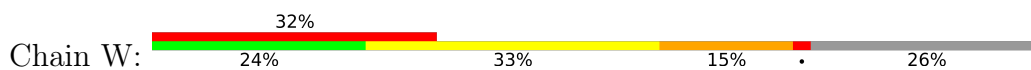
• Molecule 28: 26S PROTEASOME REGULATORY SUBUNIT RPN8



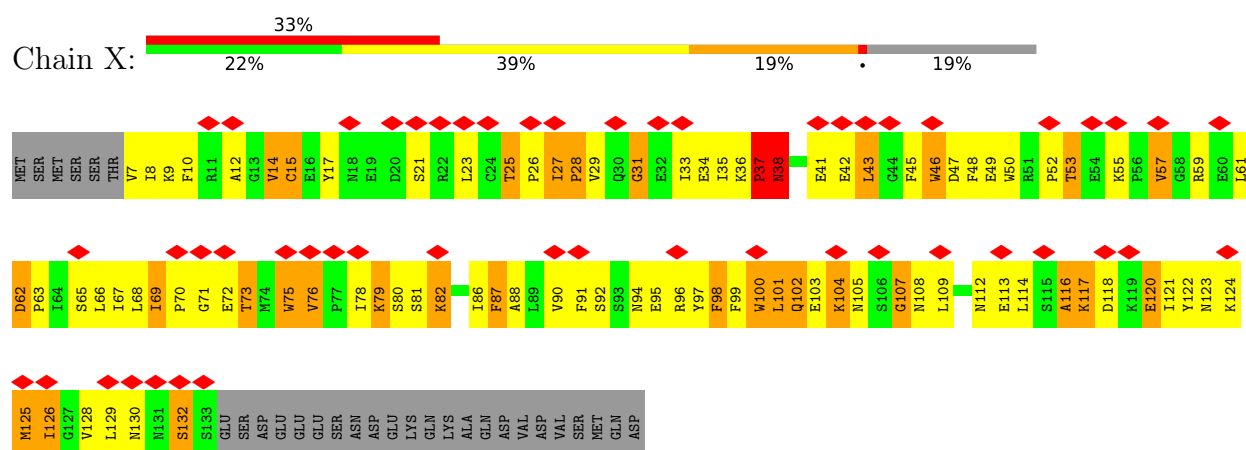
- Molecule 29: 26S PROTEASOME REGULATORY SUBUNIT RPN11



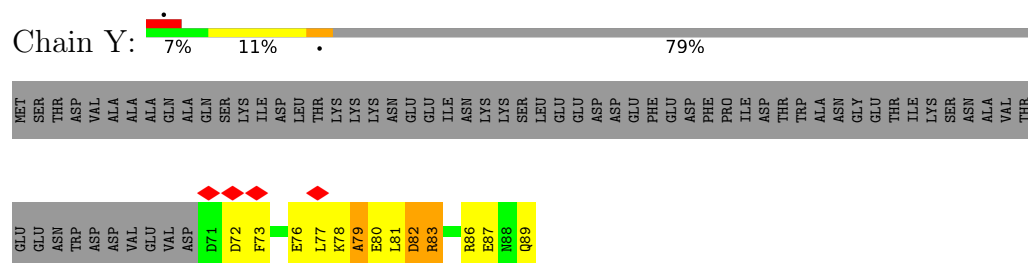
● Molecule 30: 26S PROTEASOME REGULATORY SUBUNIT RPN10



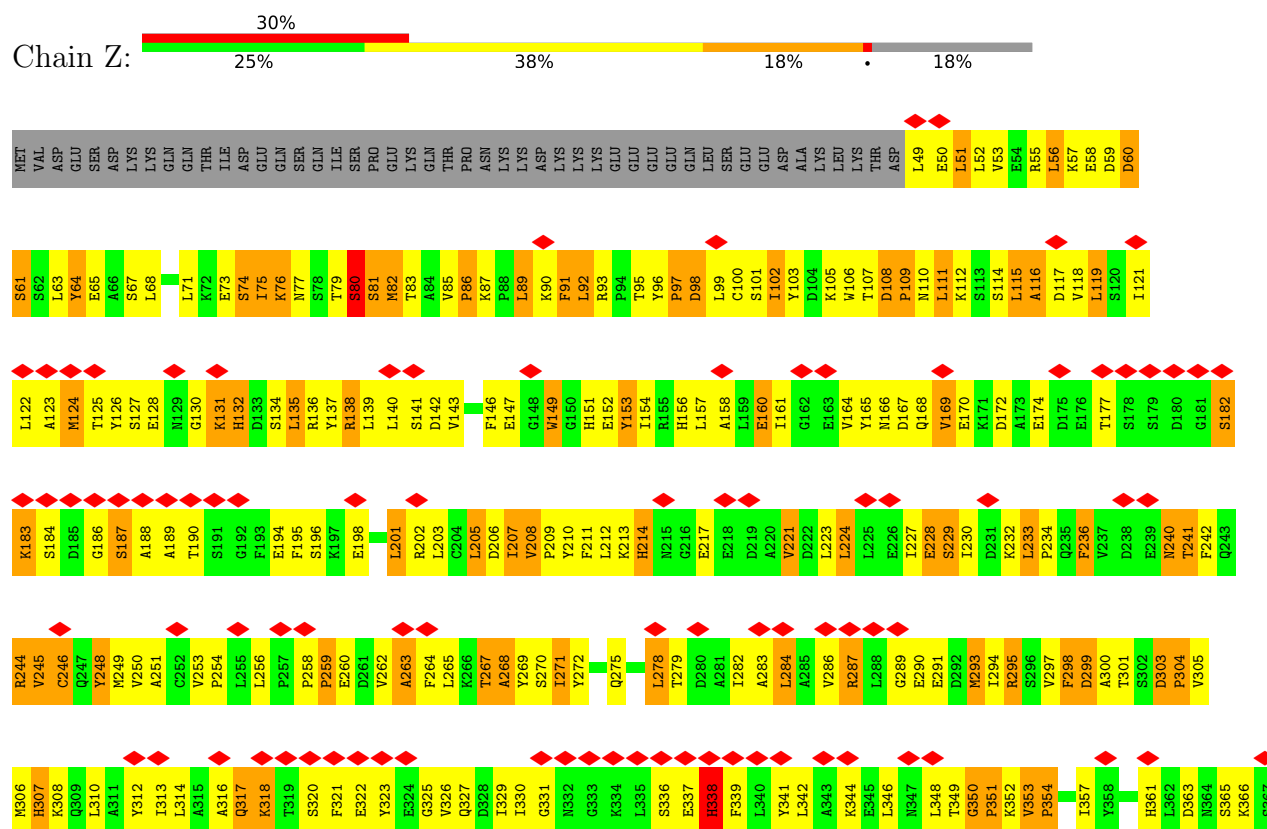
- Molecule 31: 26S PROTEASOME REGULATORY SUBUNIT RPN13

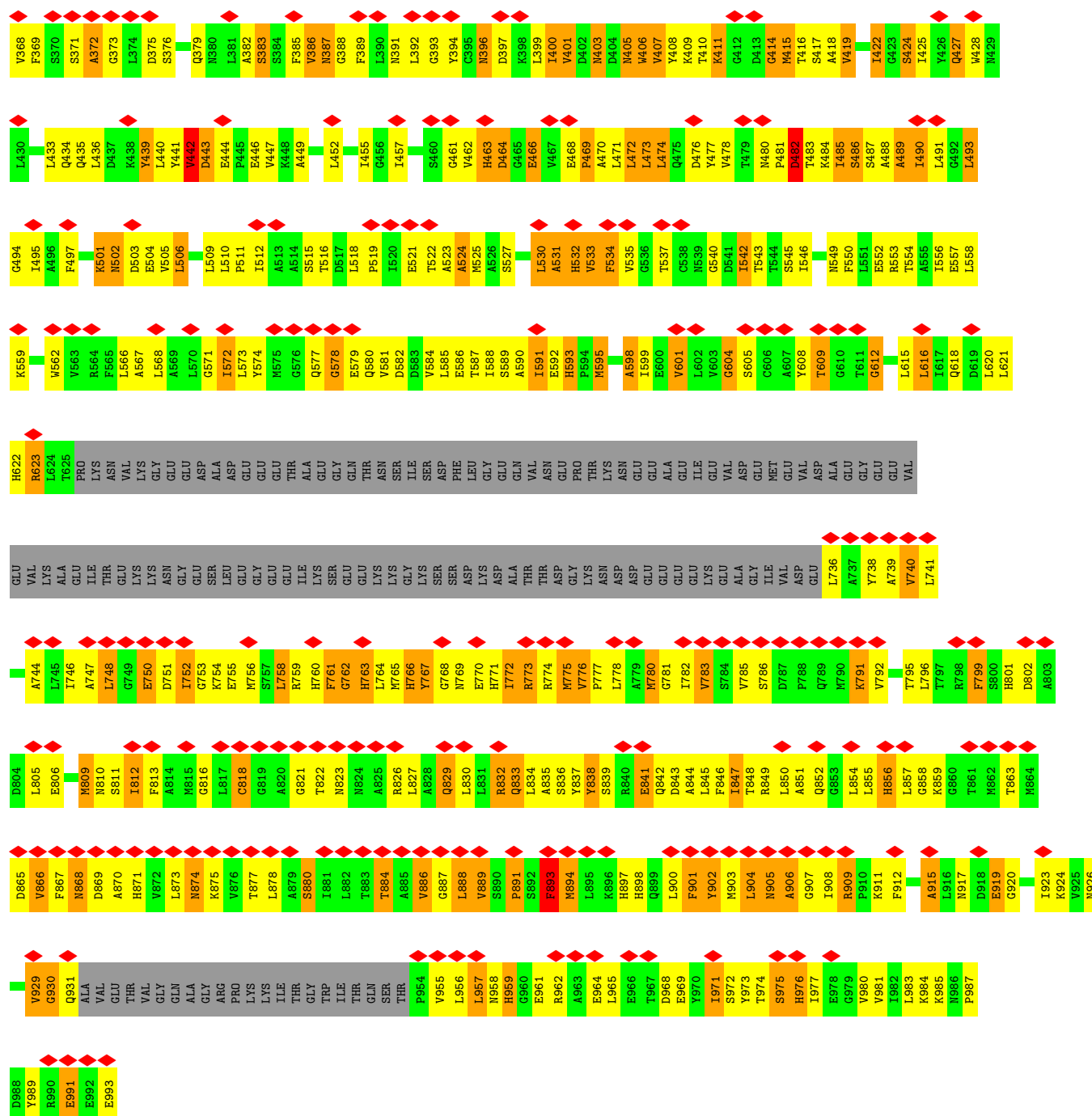


• Molecule 32: 26S PROTEASOME COMPLEX SUBUNIT SEM1



• Molecule 33: 26S PROTEASOME REGULATORY SUBUNIT RPN1





## 4 Experimental information

| Property                             | Value                       | Source    |
|--------------------------------------|-----------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE             | Depositor |
| Imposed symmetry                     | POINT, C1                   | Depositor |
| Number of particles used             | 1300000                     | Depositor |
| Resolution determination method      | Not provided                |           |
| CTF correction method                | MICROGRAPH                  | Depositor |
| Microscope                           | FEI TITAN KRIOS             | Depositor |
| Voltage (kV)                         | 200                         | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 25                          | Depositor |
| Minimum defocus (nm)                 | 1000                        | Depositor |
| Maximum defocus (nm)                 | 3500                        | Depositor |
| Magnification                        | Not provided                |           |
| Image detector                       | TVIPS TEMCAM-F816 (8k x 8k) | Depositor |
| Maximum map value                    | 6.242                       | Depositor |
| Minimum map value                    | -4.111                      | Depositor |
| Average map value                    | 0.010                       | Depositor |
| Map value standard deviation         | 0.157                       | Depositor |
| Recommended contour level            | 0.74                        | Depositor |
| Map size ( $\text{\AA}$ )            | 557.2, 557.2, 557.2         | wwPDB     |
| Map dimensions                       | 280, 280, 280               | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0            | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.99, 1.99, 1.99            | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                   | Bond angles |                    |
|-----|-------|--------------|-------------------|-------------|--------------------|
|     |       | RMSZ         | $\# Z  > 5$       | RMSZ        | $\# Z  > 5$        |
| 1   | 1     | 1.93         | 53/1605 (3.3%)    | 1.99        | 76/2171 (3.5%)     |
| 2   | 2     | 1.96         | 51/1723 (3.0%)    | 2.05        | 93/2337 (4.0%)     |
| 3   | 3     | 1.91         | 49/1611 (3.0%)    | 1.96        | 77/2174 (3.5%)     |
| 4   | 4     | 1.90         | 53/1613 (3.3%)    | 1.96        | 75/2173 (3.5%)     |
| 5   | 5     | 1.89         | 48/1683 (2.9%)    | 1.91        | 68/2277 (3.0%)     |
| 6   | 6     | 1.90         | 55/1795 (3.1%)    | 2.00        | 100/2420 (4.1%)    |
| 7   | 7     | 1.91         | 64/1855 (3.5%)    | 1.97        | 86/2514 (3.4%)     |
| 8   | A     | 1.95         | 64/1959 (3.3%)    | 2.01        | 89/2652 (3.4%)     |
| 9   | B     | 1.94         | 64/1952 (3.3%)    | 1.97        | 98/2642 (3.7%)     |
| 10  | C     | 1.86         | 50/1943 (2.6%)    | 2.05        | 99/2629 (3.8%)     |
| 11  | D     | 1.91         | 65/1928 (3.4%)    | 2.05        | 111/2610 (4.3%)    |
| 12  | E     | 2.01         | 71/1892 (3.8%)    | 2.08        | 91/2549 (3.6%)     |
| 13  | F     | 1.92         | 56/1823 (3.1%)    | 2.07        | 100/2463 (4.1%)    |
| 14  | G     | 2.03         | 75/1940 (3.9%)    | 2.12        | 118/2619 (4.5%)    |
| 15  | H     | 1.74         | 68/2831 (2.4%)    | 2.05        | 153/3808 (4.0%)    |
| 16  | I     | 1.84         | 89/2859 (3.1%)    | 1.95        | 116/3853 (3.0%)    |
| 17  | J     | 1.95         | 85/2963 (2.9%)    | 2.08        | 168/3978 (4.2%)    |
| 18  | K     | 1.85         | 91/3061 (3.0%)    | 2.02        | 140/4129 (3.4%)    |
| 19  | L     | 1.94         | 96/2896 (3.3%)    | 2.23        | 178/3895 (4.6%)    |
| 20  | M     | 1.93         | 76/2903 (2.6%)    | 2.18        | 177/3909 (4.5%)    |
| 21  | N     | 1.84         | 194/6670 (2.9%)   | 2.15        | 418/9023 (4.6%)    |
| 22  | O     | 1.82         | 81/3243 (2.5%)    | 2.08        | 193/4374 (4.4%)    |
| 23  | P     | 1.77         | 82/3452 (2.4%)    | 2.08        | 184/4657 (4.0%)    |
| 24  | Q     | 1.84         | 105/3527 (3.0%)   | 2.09        | 192/4748 (4.0%)    |
| 25  | R     | 1.75         | 95/3272 (2.9%)    | 1.95        | 153/4412 (3.5%)    |
| 26  | S     | 1.84         | 93/2945 (3.2%)    | 2.06        | 150/3976 (3.8%)    |
| 27  | T     | 1.75         | 62/2279 (2.7%)    | 2.09        | 131/3077 (4.3%)    |
| 28  | U     | 1.92         | 60/2087 (2.9%)    | 2.04        | 99/2811 (3.5%)     |
| 29  | V     | 1.97         | 72/1969 (3.7%)    | 2.06        | 103/2652 (3.9%)    |
| 30  | W     | 1.92         | 49/1557 (3.1%)    | 2.13        | 86/2111 (4.1%)     |
| 31  | X     | 1.83         | 38/1058 (3.6%)    | 1.85        | 35/1432 (2.4%)     |
| 32  | Y     | 1.81         | 5/169 (3.0%)      | 2.17        | 11/223 (4.9%)      |
| 33  | Z     | 1.83         | 185/6403 (2.9%)   | 2.09        | 346/8686 (4.0%)    |
| All | All   | 1.87         | 2444/81466 (3.0%) | 2.06        | 4314/109984 (3.9%) |

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 |
|-----|-------|---------------------|---------------------|
| 7   | 7     | 0                   | 1                   |
| 11  | D     | 0                   | 1                   |
| 12  | E     | 0                   | 3                   |
| 13  | F     | 0                   | 1                   |
| 15  | H     | 0                   | 8                   |
| 16  | I     | 0                   | 4                   |
| 18  | K     | 0                   | 2                   |
| 19  | L     | 0                   | 4                   |
| 20  | M     | 0                   | 2                   |
| 21  | N     | 0                   | 1                   |
| 22  | O     | 0                   | 4                   |
| 23  | P     | 0                   | 2                   |
| 24  | Q     | 0                   | 1                   |
| 25  | R     | 0                   | 2                   |
| 27  | T     | 0                   | 4                   |
| 29  | V     | 0                   | 1                   |
| 30  | W     | 0                   | 1                   |
| 33  | Z     | 0                   | 2                   |
| All | All   | 0                   | 44                  |

All (2444) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 20  | M     | 251 | LEU  | C-N   | -36.43 | 0.84        | 1.33     |
| 17  | J     | 224 | GLY  | C-N   | 28.21  | 1.73        | 1.33     |
| 19  | L     | 257 | GLY  | C-N   | -13.69 | 1.14        | 1.33     |
| 17  | J     | 190 | PRO  | CA-C  | 11.38  | 1.62        | 1.52     |
| 13  | F     | 220 | THR  | C-O   | -10.97 | 1.16        | 1.25     |
| 12  | E     | 148 | ASP  | CA-C  | -10.59 | 1.39        | 1.52     |
| 3   | 3     | 43  | GLY  | CA-C  | -10.57 | 1.44        | 1.52     |
| 11  | D     | 143 | ASP  | CA-C  | -10.47 | 1.41        | 1.52     |
| 19  | L     | 203 | ASN  | C-O   | -10.21 | 1.16        | 1.25     |
| 7   | 7     | 144 | ASN  | N-CA  | -9.98  | 1.35        | 1.46     |
| 13  | F     | 130 | VAL  | CA-C  | -9.96  | 1.40        | 1.52     |
| 23  | P     | 183 | GLN  | CA-C  | -9.85  | 1.40        | 1.52     |
| 26  | S     | 421 | TYR  | CA-C  | -9.81  | 1.40        | 1.52     |
| 16  | I     | 316 | PHE  | CA-C  | -9.68  | 1.40        | 1.52     |
| 29  | V     | 56  | GLU  | CA-C  | -9.65  | 1.40        | 1.52     |
| 27  | T     | 229 | VAL  | CA-C  | -9.58  | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 22  | O     | 120 | LYS  | CA-C   | -9.47 | 1.40        | 1.52     |
| 19  | L     | 362 | LYS  | CA-C   | -9.47 | 1.40        | 1.52     |
| 30  | W     | 115 | CYS  | CA-C   | -9.44 | 1.40        | 1.52     |
| 26  | S     | 468 | ALA  | C-N    | 9.43  | 1.46        | 1.33     |
| 14  | G     | 163 | ALA  | CA-C   | -9.42 | 1.41        | 1.52     |
| 21  | N     | 600 | THR  | N-CA   | -9.41 | 1.34        | 1.46     |
| 16  | I     | 156 | ILE  | CA-C   | -9.41 | 1.43        | 1.53     |
| 20  | M     | 220 | MET  | N-CA   | -9.39 | 1.34        | 1.46     |
| 24  | Q     | 80  | HIS  | CG-CD2 | 9.35  | 1.46        | 1.35     |
| 16  | I     | 117 | HIS  | CG-CD2 | 9.33  | 1.46        | 1.35     |
| 14  | G     | 146 | HIS  | CG-CD2 | 9.33  | 1.46        | 1.35     |
| 16  | I     | 150 | HIS  | CG-CD2 | 9.33  | 1.46        | 1.35     |
| 22  | O     | 236 | HIS  | CG-CD2 | 9.33  | 1.46        | 1.35     |
| 6   | 6     | 67  | HIS  | CG-CD2 | 9.32  | 1.46        | 1.35     |
| 28  | U     | 173 | HIS  | CG-CD2 | 9.32  | 1.46        | 1.35     |
| 29  | V     | 109 | HIS  | CG-CD2 | 9.32  | 1.46        | 1.35     |
| 12  | E     | 73  | HIS  | CG-CD2 | 9.32  | 1.46        | 1.35     |
| 14  | G     | 122 | HIS  | CG-CD2 | 9.32  | 1.46        | 1.35     |
| 1   | 1     | 157 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 33  | Z     | 898 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 1   | 1     | 62  | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 14  | G     | 72  | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 20  | M     | 364 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 23  | P     | 282 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 24  | Q     | 334 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 28  | U     | 21  | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 27  | T     | 251 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 11  | D     | 16  | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 26  | S     | 334 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 12  | E     | 147 | HIS  | CG-CD2 | 9.31  | 1.46        | 1.35     |
| 23  | P     | 417 | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 24  | Q     | 135 | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 9   | B     | 94  | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 23  | P     | 440 | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 25  | R     | 81  | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 1   | 1     | 38  | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 3   | 3     | 36  | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 10  | C     | 125 | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 33  | Z     | 132 | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 6   | 6     | 99  | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 9   | B     | 139 | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |
| 22  | O     | 5   | HIS  | CG-CD2 | 9.30  | 1.46        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 26  | S     | 438 | HIS  | CG-CD2 | 9.30 | 1.46        | 1.35     |
| 24  | Q     | 247 | HIS  | CG-CD2 | 9.30 | 1.46        | 1.35     |
| 15  | H     | 95  | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 24  | Q     | 186 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 9   | B     | 190 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 20  | M     | 53  | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 25  | R     | 325 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 29  | V     | 190 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 33  | Z     | 214 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 29  | V     | 195 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 4   | 4     | 40  | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 5   | 5     | 188 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 33  | Z     | 760 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 33  | Z     | 871 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 33  | Z     | 463 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 33  | Z     | 976 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 5   | 5     | 179 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 6   | 6     | 86  | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 8   | A     | 193 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 12  | E     | 99  | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 14  | G     | 182 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 17  | J     | 123 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 17  | J     | 376 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 21  | N     | 573 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 23  | P     | 336 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 33  | Z     | 771 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 33  | Z     | 856 | HIS  | CG-CD2 | 9.29 | 1.46        | 1.35     |
| 14  | G     | 227 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 27  | T     | 123 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 21  | N     | 616 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 26  | S     | 472 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 13  | F     | 69  | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 13  | F     | 110 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 14  | G     | 86  | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 26  | S     | 261 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 23  | P     | 425 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 26  | S     | 317 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 5   | 5     | 66  | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 7   | 7     | 141 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 30  | W     | 86  | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 22  | O     | 235 | HIS  | CG-CD2 | 9.28 | 1.46        | 1.35     |
| 14  | G     | 203 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 17  | J     | 331 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 18  | K     | 142 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 19  | L     | 364 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 21  | N     | 690 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 29  | V     | 204 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 30  | W     | 170 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 7   | 7     | 54  | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 8   | A     | 15  | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 12  | E     | 157 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 21  | N     | 340 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 24  | Q     | 178 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 26  | S     | 191 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 28  | U     | 70  | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 33  | Z     | 361 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 33  | Z     | 593 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 13  | F     | 43  | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 22  | O     | 122 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 16  | I     | 204 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 21  | N     | 375 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 33  | Z     | 801 | HIS  | CG-CD2 | 9.27 | 1.46        | 1.35     |
| 2   | 2     | 109 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 18  | K     | 140 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 22  | O     | 23  | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 16  | I     | 151 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 18  | K     | 244 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 29  | V     | 111 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 33  | Z     | 959 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 26  | S     | 347 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 28  | U     | 5   | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 33  | Z     | 151 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 11  | D     | 96  | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 14  | G     | 181 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 16  | I     | 365 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 27  | T     | 132 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 28  | U     | 94  | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 33  | Z     | 338 | HIS  | CG-CD2 | 9.26 | 1.46        | 1.35     |
| 2   | 2     | 66  | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 23  | P     | 263 | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 29  | V     | 40  | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 25  | R     | 401 | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 19  | L     | 409 | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 26  | S     | 302 | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 33  | Z     | 307 | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 5   | 5     | 166 | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 6   | 6     | 70  | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 2   | 2     | 35  | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 2   | 2     | 116 | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 18  | K     | 74  | HIS  | CG-CD2 | 9.25 | 1.46        | 1.35     |
| 2   | 2     | 141 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 8   | A     | 209 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 21  | N     | 329 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 22  | O     | 326 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 24  | Q     | 226 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 28  | U     | 223 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 12  | E     | 91  | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 30  | W     | 77  | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 30  | W     | 100 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 33  | Z     | 532 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 17  | J     | 170 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 17  | J     | 205 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 29  | V     | 217 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 29  | V     | 279 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 11  | D     | 70  | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 22  | O     | 283 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 1   | 1     | 120 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 2   | 2     | 93  | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 21  | N     | 444 | HIS  | CG-CD2 | 9.24 | 1.46        | 1.35     |
| 2   | 2     | 114 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 12  | E     | 188 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 24  | Q     | 145 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 19  | L     | 67  | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 4   | 4     | 132 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 4   | 4     | 145 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 10  | C     | 31  | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 15  | H     | 392 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 23  | P     | 431 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 21  | N     | 613 | HIS  | CG-CD2 | 9.23 | 1.46        | 1.35     |
| 5   | 5     | 191 | HIS  | CG-CD2 | 9.22 | 1.46        | 1.35     |
| 8   | A     | 185 | HIS  | CG-CD2 | 9.22 | 1.46        | 1.35     |
| 13  | F     | 143 | HIS  | CG-CD2 | 9.22 | 1.46        | 1.35     |
| 21  | N     | 510 | HIS  | CG-CD2 | 9.22 | 1.46        | 1.35     |
| 2   | 2     | 86  | HIS  | CG-CD2 | 9.22 | 1.46        | 1.35     |
| 26  | S     | 139 | HIS  | CG-CD2 | 9.22 | 1.46        | 1.35     |
| 27  | T     | 94  | HIS  | CG-CD2 | 9.22 | 1.46        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 747 | HIS  | CG-CD2 | 9.22  | 1.46        | 1.35     |
| 33  | Z     | 766 | HIS  | CG-CD2 | 9.22  | 1.46        | 1.35     |
| 6   | 6     | 186 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 19  | L     | 273 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 26  | S     | 225 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 33  | Z     | 763 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 4   | 4     | 146 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 14  | G     | 216 | SER  | N-CA   | -9.21 | 1.35        | 1.46     |
| 23  | P     | 230 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 24  | Q     | 361 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 33  | Z     | 622 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 30  | W     | 107 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 33  | Z     | 897 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 10  | C     | 94  | HIS  | CG-CD2 | 9.20  | 1.46        | 1.35     |
| 17  | J     | 240 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 33  | Z     | 156 | HIS  | CG-CD2 | 9.21  | 1.46        | 1.35     |
| 20  | M     | 412 | HIS  | CG-CD2 | 9.20  | 1.46        | 1.35     |
| 6   | 6     | 207 | PHE  | CA-C   | -9.20 | 1.41        | 1.52     |
| 21  | N     | 499 | HIS  | CG-CD2 | 9.20  | 1.46        | 1.35     |
| 28  | U     | 156 | HIS  | CG-CD2 | 9.20  | 1.46        | 1.35     |
| 23  | P     | 348 | HIS  | CG-CD2 | 9.19  | 1.46        | 1.35     |
| 16  | I     | 343 | ARG  | C-N    | 9.19  | 1.43        | 1.33     |
| 25  | R     | 217 | HIS  | CG-CD2 | 9.19  | 1.46        | 1.35     |
| 22  | O     | 318 | HIS  | CG-CD2 | 9.19  | 1.46        | 1.35     |
| 24  | Q     | 252 | HIS  | CG-CD2 | 9.19  | 1.46        | 1.35     |
| 23  | P     | 337 | HIS  | CG-CD2 | 9.19  | 1.46        | 1.35     |
| 17  | J     | 204 | HIS  | CG-CD2 | 9.18  | 1.46        | 1.35     |
| 3   | 3     | 39  | HIS  | CG-CD2 | 9.18  | 1.46        | 1.35     |
| 24  | Q     | 329 | GLU  | CA-C   | -9.09 | 1.40        | 1.52     |
| 1   | 1     | 26  | ILE  | CA-C   | -8.99 | 1.45        | 1.53     |
| 21  | N     | 250 | ASP  | N-CA   | -8.98 | 1.35        | 1.46     |
| 15  | H     | 240 | ILE  | CA-C   | -8.97 | 1.42        | 1.52     |
| 15  | H     | 370 | ARG  | C-N    | 8.95  | 1.44        | 1.33     |
| 33  | Z     | 208 | VAL  | CA-C   | 8.95  | 1.60        | 1.52     |
| 22  | O     | 361 | ASP  | CA-C   | -8.94 | 1.43        | 1.52     |
| 7   | 7     | -1  | GLY  | CA-C   | -8.92 | 1.44        | 1.52     |
| 12  | E     | 190 | SER  | N-CA   | -8.92 | 1.39        | 1.47     |
| 17  | J     | 131 | ASP  | C-N    | 8.89  | 1.44        | 1.33     |
| 23  | P     | 219 | GLU  | CA-C   | 8.85  | 1.64        | 1.52     |
| 18  | K     | 112 | SER  | CA-C   | -8.85 | 1.41        | 1.52     |
| 24  | Q     | 288 | LYS  | CA-C   | -8.83 | 1.41        | 1.52     |
| 23  | P     | 276 | LEU  | N-CA   | -8.82 | 1.35        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 5     | 14  | VAL  | CA-C  | -8.76 | 1.41        | 1.52     |
| 33  | Z     | 116 | ALA  | N-CA  | -8.75 | 1.35        | 1.46     |
| 10  | C     | 223 | GLY  | CA-C  | -8.74 | 1.41        | 1.51     |
| 6   | 6     | 112 | ALA  | N-CA  | -8.74 | 1.35        | 1.46     |
| 21  | N     | 620 | GLY  | CA-C  | -8.73 | 1.41        | 1.52     |
| 25  | R     | 143 | GLN  | N-CA  | -8.71 | 1.35        | 1.46     |
| 21  | N     | 404 | SER  | CA-C  | -8.66 | 1.41        | 1.52     |
| 19  | L     | 312 | MET  | CA-C  | -8.65 | 1.42        | 1.52     |
| 25  | R     | 327 | ASP  | CA-C  | -8.65 | 1.40        | 1.52     |
| 26  | S     | 319 | CYS  | CA-C  | -8.65 | 1.41        | 1.52     |
| 22  | O     | 339 | GLY  | CA-C  | 8.65  | 1.62        | 1.51     |
| 8   | A     | 47  | GLY  | N-CA  | -8.64 | 1.35        | 1.45     |
| 20  | M     | 360 | ILE  | N-CA  | -8.63 | 1.36        | 1.46     |
| 29  | V     | 104 | VAL  | C-N   | 8.63  | 1.43        | 1.33     |
| 25  | R     | 306 | PRO  | N-CD  | 8.62  | 1.59        | 1.47     |
| 23  | P     | 212 | LYS  | C-N   | 8.61  | 1.44        | 1.33     |
| 29  | V     | 142 | ASP  | C-N   | 8.60  | 1.40        | 1.33     |
| 4   | 4     | 190 | GLN  | C-N   | 8.58  | 1.41        | 1.33     |
| 16  | I     | 387 | LEU  | CA-C  | -8.58 | 1.42        | 1.52     |
| 29  | V     | 140 | VAL  | CA-C  | -8.55 | 1.42        | 1.52     |
| 24  | Q     | 195 | LYS  | C-N   | 8.54  | 1.45        | 1.34     |
| 29  | V     | 46  | PRO  | C-N   | 8.51  | 1.45        | 1.33     |
| 14  | G     | 68  | VAL  | N-CA  | -8.50 | 1.35        | 1.46     |
| 19  | L     | 224 | PRO  | C-N   | 8.50  | 1.42        | 1.33     |
| 23  | P     | 399 | ILE  | C-N   | 8.49  | 1.44        | 1.33     |
| 15  | H     | 353 | PHE  | CA-C  | -8.47 | 1.42        | 1.52     |
| 28  | U     | 214 | VAL  | N-CA  | -8.43 | 1.37        | 1.46     |
| 21  | N     | 761 | ILE  | N-CA  | -8.41 | 1.36        | 1.46     |
| 7   | 7     | 162 | VAL  | N-CA  | 8.39  | 1.56        | 1.46     |
| 12  | E     | 136 | ARG  | CD-NE | 8.38  | 1.57        | 1.46     |
| 12  | E     | 146 | GLY  | N-CA  | -8.38 | 1.36        | 1.45     |
| 9   | B     | 44  | VAL  | CA-C  | -8.38 | 1.42        | 1.52     |
| 26  | S     | 227 | ASN  | C-N   | 8.36  | 1.45        | 1.33     |
| 19  | L     | 106 | GLY  | CA-C  | -8.34 | 1.42        | 1.51     |
| 19  | L     | 67  | HIS  | C-N   | 8.32  | 1.44        | 1.33     |
| 21  | N     | 21  | LYS  | CA-C  | 8.30  | 1.63        | 1.52     |
| 28  | U     | 102 | SER  | CA-C  | -8.30 | 1.41        | 1.52     |
| 33  | Z     | 494 | GLY  | CA-C  | -8.30 | 1.42        | 1.52     |
| 22  | O     | 201 | PRO  | N-CD  | 8.30  | 1.59        | 1.47     |
| 24  | Q     | 209 | TYR  | C-N   | 8.30  | 1.43        | 1.33     |
| 1   | 1     | 69  | GLN  | CA-C  | -8.28 | 1.42        | 1.52     |
| 28  | U     | 191 | THR  | N-CA  | 8.28  | 1.56        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 17  | J     | 117 | SER  | CA-C  | -8.27 | 1.40        | 1.52     |
| 15  | H     | 281 | GLN  | CA-C  | 8.26  | 1.62        | 1.52     |
| 33  | Z     | 305 | VAL  | N-CA  | -8.26 | 1.36        | 1.46     |
| 9   | B     | 157 | PHE  | CA-C  | -8.26 | 1.42        | 1.52     |
| 14  | G     | 162 | ALA  | CA-C  | -8.24 | 1.42        | 1.52     |
| 30  | W     | 86  | HIS  | CA-C  | -8.24 | 1.45        | 1.53     |
| 3   | 3     | 75  | PRO  | N-CD  | 8.23  | 1.59        | 1.47     |
| 18  | K     | 252 | ARG  | CD-NE | 8.21  | 1.57        | 1.46     |
| 8   | A     | 60  | PRO  | N-CD  | 8.21  | 1.59        | 1.47     |
| 11  | D     | 54  | LEU  | N-CA  | -8.20 | 1.38        | 1.46     |
| 10  | C     | 47  | ALA  | CA-C  | -8.19 | 1.42        | 1.52     |
| 29  | V     | 143 | PRO  | N-CD  | 8.18  | 1.59        | 1.47     |
| 4   | 4     | 132 | HIS  | CA-C  | -8.17 | 1.42        | 1.52     |
| 22  | O     | 122 | HIS  | N-CA  | -8.15 | 1.35        | 1.46     |
| 18  | K     | 98  | GLN  | CA-C  | -8.15 | 1.42        | 1.52     |
| 3   | 3     | 159 | SER  | CA-C  | -8.14 | 1.42        | 1.52     |
| 31  | X     | 104 | LYS  | CA-C  | -8.12 | 1.42        | 1.52     |
| 23  | P     | 390 | TYR  | C-N   | 8.11  | 1.43        | 1.33     |
| 16  | I     | 324 | VAL  | CA-C  | -8.11 | 1.43        | 1.52     |
| 25  | R     | 227 | ALA  | N-CA  | -8.09 | 1.36        | 1.46     |
| 6   | 6     | 176 | ARG  | CA-C  | -8.08 | 1.42        | 1.52     |
| 13  | F     | 123 | TYR  | CA-C  | -8.07 | 1.42        | 1.52     |
| 8   | A     | 210 | MET  | C-N   | 8.06  | 1.44        | 1.33     |
| 26  | S     | 233 | LEU  | CA-C  | -8.06 | 1.42        | 1.52     |
| 21  | N     | 785 | PRO  | CA-C  | -8.01 | 1.41        | 1.52     |
| 20  | M     | 376 | TRP  | CA-C  | -8.01 | 1.42        | 1.52     |
| 21  | N     | 267 | GLN  | N-CA  | -8.00 | 1.36        | 1.46     |
| 18  | K     | 398 | ASN  | CA-C  | -8.00 | 1.45        | 1.53     |
| 33  | Z     | 604 | GLY  | CA-C  | 7.97  | 1.61        | 1.52     |
| 28  | U     | 41  | ALA  | CA-C  | -7.97 | 1.42        | 1.52     |
| 21  | N     | 259 | PHE  | C-N   | 7.97  | 1.43        | 1.33     |
| 25  | R     | 356 | ALA  | C-N   | 7.96  | 1.43        | 1.33     |
| 10  | C     | 49  | GLU  | CA-C  | -7.93 | 1.43        | 1.52     |
| 9   | B     | 240 | SER  | C-N   | 7.93  | 1.44        | 1.33     |
| 23  | P     | 363 | LEU  | CA-C  | -7.92 | 1.42        | 1.52     |
| 6   | 6     | 112 | ALA  | CA-C  | -7.92 | 1.42        | 1.52     |
| 22  | O     | 79  | VAL  | C-N   | 7.91  | 1.43        | 1.33     |
| 21  | N     | 273 | LEU  | N-CA  | -7.91 | 1.36        | 1.46     |
| 29  | V     | 295 | VAL  | N-CA  | 7.91  | 1.55        | 1.46     |
| 33  | Z     | 622 | HIS  | CA-C  | -7.90 | 1.42        | 1.52     |
| 11  | D     | 68  | ASP  | CA-C  | -7.90 | 1.43        | 1.52     |
| 8   | A     | 231 | ASP  | C-N   | 7.89  | 1.43        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 16  | I     | 312 | GLN  | C-N   | 7.89  | 1.44        | 1.33     |
| 18  | K     | 294 | ARG  | CA-CB | 7.88  | 1.65        | 1.53     |
| 25  | R     | 347 | THR  | N-CA  | -7.86 | 1.36        | 1.46     |
| 15  | H     | 358 | PRO  | N-CD  | 7.85  | 1.58        | 1.47     |
| 21  | N     | 34  | GLN  | C-N   | 7.85  | 1.43        | 1.33     |
| 12  | E     | 21  | LEU  | CA-C  | -7.85 | 1.42        | 1.52     |
| 28  | U     | 226 | LEU  | CA-C  | -7.84 | 1.42        | 1.52     |
| 2   | 2     | 16  | ALA  | CA-C  | -7.83 | 1.43        | 1.52     |
| 30  | W     | 171 | LEU  | CA-C  | -7.83 | 1.43        | 1.52     |
| 8   | A     | 146 | VAL  | CA-C  | -7.82 | 1.45        | 1.52     |
| 8   | A     | 202 | VAL  | N-CA  | 7.81  | 1.55        | 1.46     |
| 20  | M     | 422 | VAL  | CA-C  | -7.81 | 1.42        | 1.52     |
| 3   | 3     | 95  | PHE  | CA-C  | -7.80 | 1.45        | 1.53     |
| 33  | Z     | 901 | PHE  | C-N   | 7.80  | 1.44        | 1.33     |
| 24  | Q     | 175 | VAL  | N-CA  | -7.80 | 1.37        | 1.46     |
| 7   | 7     | 169 | ILE  | N-CA  | -7.80 | 1.37        | 1.46     |
| 16  | I     | 133 | LEU  | N-CA  | -7.79 | 1.36        | 1.45     |
| 16  | I     | 390 | ALA  | CA-C  | -7.79 | 1.42        | 1.52     |
| 20  | M     | 126 | THR  | CA-C  | -7.78 | 1.43        | 1.52     |
| 13  | F     | 126 | ARG  | CA-C  | -7.78 | 1.42        | 1.52     |
| 24  | Q     | 212 | THR  | N-CA  | 7.78  | 1.55        | 1.46     |
| 21  | N     | 919 | THR  | CA-C  | -7.77 | 1.43        | 1.52     |
| 3   | 3     | 115 | PHE  | N-CA  | -7.77 | 1.35        | 1.45     |
| 13  | F     | 149 | PRO  | N-CD  | 7.77  | 1.58        | 1.47     |
| 33  | Z     | 482 | ASP  | CA-C  | -7.77 | 1.42        | 1.52     |
| 29  | V     | 132 | LEU  | CA-C  | -7.75 | 1.43        | 1.53     |
| 9   | B     | 82  | TYR  | C-N   | 7.75  | 1.44        | 1.33     |
| 8   | A     | 188 | LYS  | N-CA  | -7.75 | 1.36        | 1.46     |
| 6   | 6     | 128 | ARG  | CA-C  | -7.73 | 1.43        | 1.52     |
| 9   | B     | 183 | LEU  | C-N   | 7.73  | 1.44        | 1.33     |
| 15  | H     | 200 | VAL  | CA-C  | -7.73 | 1.43        | 1.52     |
| 10  | C     | 103 | ASN  | C-N   | 7.72  | 1.43        | 1.33     |
| 33  | Z     | 891 | PRO  | N-CD  | 7.71  | 1.58        | 1.47     |
| 14  | G     | 44  | GLY  | CA-C  | -7.71 | 1.40        | 1.51     |
| 17  | J     | 97  | ASP  | CA-C  | -7.71 | 1.43        | 1.52     |
| 21  | N     | 8   | PRO  | N-CD  | 7.70  | 1.58        | 1.47     |
| 24  | Q     | 187 | LYS  | CA-C  | -7.68 | 1.42        | 1.52     |
| 1   | 1     | 14  | LEU  | N-CA  | -7.68 | 1.36        | 1.46     |
| 27  | T     | 7   | LEU  | CA-C  | -7.67 | 1.42        | 1.52     |
| 33  | Z     | 441 | TYR  | C-N   | 7.66  | 1.44        | 1.33     |
| 24  | Q     | 111 | LEU  | CA-C  | -7.66 | 1.43        | 1.52     |
| 7   | 7     | 109 | ALA  | CA-C  | -7.65 | 1.43        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11  | D     | 16  | HIS  | CA-C  | -7.65 | 1.43        | 1.52     |
| 29  | V     | 276 | PRO  | C-N   | 7.64  | 1.44        | 1.33     |
| 12  | E     | 246 | LYS  | N-CA  | -7.64 | 1.36        | 1.46     |
| 25  | R     | 333 | MET  | CA-C  | -7.64 | 1.42        | 1.52     |
| 28  | U     | 54  | LEU  | CA-C  | -7.63 | 1.43        | 1.52     |
| 4   | 4     | 55  | PHE  | CA-C  | -7.63 | 1.43        | 1.52     |
| 26  | S     | 163 | VAL  | CA-C  | -7.63 | 1.43        | 1.52     |
| 31  | X     | 116 | ALA  | CA-C  | -7.63 | 1.42        | 1.52     |
| 16  | I     | 170 | VAL  | C-N   | 7.62  | 1.43        | 1.33     |
| 4   | 4     | 38  | SER  | N-CA  | -7.61 | 1.39        | 1.46     |
| 26  | S     | 443 | ILE  | C-N   | 7.61  | 1.43        | 1.33     |
| 19  | L     | 172 | SER  | CA-C  | -7.61 | 1.43        | 1.52     |
| 33  | Z     | 337 | GLU  | CA-C  | -7.60 | 1.42        | 1.52     |
| 9   | B     | 182 | GLU  | N-CA  | -7.60 | 1.36        | 1.46     |
| 26  | S     | 286 | TYR  | C-N   | 7.59  | 1.43        | 1.33     |
| 15  | H     | 207 | THR  | C-N   | 7.59  | 1.44        | 1.33     |
| 2   | 2     | 15  | ALA  | N-CA  | -7.59 | 1.36        | 1.46     |
| 16  | I     | 282 | ASP  | CA-C  | -7.59 | 1.43        | 1.52     |
| 17  | J     | 269 | GLN  | N-CA  | -7.58 | 1.36        | 1.46     |
| 23  | P     | 70  | ASN  | C-N   | 7.58  | 1.43        | 1.33     |
| 30  | W     | 136 | ASN  | N-CA  | 7.58  | 1.55        | 1.46     |
| 12  | E     | 248 | ALA  | CA-C  | 7.57  | 1.62        | 1.52     |
| 22  | O     | 166 | ARG  | N-CA  | -7.57 | 1.36        | 1.46     |
| 23  | P     | 342 | GLN  | N-CA  | -7.57 | 1.37        | 1.46     |
| 3   | 3     | 16  | CYS  | CA-C  | -7.56 | 1.43        | 1.52     |
| 12  | E     | 75  | GLY  | CA-C  | -7.56 | 1.44        | 1.52     |
| 17  | J     | 32  | LEU  | N-CA  | -7.56 | 1.37        | 1.46     |
| 17  | J     | 27  | ILE  | C-N   | 7.55  | 1.43        | 1.33     |
| 21  | N     | 58  | ARG  | C-N   | 7.54  | 1.44        | 1.33     |
| 24  | Q     | 343 | LEU  | N-CA  | -7.51 | 1.37        | 1.46     |
| 10  | C     | 148 | LEU  | N-CA  | -7.51 | 1.37        | 1.46     |
| 9   | B     | 216 | ASP  | CA-C  | -7.51 | 1.43        | 1.52     |
| 22  | O     | 180 | LYS  | C-N   | 7.51  | 1.43        | 1.33     |
| 23  | P     | 286 | ASN  | CA-C  | 7.51  | 1.62        | 1.52     |
| 11  | D     | 121 | THR  | CA-C  | -7.49 | 1.43        | 1.52     |
| 33  | Z     | 201 | LEU  | N-CA  | -7.49 | 1.37        | 1.46     |
| 33  | Z     | 866 | VAL  | C-N   | 7.49  | 1.44        | 1.33     |
| 31  | X     | 37  | PRO  | N-CD  | 7.49  | 1.58        | 1.47     |
| 8   | A     | 199 | TRP  | CA-C  | -7.48 | 1.42        | 1.52     |
| 31  | X     | 132 | SER  | N-CA  | -7.48 | 1.37        | 1.46     |
| 25  | R     | 180 | PHE  | CA-C  | -7.48 | 1.43        | 1.52     |
| 33  | Z     | 354 | PRO  | N-CD  | 7.48  | 1.58        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 21  | N     | 274 | VAL  | C-N   | 7.48  | 1.43        | 1.33     |
| 5   | 5     | 50  | ALA  | C-N   | 7.47  | 1.43        | 1.33     |
| 10  | C     | 52  | VAL  | C-N   | 7.47  | 1.44        | 1.33     |
| 33  | Z     | 501 | LYS  | CA-C  | -7.47 | 1.43        | 1.52     |
| 26  | S     | 157 | GLU  | CA-C  | -7.47 | 1.43        | 1.52     |
| 6   | 6     | 56  | VAL  | N-CA  | -7.46 | 1.37        | 1.46     |
| 14  | G     | 81  | ILE  | CA-C  | 7.45  | 1.59        | 1.52     |
| 20  | M     | 154 | LEU  | CA-C  | -7.45 | 1.43        | 1.52     |
| 26  | S     | 291 | GLU  | N-CA  | -7.45 | 1.37        | 1.46     |
| 10  | C     | 120 | GLN  | N-CA  | -7.45 | 1.37        | 1.46     |
| 12  | E     | 167 | TYR  | CA-C  | -7.45 | 1.43        | 1.52     |
| 13  | F     | 105 | VAL  | CA-C  | -7.44 | 1.43        | 1.52     |
| 22  | O     | 50  | ASP  | C-N   | 7.43  | 1.43        | 1.33     |
| 12  | E     | 79  | SER  | N-CA  | -7.43 | 1.37        | 1.46     |
| 25  | R     | 51  | LEU  | N-CA  | -7.43 | 1.37        | 1.46     |
| 28  | U     | 67  | PHE  | CA-C  | -7.43 | 1.43        | 1.52     |
| 6   | 6     | 27  | ASN  | N-CA  | -7.42 | 1.36        | 1.46     |
| 26  | S     | 376 | THR  | C-N   | 7.41  | 1.44        | 1.34     |
| 7   | 7     | 103 | TRP  | CA-C  | -7.41 | 1.45        | 1.53     |
| 21  | N     | 373 | VAL  | CA-C  | -7.41 | 1.43        | 1.52     |
| 19  | L     | 276 | CYS  | N-CA  | -7.41 | 1.36        | 1.46     |
| 31  | X     | 70  | PRO  | N-CD  | 7.40  | 1.58        | 1.47     |
| 9   | B     | 135 | LEU  | CA-C  | -7.39 | 1.44        | 1.52     |
| 5   | 5     | 208 | ASN  | N-CA  | -7.39 | 1.36        | 1.46     |
| 18  | K     | 287 | GLY  | CA-C  | -7.38 | 1.41        | 1.51     |
| 15  | H     | 454 | TYR  | CA-C  | -7.38 | 1.43        | 1.52     |
| 11  | D     | 140 | PRO  | C-N   | 7.37  | 1.44        | 1.33     |
| 17  | J     | 86  | VAL  | CA-C  | -7.37 | 1.43        | 1.52     |
| 2   | 2     | 108 | SER  | CA-C  | -7.37 | 1.43        | 1.52     |
| 25  | R     | 234 | SER  | CA-C  | -7.37 | 1.43        | 1.52     |
| 33  | Z     | 80  | SER  | CA-C  | -7.35 | 1.43        | 1.52     |
| 21  | N     | 627 | ILE  | CA-C  | -7.35 | 1.44        | 1.52     |
| 16  | I     | 159 | VAL  | C-N   | 7.34  | 1.43        | 1.33     |
| 5   | 5     | 142 | SER  | C-N   | 7.34  | 1.43        | 1.33     |
| 29  | V     | 154 | ASP  | CA-C  | -7.33 | 1.43        | 1.52     |
| 19  | L     | 297 | ALA  | N-CA  | -7.31 | 1.39        | 1.46     |
| 7   | 7     | -5  | PRO  | N-CD  | 7.31  | 1.57        | 1.47     |
| 5   | 5     | 101 | ILE  | CA-C  | -7.30 | 1.43        | 1.52     |
| 9   | B     | 231 | LYS  | CA-C  | -7.30 | 1.43        | 1.52     |
| 15  | H     | 242 | PRO  | CA-C  | -7.30 | 1.45        | 1.52     |
| 2   | 2     | 149 | GLU  | N-CA  | -7.30 | 1.37        | 1.46     |
| 21  | N     | 643 | PRO  | N-CD  | 7.30  | 1.57        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 30  | W     | 191 | ILE  | C-N   | 7.30  | 1.44        | 1.33     |
| 33  | Z     | 278 | LEU  | CA-C  | -7.29 | 1.42        | 1.52     |
| 30  | W     | 71  | LYS  | CA-C  | -7.29 | 1.43        | 1.52     |
| 12  | E     | 236 | THR  | C-N   | 7.29  | 1.43        | 1.33     |
| 9   | B     | 108 | LYS  | CA-C  | -7.29 | 1.43        | 1.52     |
| 21  | N     | 207 | LEU  | N-CA  | -7.28 | 1.37        | 1.46     |
| 15  | H     | 378 | SER  | CA-C  | -7.27 | 1.44        | 1.52     |
| 7   | 7     | 193 | ASP  | CA-C  | -7.26 | 1.43        | 1.52     |
| 16  | I     | 246 | ARG  | CA-C  | -7.26 | 1.43        | 1.52     |
| 20  | M     | 388 | GLY  | CA-C  | 7.25  | 1.60        | 1.52     |
| 13  | F     | 109 | GLY  | CA-C  | -7.25 | 1.44        | 1.52     |
| 8   | A     | 226 | GLY  | CA-C  | -7.25 | 1.45        | 1.51     |
| 7   | 7     | 34  | LEU  | C-N   | 7.24  | 1.41        | 1.33     |
| 18  | K     | 128 | ARG  | CA-C  | 7.23  | 1.62        | 1.52     |
| 20  | M     | 333 | LEU  | N-CA  | -7.23 | 1.37        | 1.46     |
| 8   | A     | 191 | ILE  | CA-C  | -7.22 | 1.43        | 1.52     |
| 24  | Q     | 9   | GLU  | CA-C  | -7.21 | 1.43        | 1.52     |
| 33  | Z     | 411 | LYS  | CA-C  | -7.19 | 1.44        | 1.52     |
| 9   | B     | 210 | GLU  | CA-C  | -7.19 | 1.44        | 1.52     |
| 21  | N     | 615 | ALA  | C-N   | 7.19  | 1.43        | 1.34     |
| 15  | H     | 65  | GLU  | C-N   | 7.18  | 1.43        | 1.33     |
| 1   | 1     | 108 | GLY  | CA-C  | -7.17 | 1.43        | 1.52     |
| 16  | I     | 422 | ARG  | CA-C  | -7.17 | 1.43        | 1.52     |
| 26  | S     | 193 | THR  | CA-C  | -7.17 | 1.44        | 1.52     |
| 18  | K     | 160 | VAL  | CA-C  | -7.17 | 1.43        | 1.52     |
| 24  | Q     | 153 | ASP  | CA-C  | 7.16  | 1.62        | 1.52     |
| 33  | Z     | 414 | GLY  | CA-C  | 7.16  | 1.60        | 1.52     |
| 33  | Z     | 391 | ASN  | CA-C  | -7.15 | 1.43        | 1.53     |
| 3   | 3     | 192 | LYS  | C-N   | 7.15  | 1.42        | 1.33     |
| 1   | 1     | 57  | ASP  | CA-C  | -7.15 | 1.43        | 1.52     |
| 4   | 4     | 18  | LYS  | CA-C  | -7.14 | 1.43        | 1.52     |
| 28  | U     | 80  | CYS  | CA-C  | -7.14 | 1.43        | 1.52     |
| 19  | L     | 237 | ALA  | CA-C  | -7.14 | 1.43        | 1.52     |
| 21  | N     | 671 | LEU  | CA-C  | -7.14 | 1.43        | 1.52     |
| 13  | F     | 56  | LEU  | N-CA  | 7.13  | 1.55        | 1.46     |
| 16  | I     | 80  | GLU  | CA-C  | -7.13 | 1.43        | 1.52     |
| 27  | T     | 12  | SER  | C-N   | 7.13  | 1.42        | 1.33     |
| 9   | B     | 69  | PRO  | N-CD  | 7.13  | 1.57        | 1.47     |
| 9   | B     | 228 | PRO  | N-CA  | -7.13 | 1.38        | 1.47     |
| 33  | Z     | 870 | ALA  | N-CA  | -7.13 | 1.38        | 1.46     |
| 2   | 2     | 183 | ASP  | C-N   | 7.13  | 1.43        | 1.33     |
| 15  | H     | 317 | ALA  | CA-C  | -7.12 | 1.43        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 29  | V     | 46  | PRO  | N-CD  | 7.12  | 1.57        | 1.47     |
| 25  | R     | 187 | VAL  | N-CA  | -7.11 | 1.37        | 1.46     |
| 26  | S     | 254 | ILE  | C-N   | 7.11  | 1.43        | 1.33     |
| 33  | Z     | 592 | GLU  | C-N   | 7.11  | 1.41        | 1.33     |
| 4   | 4     | 133 | GLY  | CA-C  | -7.11 | 1.44        | 1.52     |
| 17  | J     | 281 | GLY  | CA-C  | -7.11 | 1.41        | 1.51     |
| 5   | 5     | 45  | MET  | CA-C  | -7.10 | 1.44        | 1.52     |
| 29  | V     | 289 | GLU  | CA-C  | -7.10 | 1.43        | 1.52     |
| 15  | H     | 331 | ARG  | C-N   | 7.10  | 1.43        | 1.33     |
| 15  | H     | 451 | ILE  | N-CA  | 7.10  | 1.54        | 1.46     |
| 18  | K     | 399 | ARG  | CA-C  | -7.09 | 1.43        | 1.52     |
| 6   | 6     | 5   | GLY  | CA-C  | -7.08 | 1.46        | 1.52     |
| 29  | V     | 293 | VAL  | N-CA  | -7.08 | 1.38        | 1.46     |
| 10  | C     | 128 | LEU  | N-CA  | -7.08 | 1.37        | 1.45     |
| 19  | L     | 248 | ALA  | C-O   | -7.08 | 1.15        | 1.24     |
| 26  | S     | 320 | ILE  | N-CA  | -7.08 | 1.38        | 1.46     |
| 21  | N     | 638 | ILE  | CA-C  | -7.07 | 1.43        | 1.52     |
| 25  | R     | 237 | THR  | CA-C  | -7.07 | 1.42        | 1.52     |
| 24  | Q     | 319 | LYS  | C-N   | 7.07  | 1.43        | 1.33     |
| 33  | Z     | 134 | SER  | C-N   | 7.07  | 1.43        | 1.33     |
| 11  | D     | 230 | ASN  | CA-C  | -7.07 | 1.43        | 1.52     |
| 26  | S     | 207 | ASN  | C-N   | 7.07  | 1.42        | 1.33     |
| 28  | U     | 133 | PRO  | N-CD  | 7.07  | 1.57        | 1.47     |
| 14  | G     | 156 | TYR  | N-CA  | -7.06 | 1.37        | 1.46     |
| 31  | X     | 80  | SER  | C-N   | 7.06  | 1.43        | 1.33     |
| 18  | K     | 132 | LYS  | N-CA  | 7.06  | 1.52        | 1.45     |
| 21  | N     | 497 | ALA  | N-CA  | -7.06 | 1.38        | 1.46     |
| 13  | F     | 151 | GLY  | CA-C  | -7.05 | 1.42        | 1.51     |
| 14  | G     | 50  | GLU  | N-CA  | -7.05 | 1.37        | 1.46     |
| 30  | W     | 4   | GLU  | CA-C  | -7.05 | 1.43        | 1.52     |
| 22  | O     | 317 | THR  | N-CA  | -7.05 | 1.37        | 1.46     |
| 21  | N     | 886 | LYS  | CA-C  | -7.05 | 1.44        | 1.53     |
| 3   | 3     | 182 | LYS  | CA-C  | -7.05 | 1.44        | 1.52     |
| 25  | R     | 176 | ARG  | CA-C  | -7.04 | 1.44        | 1.52     |
| 19  | L     | 342 | ARG  | CA-C  | -7.04 | 1.43        | 1.52     |
| 10  | C     | 215 | THR  | N-CA  | -7.04 | 1.36        | 1.45     |
| 1   | 1     | 19  | ARG  | N-CA  | -7.04 | 1.37        | 1.46     |
| 17  | J     | 121 | MET  | CA-C  | -7.03 | 1.43        | 1.52     |
| 33  | Z     | 56  | LEU  | N-CA  | -7.03 | 1.37        | 1.46     |
| 6   | 6     | 41  | ILE  | CA-C  | -7.03 | 1.43        | 1.52     |
| 32  | Y     | 73  | PHE  | N-CA  | -7.02 | 1.38        | 1.46     |
| 9   | B     | 140 | ASP  | CA-C  | -7.02 | 1.43        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23  | P     | 176 | LYS  | N-CA  | -7.02 | 1.37        | 1.46     |
| 24  | Q     | 37  | GLN  | N-CA  | 7.02  | 1.55        | 1.46     |
| 31  | X     | 100 | TRP  | CA-C  | -7.01 | 1.44        | 1.52     |
| 1   | 1     | 190 | PRO  | N-CD  | 7.01  | 1.57        | 1.47     |
| 22  | O     | 230 | PHE  | C-N   | 7.00  | 1.43        | 1.33     |
| 23  | P     | 122 | ILE  | CA-C  | -7.00 | 1.45        | 1.53     |
| 18  | K     | 50  | LYS  | N-CA  | -6.99 | 1.38        | 1.46     |
| 18  | K     | 355 | THR  | C-N   | 6.99  | 1.42        | 1.33     |
| 9   | B     | 90  | ARG  | C-N   | 6.98  | 1.43        | 1.33     |
| 14  | G     | 63  | ASN  | C-N   | 6.98  | 1.42        | 1.33     |
| 29  | V     | 101 | ASP  | CA-C  | -6.98 | 1.44        | 1.52     |
| 33  | Z     | 186 | GLY  | C-N   | 6.97  | 1.42        | 1.33     |
| 13  | F     | 50  | LYS  | C-N   | 6.97  | 1.43        | 1.33     |
| 16  | I     | 145 | CYS  | C-N   | 6.96  | 1.43        | 1.33     |
| 8   | A     | 136 | PRO  | CA-C  | -6.96 | 1.45        | 1.52     |
| 20  | M     | 286 | ILE  | N-CA  | -6.96 | 1.38        | 1.46     |
| 20  | M     | 413 | GLU  | CA-C  | -6.96 | 1.43        | 1.52     |
| 5   | 5     | 8   | PHE  | N-CA  | -6.96 | 1.36        | 1.46     |
| 3   | 3     | 21  | GLY  | N-CA  | -6.95 | 1.38        | 1.44     |
| 12  | E     | 230 | ILE  | N-CA  | -6.94 | 1.37        | 1.46     |
| 22  | O     | 26  | PHE  | CA-C  | -6.94 | 1.43        | 1.52     |
| 33  | Z     | 616 | LEU  | CA-C  | -6.94 | 1.43        | 1.52     |
| 17  | J     | 161 | LYS  | CA-C  | -6.94 | 1.44        | 1.52     |
| 26  | S     | 260 | PRO  | N-CD  | 6.93  | 1.57        | 1.47     |
| 6   | 6     | 193 | LEU  | CA-C  | -6.93 | 1.44        | 1.52     |
| 4   | 4     | 127 | LEU  | N-CA  | -6.93 | 1.36        | 1.46     |
| 29  | V     | 260 | GLU  | C-N   | 6.93  | 1.42        | 1.33     |
| 16  | I     | 143 | PRO  | C-N   | 6.92  | 1.44        | 1.33     |
| 21  | N     | 605 | ILE  | C-N   | 6.92  | 1.41        | 1.34     |
| 13  | F     | 137 | TYR  | N-CA  | -6.92 | 1.38        | 1.46     |
| 8   | A     | 117 | LEU  | C-N   | 6.91  | 1.42        | 1.33     |
| 10  | C     | 104 | GLU  | C-N   | 6.90  | 1.42        | 1.33     |
| 21  | N     | 474 | SER  | CA-C  | -6.90 | 1.44        | 1.52     |
| 7   | 7     | 189 | LEU  | N-CA  | -6.90 | 1.37        | 1.46     |
| 2   | 2     | 20  | SER  | CA-C  | -6.89 | 1.44        | 1.52     |
| 15  | H     | 289 | ARG  | N-CA  | -6.89 | 1.37        | 1.46     |
| 20  | M     | 326 | ALA  | CA-C  | -6.88 | 1.44        | 1.52     |
| 24  | Q     | 246 | TYR  | N-CA  | -6.88 | 1.37        | 1.46     |
| 33  | Z     | 907 | GLY  | C-N   | 6.88  | 1.42        | 1.33     |
| 14  | G     | 19  | ARG  | N-CA  | -6.88 | 1.37        | 1.46     |
| 19  | L     | 76  | GLN  | CA-C  | -6.88 | 1.44        | 1.52     |
| 33  | Z     | 969 | GLU  | C-N   | 6.88  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | 6     | 88  | LEU  | CA-C  | -6.88 | 1.44        | 1.52     |
| 10  | C     | 195 | LYS  | CA-C  | -6.87 | 1.44        | 1.52     |
| 27  | T     | 42  | PRO  | CA-C  | -6.87 | 1.45        | 1.52     |
| 14  | G     | 50  | GLU  | C-N   | 6.87  | 1.42        | 1.33     |
| 14  | G     | 16  | PRO  | N-CD  | 6.87  | 1.57        | 1.47     |
| 15  | H     | 381 | ASP  | N-CA  | 6.87  | 1.54        | 1.45     |
| 31  | X     | 62  | ASP  | N-CA  | -6.86 | 1.41        | 1.46     |
| 24  | Q     | 129 | LYS  | C-N   | 6.86  | 1.42        | 1.33     |
| 20  | M     | 380 | ALA  | C-N   | 6.85  | 1.43        | 1.33     |
| 12  | E     | 124 | GLY  | CA-C  | -6.85 | 1.44        | 1.51     |
| 25  | R     | 255 | VAL  | CA-C  | 6.84  | 1.61        | 1.52     |
| 17  | J     | 326 | GLU  | N-CA  | -6.83 | 1.38        | 1.46     |
| 24  | Q     | 149 | LYS  | CA-C  | -6.83 | 1.43        | 1.52     |
| 26  | S     | 145 | PHE  | C-N   | 6.83  | 1.43        | 1.33     |
| 26  | S     | 370 | LEU  | CA-C  | -6.83 | 1.44        | 1.52     |
| 7   | 7     | 26  | LEU  | N-CA  | -6.83 | 1.38        | 1.46     |
| 18  | K     | 208 | GLY  | CA-C  | -6.83 | 1.46        | 1.51     |
| 16  | I     | 309 | LEU  | N-CA  | -6.82 | 1.38        | 1.46     |
| 6   | 6     | 178 | SER  | CA-C  | -6.81 | 1.44        | 1.52     |
| 4   | 4     | 99  | VAL  | CA-C  | -6.81 | 1.44        | 1.52     |
| 10  | C     | 185 | LYS  | C-N   | 6.81  | 1.42        | 1.33     |
| 24  | Q     | 421 | LYS  | C-N   | 6.81  | 1.42        | 1.33     |
| 1   | 1     | 2   | SER  | CA-C  | 6.81  | 1.60        | 1.53     |
| 18  | K     | 232 | ALA  | N-CA  | -6.81 | 1.37        | 1.45     |
| 33  | Z     | 300 | ALA  | CA-C  | -6.80 | 1.43        | 1.52     |
| 23  | P     | 188 | ILE  | N-CA  | -6.80 | 1.38        | 1.46     |
| 24  | Q     | 403 | PRO  | N-CD  | 6.80  | 1.57        | 1.47     |
| 21  | N     | 213 | PHE  | CA-C  | -6.80 | 1.43        | 1.52     |
| 28  | U     | 70  | HIS  | CA-C  | -6.80 | 1.44        | 1.52     |
| 11  | D     | 58  | ARG  | C-N   | 6.80  | 1.40        | 1.33     |
| 19  | L     | 296 | SER  | C-O   | -6.79 | 1.16        | 1.24     |
| 13  | F     | 2   | PHE  | C-N   | 6.79  | 1.42        | 1.33     |
| 14  | G     | 49  | VAL  | CA-C  | -6.78 | 1.44        | 1.52     |
| 6   | 6     | 44  | SER  | CA-C  | -6.78 | 1.44        | 1.52     |
| 11  | D     | 9   | SER  | CA-C  | -6.77 | 1.44        | 1.52     |
| 23  | P     | 130 | ILE  | N-CA  | -6.76 | 1.37        | 1.46     |
| 29  | V     | 207 | ALA  | C-N   | 6.76  | 1.43        | 1.33     |
| 33  | Z     | 886 | VAL  | CA-C  | -6.76 | 1.44        | 1.52     |
| 25  | R     | 282 | THR  | C-N   | 6.76  | 1.42        | 1.33     |
| 31  | X     | 26  | PRO  | N-CD  | 6.75  | 1.57        | 1.47     |
| 33  | Z     | 818 | CYS  | C-N   | 6.75  | 1.42        | 1.33     |
| 17  | J     | 274 | GLU  | N-CA  | -6.75 | 1.38        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23  | P     | 72  | TRP  | N-CA  | -6.74 | 1.38        | 1.46     |
| 29  | V     | 136 | ALA  | CA-C  | -6.74 | 1.44        | 1.52     |
| 18  | K     | 139 | LEU  | CA-C  | -6.74 | 1.44        | 1.52     |
| 33  | Z     | 289 | GLY  | CA-C  | -6.74 | 1.42        | 1.51     |
| 15  | H     | 163 | VAL  | CA-C  | 6.74  | 1.60        | 1.52     |
| 21  | N     | 538 | LYS  | CA-C  | -6.73 | 1.43        | 1.52     |
| 13  | F     | 9   | ASP  | C-N   | 6.73  | 1.43        | 1.33     |
| 14  | G     | 189 | ARG  | C-N   | 6.73  | 1.42        | 1.33     |
| 21  | N     | 748 | PHE  | N-CA  | -6.72 | 1.37        | 1.46     |
| 33  | Z     | 571 | GLY  | CA-C  | -6.72 | 1.44        | 1.52     |
| 15  | H     | 327 | ASN  | CA-C  | -6.72 | 1.43        | 1.52     |
| 30  | W     | 50  | GLY  | C-N   | 6.72  | 1.42        | 1.33     |
| 19  | L     | 148 | LEU  | N-CA  | -6.71 | 1.37        | 1.45     |
| 14  | G     | 219 | SER  | N-CA  | -6.71 | 1.37        | 1.46     |
| 18  | K     | 215 | PRO  | N-CD  | 6.71  | 1.57        | 1.47     |
| 12  | E     | 166 | ARG  | CA-C  | 6.70  | 1.61        | 1.52     |
| 21  | N     | 251 | GLU  | C-N   | 6.70  | 1.41        | 1.33     |
| 24  | Q     | 307 | ASN  | C-N   | 6.70  | 1.43        | 1.33     |
| 19  | L     | 271 | LYS  | CA-C  | -6.70 | 1.43        | 1.52     |
| 24  | Q     | 234 | THR  | CA-C  | 6.70  | 1.61        | 1.52     |
| 5   | 5     | 151 | GLU  | CA-C  | -6.69 | 1.44        | 1.52     |
| 11  | D     | 170 | THR  | C-N   | 6.69  | 1.41        | 1.34     |
| 23  | P     | 377 | GLU  | CA-C  | 6.69  | 1.61        | 1.52     |
| 20  | M     | 387 | ASN  | CA-C  | -6.69 | 1.44        | 1.52     |
| 28  | U     | 261 | LEU  | C-O   | -6.69 | 1.16        | 1.24     |
| 29  | V     | 78  | VAL  | N-CA  | -6.69 | 1.38        | 1.46     |
| 24  | Q     | 208 | ILE  | C-N   | 6.68  | 1.42        | 1.33     |
| 20  | M     | 315 | PHE  | C-N   | 6.68  | 1.42        | 1.33     |
| 10  | C     | 135 | PHE  | N-CA  | -6.67 | 1.37        | 1.46     |
| 2   | 2     | 97  | TYR  | CA-C  | -6.67 | 1.44        | 1.52     |
| 21  | N     | 139 | ARG  | CA-C  | -6.67 | 1.43        | 1.52     |
| 16  | I     | 283 | GLU  | C-N   | 6.66  | 1.39        | 1.33     |
| 21  | N     | 288 | ASN  | C-N   | 6.66  | 1.42        | 1.33     |
| 26  | S     | 227 | ASN  | N-CA  | -6.66 | 1.38        | 1.46     |
| 27  | T     | 26  | LEU  | CA-C  | 6.66  | 1.61        | 1.52     |
| 28  | U     | 69  | ASP  | N-CA  | -6.66 | 1.37        | 1.46     |
| 8   | A     | 128 | TYR  | C-N   | 6.66  | 1.43        | 1.34     |
| 17  | J     | 324 | ARG  | C-N   | 6.66  | 1.42        | 1.33     |
| 33  | Z     | 836 | SER  | C-N   | 6.65  | 1.42        | 1.33     |
| 28  | U     | 47  | ARG  | CA-C  | -6.65 | 1.44        | 1.52     |
| 14  | G     | 246 | ILE  | N-CA  | -6.64 | 1.38        | 1.46     |
| 3   | 3     | 156 | GLU  | C-N   | 6.64  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | 3     | 194 | ARG  | CA-C  | -6.64 | 1.44        | 1.52     |
| 26  | S     | 381 | VAL  | CA-C  | -6.64 | 1.44        | 1.52     |
| 3   | 3     | 72  | ALA  | N-CA  | -6.64 | 1.37        | 1.46     |
| 23  | P     | 70  | ASN  | CA-C  | -6.64 | 1.44        | 1.52     |
| 8   | A     | 15  | HIS  | C-N   | 6.64  | 1.42        | 1.33     |
| 30  | W     | 156 | GLU  | N-CA  | -6.63 | 1.38        | 1.46     |
| 9   | B     | 181 | ASP  | CA-C  | -6.63 | 1.43        | 1.52     |
| 19  | L     | 162 | GLU  | C-O   | -6.63 | 1.16        | 1.23     |
| 12  | E     | 56  | SER  | N-CA  | -6.62 | 1.39        | 1.45     |
| 4   | 4     | 135 | SER  | CA-C  | -6.62 | 1.44        | 1.52     |
| 19  | L     | 425 | VAL  | C-N   | 6.62  | 1.42        | 1.33     |
| 1   | 1     | 148 | LYS  | C-N   | 6.62  | 1.42        | 1.33     |
| 17  | J     | 72  | VAL  | CA-C  | -6.62 | 1.44        | 1.52     |
| 21  | N     | 65  | ALA  | C-N   | 6.62  | 1.42        | 1.33     |
| 26  | S     | 139 | HIS  | C-N   | 6.61  | 1.42        | 1.33     |
| 27  | T     | 122 | PHE  | N-CA  | -6.61 | 1.38        | 1.46     |
| 11  | D     | 205 | THR  | CA-C  | -6.61 | 1.44        | 1.52     |
| 22  | O     | 122 | HIS  | CA-C  | -6.61 | 1.44        | 1.52     |
| 20  | M     | 350 | PRO  | N-CD  | 6.61  | 1.57        | 1.47     |
| 3   | 3     | 180 | ILE  | N-CA  | -6.61 | 1.38        | 1.46     |
| 4   | 4     | 105 | GLY  | CA-C  | -6.61 | 1.45        | 1.51     |
| 24  | Q     | 356 | CYS  | CA-C  | -6.61 | 1.44        | 1.52     |
| 18  | K     | 81  | ARG  | CA-C  | -6.60 | 1.44        | 1.52     |
| 23  | P     | 188 | ILE  | CA-C  | -6.60 | 1.44        | 1.52     |
| 16  | I     | 118 | ALA  | CA-C  | 6.60  | 1.61        | 1.52     |
| 8   | A     | 52  | VAL  | CA-C  | 6.60  | 1.60        | 1.52     |
| 25  | R     | 91  | TRP  | N-CA  | -6.60 | 1.38        | 1.46     |
| 23  | P     | 185 | GLU  | CA-C  | 6.59  | 1.61        | 1.52     |
| 23  | P     | 389 | ILE  | N-CA  | -6.59 | 1.38        | 1.46     |
| 10  | C     | 40  | ALA  | N-CA  | -6.59 | 1.37        | 1.45     |
| 17  | J     | 269 | GLN  | C-N   | 6.58  | 1.42        | 1.34     |
| 17  | J     | 296 | ARG  | CA-C  | -6.58 | 1.44        | 1.52     |
| 6   | 6     | 72  | ASP  | CA-C  | 6.58  | 1.61        | 1.52     |
| 31  | X     | 92  | SER  | CA-C  | -6.58 | 1.46        | 1.53     |
| 33  | Z     | 902 | TYR  | C-N   | 6.58  | 1.42        | 1.33     |
| 28  | U     | 191 | THR  | CA-C  | -6.58 | 1.44        | 1.52     |
| 33  | Z     | 762 | GLY  | CA-C  | -6.57 | 1.44        | 1.52     |
| 12  | E     | 70  | ILE  | N-CA  | -6.57 | 1.37        | 1.46     |
| 14  | G     | 233 | ASP  | C-N   | 6.57  | 1.42        | 1.33     |
| 25  | R     | 33  | LEU  | N-CA  | -6.57 | 1.38        | 1.46     |
| 24  | Q     | 362 | ILE  | N-CA  | 6.56  | 1.54        | 1.46     |
| 27  | T     | 271 | GLU  | C-N   | 6.56  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 19  | L     | 382 | MET  | CA-C  | -6.55 | 1.43        | 1.52     |
| 17  | J     | 141 | LYS  | C-N   | 6.55  | 1.40        | 1.33     |
| 12  | E     | 196 | ALA  | N-CA  | -6.55 | 1.38        | 1.46     |
| 18  | K     | 81  | ARG  | C-N   | 6.54  | 1.42        | 1.33     |
| 7   | 7     | 47  | GLY  | CA-C  | -6.53 | 1.44        | 1.52     |
| 21  | N     | 776 | TYR  | CA-C  | -6.53 | 1.45        | 1.53     |
| 7   | 7     | 98  | LYS  | N-CA  | -6.52 | 1.38        | 1.46     |
| 20  | M     | 329 | ARG  | N-CA  | -6.52 | 1.38        | 1.46     |
| 10  | C     | 28  | SER  | CA-C  | -6.51 | 1.44        | 1.52     |
| 10  | C     | 130 | PRO  | N-CD  | 6.51  | 1.56        | 1.47     |
| 21  | N     | 410 | LEU  | C-N   | 6.51  | 1.42        | 1.33     |
| 22  | O     | 130 | ASP  | C-N   | 6.51  | 1.42        | 1.33     |
| 15  | H     | 382 | LEU  | N-CA  | -6.51 | 1.38        | 1.46     |
| 21  | N     | 634 | LEU  | CA-C  | -6.51 | 1.44        | 1.52     |
| 10  | C     | 189 | ALA  | CA-C  | -6.51 | 1.44        | 1.52     |
| 7   | 7     | 34  | LEU  | CA-C  | -6.50 | 1.44        | 1.52     |
| 15  | H     | 199 | THR  | CA-C  | -6.50 | 1.44        | 1.52     |
| 25  | R     | 290 | SER  | C-N   | 6.50  | 1.42        | 1.33     |
| 5   | 5     | 158 | LYS  | N-CA  | -6.50 | 1.38        | 1.46     |
| 11  | D     | 133 | THR  | C-N   | 6.49  | 1.42        | 1.33     |
| 17  | J     | 68  | PRO  | N-CD  | 6.49  | 1.56        | 1.47     |
| 11  | D     | 196 | VAL  | N-CA  | -6.48 | 1.38        | 1.46     |
| 16  | I     | 382 | THR  | C-N   | 6.48  | 1.43        | 1.33     |
| 18  | K     | 93  | PRO  | N-CD  | 6.48  | 1.56        | 1.47     |
| 25  | R     | 32  | LEU  | CA-C  | 6.48  | 1.61        | 1.52     |
| 2   | 2     | 160 | GLN  | C-N   | 6.47  | 1.42        | 1.33     |
| 18  | K     | 108 | GLY  | CA-C  | -6.47 | 1.46        | 1.52     |
| 24  | Q     | 140 | LYS  | C-N   | 6.47  | 1.42        | 1.33     |
| 17  | J     | 119 | SER  | CA-C  | -6.47 | 1.44        | 1.52     |
| 25  | R     | 250 | ALA  | N-CA  | -6.47 | 1.38        | 1.46     |
| 19  | L     | 217 | GLY  | CA-C  | -6.46 | 1.46        | 1.51     |
| 23  | P     | 72  | TRP  | CA-C  | -6.46 | 1.44        | 1.52     |
| 5   | 5     | 18  | SER  | N-CA  | -6.46 | 1.38        | 1.46     |
| 16  | I     | 271 | ALA  | N-CA  | -6.46 | 1.38        | 1.46     |
| 21  | N     | 82  | ALA  | N-CA  | -6.45 | 1.38        | 1.46     |
| 1   | 1     | 104 | ASP  | CA-C  | -6.45 | 1.43        | 1.52     |
| 10  | C     | 52  | VAL  | CA-C  | -6.45 | 1.44        | 1.52     |
| 18  | K     | 354 | GLY  | CA-C  | -6.45 | 1.44        | 1.52     |
| 25  | R     | 73  | ASN  | CA-C  | -6.44 | 1.44        | 1.52     |
| 3   | 3     | 94  | TYR  | N-CA  | -6.44 | 1.38        | 1.45     |
| 15  | H     | 334 | LEU  | N-CA  | -6.44 | 1.38        | 1.46     |
| 23  | P     | 271 | SER  | CA-C  | 6.44  | 1.61        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 13  | F     | 26  | LEU  | N-CA  | -6.43 | 1.38        | 1.46     |
| 18  | K     | 333 | ARG  | N-CA  | -6.43 | 1.37        | 1.46     |
| 25  | R     | 76  | GLN  | CA-C  | -6.43 | 1.44        | 1.52     |
| 24  | Q     | 314 | PHE  | C-N   | 6.43  | 1.42        | 1.33     |
| 13  | F     | 103 | LEU  | C-N   | 6.42  | 1.42        | 1.33     |
| 19  | L     | 120 | LYS  | CA-C  | -6.42 | 1.44        | 1.52     |
| 11  | D     | 31  | THR  | CA-C  | 6.42  | 1.62        | 1.53     |
| 16  | I     | 307 | LEU  | N-CA  | 6.42  | 1.54        | 1.46     |
| 20  | M     | 119 | VAL  | CA-C  | -6.42 | 1.45        | 1.52     |
| 6   | 6     | 54  | ALA  | N-CA  | -6.42 | 1.38        | 1.46     |
| 33  | Z     | 416 | THR  | CA-C  | -6.42 | 1.44        | 1.52     |
| 19  | L     | 355 | ALA  | N-CA  | -6.42 | 1.38        | 1.46     |
| 8   | A     | 18  | ILE  | C-N   | 6.41  | 1.42        | 1.33     |
| 10  | C     | 220 | ALA  | C-N   | 6.41  | 1.42        | 1.33     |
| 19  | L     | 153 | LEU  | CA-C  | -6.41 | 1.46        | 1.53     |
| 33  | Z     | 605 | SER  | CA-C  | -6.41 | 1.44        | 1.52     |
| 8   | A     | 158 | ASP  | CA-C  | -6.41 | 1.46        | 1.52     |
| 19  | L     | 106 | GLY  | C-N   | 6.41  | 1.42        | 1.33     |
| 2   | 2     | 137 | VAL  | CA-C  | -6.41 | 1.45        | 1.52     |
| 23  | P     | 319 | GLU  | C-N   | 6.41  | 1.41        | 1.34     |
| 25  | R     | 335 | ARG  | C-N   | 6.41  | 1.42        | 1.33     |
| 16  | I     | 357 | THR  | CA-C  | -6.41 | 1.44        | 1.52     |
| 28  | U     | 116 | ASN  | N-CA  | -6.41 | 1.38        | 1.46     |
| 16  | I     | 343 | ARG  | CA-C  | -6.40 | 1.44        | 1.52     |
| 24  | Q     | 338 | LEU  | CA-C  | 6.40  | 1.61        | 1.52     |
| 4   | 4     | 193 | ASP  | N-CA  | -6.40 | 1.38        | 1.45     |
| 6   | 6     | 176 | ARG  | C-O   | -6.40 | 1.16        | 1.24     |
| 18  | K     | 100 | LEU  | CA-C  | -6.40 | 1.44        | 1.52     |
| 33  | Z     | 534 | PHE  | C-N   | 6.40  | 1.41        | 1.33     |
| 19  | L     | 111 | GLU  | C-N   | 6.39  | 1.43        | 1.33     |
| 29  | V     | 152 | VAL  | CA-C  | -6.39 | 1.45        | 1.52     |
| 14  | G     | 117 | GLN  | C-O   | -6.39 | 1.16        | 1.24     |
| 3   | 3     | 132 | THR  | CA-C  | -6.38 | 1.44        | 1.52     |
| 18  | K     | 332 | GLY  | CA-C  | -6.38 | 1.43        | 1.51     |
| 30  | W     | 109 | ARG  | CA-C  | -6.38 | 1.44        | 1.52     |
| 18  | K     | 328 | LEU  | C-N   | 6.38  | 1.42        | 1.34     |
| 22  | O     | 281 | ALA  | N-CA  | -6.38 | 1.38        | 1.46     |
| 33  | Z     | 442 | VAL  | C-N   | 6.38  | 1.42        | 1.33     |
| 14  | G     | 85  | ARG  | N-CA  | -6.38 | 1.38        | 1.46     |
| 21  | N     | 757 | THR  | C-O   | -6.38 | 1.16        | 1.24     |
| 25  | R     | 364 | LEU  | CA-C  | -6.37 | 1.44        | 1.52     |
| 33  | Z     | 51  | LEU  | C-N   | 6.37  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | 4     | 111 | ASN  | C-N   | 6.37  | 1.41        | 1.33     |
| 17  | J     | 134 | VAL  | C-N   | 6.37  | 1.42        | 1.33     |
| 28  | U     | 118 | PRO  | N-CD  | 6.37  | 1.56        | 1.47     |
| 12  | E     | 245 | GLU  | C-N   | 6.37  | 1.42        | 1.33     |
| 10  | C     | 143 | ARG  | C-N   | 6.36  | 1.42        | 1.33     |
| 12  | E     | 44  | GLU  | C-N   | 6.36  | 1.42        | 1.33     |
| 1   | 1     | 148 | LYS  | N-CA  | -6.36 | 1.38        | 1.46     |
| 16  | I     | 293 | ASP  | N-CA  | -6.36 | 1.37        | 1.45     |
| 8   | A     | 27  | GLN  | CA-C  | -6.36 | 1.44        | 1.52     |
| 10  | C     | 206 | LEU  | N-CA  | -6.35 | 1.38        | 1.46     |
| 27  | T     | 267 | ALA  | CA-C  | 6.35  | 1.61        | 1.52     |
| 18  | K     | 259 | ARG  | N-CA  | -6.35 | 1.38        | 1.46     |
| 19  | L     | 208 | GLN  | C-N   | 6.35  | 1.42        | 1.33     |
| 22  | O     | 73  | ILE  | CA-C  | -6.35 | 1.45        | 1.52     |
| 8   | A     | 12  | TYR  | CA-C  | -6.35 | 1.45        | 1.52     |
| 19  | L     | 117 | TYR  | C-N   | 6.35  | 1.41        | 1.33     |
| 20  | M     | 417 | GLU  | CA-C  | -6.35 | 1.44        | 1.52     |
| 3   | 3     | 46  | GLY  | CA-C  | -6.34 | 1.43        | 1.51     |
| 14  | G     | 19  | ARG  | C-N   | 6.34  | 1.42        | 1.33     |
| 15  | H     | 445 | LYS  | N-CA  | -6.34 | 1.38        | 1.46     |
| 21  | N     | 715 | ILE  | C-N   | 6.34  | 1.41        | 1.33     |
| 10  | C     | 9   | ARG  | N-CA  | -6.34 | 1.37        | 1.46     |
| 14  | G     | 136 | ILE  | N-CA  | -6.34 | 1.38        | 1.46     |
| 17  | J     | 251 | ASP  | CA-C  | -6.34 | 1.45        | 1.52     |
| 22  | O     | 238 | ILE  | N-CA  | 6.34  | 1.54        | 1.46     |
| 23  | P     | 357 | TYR  | CA-C  | -6.34 | 1.44        | 1.53     |
| 25  | R     | 305 | PHE  | N-CA  | -6.34 | 1.39        | 1.46     |
| 29  | V     | 76  | THR  | C-N   | 6.34  | 1.41        | 1.33     |
| 33  | Z     | 858 | GLY  | C-O   | -6.34 | 1.17        | 1.24     |
| 1   | 1     | 80  | SER  | N-CA  | -6.33 | 1.38        | 1.46     |
| 21  | N     | 228 | VAL  | C-N   | 6.33  | 1.41        | 1.33     |
| 27  | T     | 70  | ILE  | N-CA  | -6.33 | 1.39        | 1.46     |
| 33  | Z     | 540 | GLY  | C-N   | 6.33  | 1.42        | 1.33     |
| 20  | M     | 374 | ILE  | CA-C  | 6.33  | 1.59        | 1.52     |
| 29  | V     | 95  | LEU  | CA-C  | -6.33 | 1.44        | 1.52     |
| 30  | W     | 172 | LEU  | CA-C  | -6.33 | 1.45        | 1.52     |
| 13  | F     | 164 | ARG  | CA-C  | -6.33 | 1.46        | 1.53     |
| 14  | G     | 105 | PRO  | CA-C  | -6.32 | 1.44        | 1.52     |
| 24  | Q     | 136 | SER  | C-N   | 6.32  | 1.42        | 1.34     |
| 4   | 4     | 76  | PRO  | N-CD  | 6.32  | 1.56        | 1.47     |
| 27  | T     | 6   | GLU  | CA-C  | -6.32 | 1.45        | 1.52     |
| 9   | B     | 222 | LEU  | C-N   | 6.32  | 1.43        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 21  | N     | 730 | VAL  | C-N   | 6.31  | 1.42        | 1.34     |
| 22  | O     | 201 | PRO  | C-N   | 6.31  | 1.41        | 1.33     |
| 28  | U     | 124 | ASP  | CA-C  | -6.31 | 1.44        | 1.52     |
| 7   | 7     | 3   | VAL  | CA-C  | -6.31 | 1.44        | 1.52     |
| 28  | U     | 87  | GLU  | C-N   | 6.31  | 1.42        | 1.33     |
| 33  | Z     | 303 | ASP  | C-N   | 6.31  | 1.42        | 1.33     |
| 17  | J     | 320 | SER  | CA-C  | -6.30 | 1.44        | 1.52     |
| 24  | Q     | 44  | ALA  | CA-C  | -6.30 | 1.45        | 1.52     |
| 8   | A     | 52  | VAL  | N-CA  | -6.30 | 1.39        | 1.46     |
| 13  | F     | 152 | ASN  | CA-C  | -6.30 | 1.45        | 1.52     |
| 26  | S     | 273 | PHE  | N-CA  | -6.30 | 1.38        | 1.46     |
| 22  | O     | 159 | LYS  | CA-C  | -6.30 | 1.44        | 1.52     |
| 22  | O     | 364 | THR  | C-N   | 6.30  | 1.42        | 1.33     |
| 4   | 4     | 145 | HIS  | C-N   | 6.30  | 1.43        | 1.33     |
| 25  | R     | 244 | THR  | C-N   | 6.30  | 1.42        | 1.33     |
| 4   | 4     | 19  | ALA  | C-N   | 6.29  | 1.41        | 1.33     |
| 5   | 5     | 186 | ILE  | N-CA  | -6.29 | 1.39        | 1.46     |
| 18  | K     | 175 | GLY  | CA-C  | -6.29 | 1.46        | 1.52     |
| 18  | K     | 249 | GLU  | N-CA  | -6.29 | 1.39        | 1.46     |
| 24  | Q     | 91  | SER  | CA-C  | -6.29 | 1.44        | 1.52     |
| 7   | 7     | 118 | PHE  | C-N   | 6.29  | 1.41        | 1.33     |
| 27  | T     | 119 | THR  | N-CA  | -6.29 | 1.38        | 1.46     |
| 4   | 4     | 93  | SER  | CA-C  | 6.28  | 1.61        | 1.53     |
| 18  | K     | 279 | THR  | C-N   | 6.28  | 1.38        | 1.33     |
| 19  | L     | 356 | GLY  | C-N   | 6.28  | 1.42        | 1.33     |
| 16  | I     | 141 | LEU  | C-N   | 6.28  | 1.40        | 1.33     |
| 24  | Q     | 325 | LEU  | N-CA  | -6.28 | 1.39        | 1.46     |
| 28  | U     | 48  | VAL  | CA-C  | -6.28 | 1.44        | 1.52     |
| 31  | X     | 52  | PRO  | N-CD  | 6.28  | 1.56        | 1.47     |
| 7   | 7     | 168 | ALA  | CA-C  | -6.27 | 1.44        | 1.52     |
| 20  | M     | 238 | GLN  | N-CA  | -6.27 | 1.38        | 1.46     |
| 5   | 5     | 54  | PHE  | CA-C  | -6.27 | 1.45        | 1.52     |
| 23  | P     | 225 | VAL  | N-CA  | -6.27 | 1.38        | 1.46     |
| 18  | K     | 345 | ASP  | CA-C  | -6.27 | 1.45        | 1.52     |
| 5   | 5     | 154 | LEU  | C-N   | 6.27  | 1.42        | 1.33     |
| 10  | C     | 42  | ASP  | CA-C  | -6.27 | 1.43        | 1.52     |
| 16  | I     | 86  | GLU  | N-CA  | -6.27 | 1.39        | 1.46     |
| 15  | H     | 235 | PHE  | C-N   | 6.27  | 1.42        | 1.33     |
| 19  | L     | 258 | GLU  | CA-C  | 6.27  | 1.61        | 1.52     |
| 21  | N     | 868 | VAL  | C-N   | 6.27  | 1.41        | 1.33     |
| 23  | P     | 242 | GLN  | CA-C  | -6.27 | 1.44        | 1.52     |
| 15  | H     | 237 | THR  | C-N   | 6.26  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 29  | V     | 195 | HIS  | CA-C  | -6.26 | 1.44        | 1.52     |
| 14  | G     | 218 | CYS  | N-CA  | -6.26 | 1.38        | 1.46     |
| 18  | K     | 376 | ASP  | CA-C  | -6.26 | 1.44        | 1.52     |
| 5   | 5     | 138 | GLY  | CA-C  | 6.26  | 1.60        | 1.51     |
| 16  | I     | 421 | GLU  | C-N   | 6.26  | 1.42        | 1.33     |
| 33  | Z     | 98  | ASP  | N-CA  | -6.26 | 1.38        | 1.46     |
| 2   | 2     | 59  | ILE  | CA-C  | -6.26 | 1.44        | 1.52     |
| 14  | G     | 218 | CYS  | C-N   | 6.26  | 1.41        | 1.33     |
| 4   | 4     | 172 | PRO  | N-CD  | 6.25  | 1.56        | 1.47     |
| 31  | X     | 26  | PRO  | C-N   | 6.25  | 1.39        | 1.33     |
| 28  | U     | 66  | TRP  | N-CA  | -6.25 | 1.38        | 1.45     |
| 8   | A     | 155 | TYR  | CA-C  | -6.25 | 1.45        | 1.52     |
| 9   | B     | 41  | ASN  | CA-C  | -6.25 | 1.44        | 1.52     |
| 4   | 4     | 61  | ALA  | N-CA  | -6.25 | 1.39        | 1.46     |
| 21  | N     | 205 | SER  | N-CA  | -6.25 | 1.38        | 1.46     |
| 7   | 7     | 127 | VAL  | CA-C  | -6.24 | 1.45        | 1.52     |
| 8   | A     | 152 | PRO  | N-CD  | 6.24  | 1.56        | 1.47     |
| 17  | J     | 143 | PRO  | N-CD  | 6.24  | 1.56        | 1.47     |
| 18  | K     | 151 | PRO  | N-CD  | 6.24  | 1.56        | 1.47     |
| 30  | W     | 160 | ALA  | CA-C  | -6.24 | 1.45        | 1.52     |
| 18  | K     | 173 | ASP  | N-CA  | -6.24 | 1.38        | 1.46     |
| 15  | H     | 67  | ALA  | C-N   | 6.23  | 1.41        | 1.33     |
| 19  | L     | 117 | TYR  | CA-C  | -6.23 | 1.45        | 1.52     |
| 21  | N     | 470 | LEU  | CA-C  | -6.23 | 1.44        | 1.52     |
| 11  | D     | 22  | TYR  | CA-C  | -6.23 | 1.44        | 1.52     |
| 3   | 3     | 163 | LEU  | N-CA  | -6.23 | 1.38        | 1.46     |
| 21  | N     | 494 | LYS  | CA-C  | -6.23 | 1.46        | 1.53     |
| 33  | Z     | 146 | PHE  | N-CA  | -6.23 | 1.38        | 1.46     |
| 13  | F     | 32  | GLY  | C-N   | 6.22  | 1.42        | 1.33     |
| 16  | I     | 287 | ILE  | C-N   | 6.22  | 1.42        | 1.33     |
| 30  | W     | 75  | GLY  | N-CA  | -6.22 | 1.37        | 1.45     |
| 1   | 1     | 192 | GLU  | C-N   | 6.22  | 1.42        | 1.34     |
| 9   | B     | 225 | THR  | CA-C  | -6.21 | 1.44        | 1.52     |
| 11  | D     | 84  | ILE  | N-CA  | -6.21 | 1.39        | 1.46     |
| 21  | N     | 570 | ARG  | N-CA  | -6.21 | 1.38        | 1.46     |
| 26  | S     | 278 | LYS  | C-N   | 6.21  | 1.41        | 1.33     |
| 33  | Z     | 336 | SER  | CA-C  | -6.21 | 1.45        | 1.52     |
| 16  | I     | 110 | GLU  | C-N   | 6.21  | 1.41        | 1.33     |
| 22  | O     | 208 | ALA  | N-CA  | -6.20 | 1.39        | 1.46     |
| 4   | 4     | 13  | ILE  | CA-C  | 6.20  | 1.60        | 1.52     |
| 22  | O     | 187 | SER  | CA-C  | -6.20 | 1.44        | 1.52     |
| 33  | Z     | 351 | PRO  | N-CD  | 6.20  | 1.56        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9   | B     | 233 | PRO  | N-CD  | 6.20  | 1.56        | 1.47     |
| 2   | 2     | 7   | LYS  | C-N   | 6.20  | 1.42        | 1.33     |
| 11  | D     | 17  | ILE  | C-N   | 6.20  | 1.41        | 1.33     |
| 33  | Z     | 202 | ARG  | C-N   | 6.20  | 1.42        | 1.33     |
| 2   | 2     | 181 | GLY  | CA-C  | -6.19 | 1.43        | 1.51     |
| 3   | 3     | 76  | GLU  | C-O   | -6.19 | 1.16        | 1.24     |
| 16  | I     | 136 | VAL  | N-CA  | -6.19 | 1.38        | 1.46     |
| 16  | I     | 242 | ALA  | CA-C  | -6.19 | 1.45        | 1.52     |
| 14  | G     | 158 | GLY  | CA-C  | -6.19 | 1.46        | 1.52     |
| 26  | S     | 327 | ILE  | N-CA  | -6.19 | 1.39        | 1.46     |
| 1   | 1     | 20  | THR  | C-N   | 6.19  | 1.42        | 1.33     |
| 14  | G     | 221 | SER  | CA-C  | -6.18 | 1.44        | 1.52     |
| 21  | N     | 370 | SER  | C-N   | 6.18  | 1.42        | 1.34     |
| 21  | N     | 672 | ASN  | N-CA  | -6.18 | 1.41        | 1.46     |
| 27  | T     | 128 | TYR  | N-CA  | -6.18 | 1.38        | 1.46     |
| 19  | L     | 244 | ILE  | CA-C  | -6.18 | 1.44        | 1.52     |
| 24  | Q     | 225 | LEU  | CA-C  | -6.18 | 1.44        | 1.52     |
| 33  | Z     | 738 | TYR  | N-CA  | 6.18  | 1.54        | 1.46     |
| 33  | Z     | 829 | GLN  | N-CA  | -6.18 | 1.38        | 1.46     |
| 24  | Q     | 416 | VAL  | C-N   | 6.18  | 1.41        | 1.33     |
| 24  | Q     | 424 | ASP  | CA-C  | 6.18  | 1.60        | 1.52     |
| 21  | N     | 397 | SER  | N-CA  | -6.18 | 1.38        | 1.46     |
| 11  | D     | 12  | SER  | CA-C  | -6.18 | 1.45        | 1.53     |
| 21  | N     | 659 | ALA  | CA-C  | -6.18 | 1.44        | 1.52     |
| 21  | N     | 530 | GLU  | N-CA  | 6.17  | 1.54        | 1.46     |
| 17  | J     | 138 | MET  | CA-C  | -6.17 | 1.45        | 1.52     |
| 25  | R     | 321 | TYR  | CA-C  | -6.17 | 1.44        | 1.52     |
| 19  | L     | 214 | PRO  | N-CD  | 6.17  | 1.56        | 1.47     |
| 28  | U     | 231 | ASP  | N-CA  | -6.17 | 1.39        | 1.46     |
| 13  | F     | 186 | PRO  | N-CD  | 6.17  | 1.56        | 1.47     |
| 19  | L     | 260 | ALA  | N-CA  | -6.17 | 1.38        | 1.46     |
| 31  | X     | 57  | VAL  | CA-C  | -6.17 | 1.45        | 1.52     |
| 33  | Z     | 843 | ASP  | CA-C  | -6.17 | 1.45        | 1.52     |
| 21  | N     | 762 | ARG  | CA-C  | -6.17 | 1.45        | 1.52     |
| 13  | F     | 78  | ALA  | CA-C  | 6.16  | 1.60        | 1.52     |
| 9   | B     | 225 | THR  | C-N   | 6.16  | 1.41        | 1.33     |
| 31  | X     | 126 | ILE  | C-N   | 6.16  | 1.41        | 1.33     |
| 17  | J     | 234 | PHE  | N-CA  | -6.16 | 1.39        | 1.46     |
| 33  | Z     | 76  | LYS  | C-N   | 6.16  | 1.42        | 1.33     |
| 3   | 3     | 23  | GLN  | N-CA  | 6.16  | 1.54        | 1.46     |
| 12  | E     | 195 | GLU  | CA-C  | -6.16 | 1.44        | 1.52     |
| 21  | N     | 361 | ASN  | C-N   | 6.16  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | M     | 222 | GLY  | CA-C  | -6.15 | 1.43        | 1.51     |
| 5   | 5     | 47  | GLY  | CA-C  | -6.15 | 1.42        | 1.51     |
| 31  | X     | 76  | VAL  | C-O   | -6.15 | 1.17        | 1.24     |
| 4   | 4     | 172 | PRO  | CA-C  | -6.15 | 1.46        | 1.52     |
| 14  | G     | 94  | GLU  | CA-C  | -6.15 | 1.44        | 1.52     |
| 18  | K     | 394 | ALA  | CA-C  | -6.15 | 1.45        | 1.52     |
| 28  | U     | 291 | LEU  | CA-C  | -6.15 | 1.44        | 1.52     |
| 8   | A     | 13  | ASP  | CA-C  | -6.15 | 1.44        | 1.52     |
| 1   | 1     | 27  | ALA  | N-CA  | -6.14 | 1.39        | 1.46     |
| 14  | G     | 15  | SER  | N-CA  | -6.14 | 1.38        | 1.45     |
| 19  | L     | 266 | MET  | C-N   | 6.14  | 1.42        | 1.33     |
| 21  | N     | 740 | TRP  | CA-C  | -6.14 | 1.44        | 1.52     |
| 5   | 5     | 175 | VAL  | CA-C  | -6.14 | 1.45        | 1.52     |
| 29  | V     | 64  | ASN  | N-CA  | -6.14 | 1.38        | 1.46     |
| 20  | M     | 348 | GLU  | CA-C  | -6.14 | 1.45        | 1.52     |
| 21  | N     | 352 | ASN  | CA-C  | -6.14 | 1.45        | 1.52     |
| 23  | P     | 71  | LYS  | N-CA  | -6.14 | 1.37        | 1.45     |
| 14  | G     | 227 | HIS  | CA-C  | -6.13 | 1.45        | 1.52     |
| 18  | K     | 131 | LEU  | N-CA  | -6.13 | 1.38        | 1.45     |
| 21  | N     | 687 | THR  | CA-C  | -6.13 | 1.44        | 1.52     |
| 21  | N     | 423 | LEU  | C-O   | -6.13 | 1.16        | 1.24     |
| 19  | L     | 252 | VAL  | CA-CB | -6.13 | 1.46        | 1.55     |
| 8   | A     | 44  | ALA  | CA-C  | -6.12 | 1.44        | 1.52     |
| 9   | B     | 136 | ILE  | CA-C  | -6.12 | 1.45        | 1.52     |
| 25  | R     | 173 | THR  | C-N   | 6.12  | 1.41        | 1.34     |
| 11  | D     | 196 | VAL  | C-N   | 6.12  | 1.42        | 1.33     |
| 10  | C     | 63  | THR  | N-CA  | -6.12 | 1.39        | 1.46     |
| 19  | L     | 354 | GLU  | CA-C  | -6.12 | 1.45        | 1.52     |
| 31  | X     | 81  | SER  | C-N   | 6.12  | 1.42        | 1.33     |
| 24  | Q     | 108 | PRO  | N-CD  | 6.12  | 1.56        | 1.47     |
| 24  | Q     | 390 | LEU  | CA-C  | -6.12 | 1.45        | 1.52     |
| 27  | T     | 236 | ASN  | CA-C  | -6.11 | 1.45        | 1.52     |
| 18  | K     | 392 | LEU  | CA-C  | -6.11 | 1.45        | 1.52     |
| 13  | F     | 38  | LEU  | CA-C  | -6.11 | 1.44        | 1.52     |
| 20  | M     | 404 | ARG  | C-N   | 6.11  | 1.42        | 1.33     |
| 21  | N     | 701 | VAL  | CA-C  | -6.11 | 1.44        | 1.52     |
| 28  | U     | 282 | VAL  | C-O   | -6.11 | 1.17        | 1.24     |
| 2   | 2     | 21  | THR  | CA-C  | -6.11 | 1.45        | 1.52     |
| 12  | E     | 169 | ALA  | N-CA  | -6.10 | 1.38        | 1.46     |
| 20  | M     | 155 | ILE  | CA-C  | -6.10 | 1.46        | 1.53     |
| 9   | B     | 165 | GLY  | CA-C  | -6.10 | 1.46        | 1.52     |
| 17  | J     | 229 | MET  | CA-C  | -6.10 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 21  | N     | 594 | VAL  | C-N   | 6.10  | 1.41        | 1.33     |
| 21  | N     | 197 | VAL  | C-N   | 6.10  | 1.42        | 1.33     |
| 24  | Q     | 229 | ASP  | C-N   | 6.10  | 1.42        | 1.33     |
| 17  | J     | 284 | THR  | CA-C  | -6.10 | 1.45        | 1.53     |
| 25  | R     | 29  | LYS  | CA-C  | -6.10 | 1.44        | 1.52     |
| 20  | M     | 130 | PRO  | N-CD  | 6.10  | 1.56        | 1.47     |
| 6   | 6     | 116 | PHE  | CA-C  | -6.09 | 1.45        | 1.52     |
| 11  | D     | 131 | VAL  | N-CA  | 6.09  | 1.53        | 1.46     |
| 18  | K     | 344 | ARG  | CA-C  | -6.09 | 1.44        | 1.52     |
| 6   | 6     | 153 | PRO  | N-CD  | 6.09  | 1.56        | 1.47     |
| 7   | 7     | 181 | ALA  | CA-C  | -6.09 | 1.44        | 1.52     |
| 6   | 6     | 172 | ILE  | C-N   | 6.08  | 1.41        | 1.33     |
| 20  | M     | 310 | ASN  | N-CA  | 6.08  | 1.53        | 1.46     |
| 23  | P     | 398 | LYS  | CA-C  | -6.08 | 1.45        | 1.53     |
| 2   | 2     | 24  | PRO  | CA-C  | -6.08 | 1.45        | 1.52     |
| 29  | V     | 91  | MET  | N-CA  | -6.08 | 1.38        | 1.46     |
| 31  | X     | 28  | PRO  | C-N   | 6.08  | 1.41        | 1.33     |
| 21  | N     | 110 | VAL  | C-N   | 6.08  | 1.41        | 1.33     |
| 28  | U     | 36  | VAL  | CA-C  | -6.08 | 1.45        | 1.52     |
| 21  | N     | 248 | GLU  | C-N   | 6.08  | 1.42        | 1.33     |
| 33  | Z     | 161 | ILE  | C-N   | 6.07  | 1.40        | 1.33     |
| 6   | 6     | 160 | LYS  | C-N   | 6.07  | 1.42        | 1.33     |
| 11  | D     | 55  | GLN  | CA-C  | -6.07 | 1.44        | 1.53     |
| 13  | F     | 142 | ALA  | C-N   | 6.07  | 1.41        | 1.33     |
| 28  | U     | 34  | VAL  | CA-C  | -6.07 | 1.45        | 1.52     |
| 28  | U     | 225 | ILE  | CA-C  | -6.07 | 1.45        | 1.52     |
| 15  | H     | 415 | THR  | N-CA  | -6.06 | 1.38        | 1.45     |
| 2   | 2     | 69  | TYR  | C-N   | 6.06  | 1.43        | 1.33     |
| 3   | 3     | 165 | ALA  | C-N   | 6.06  | 1.41        | 1.33     |
| 27  | T     | 158 | GLN  | C-N   | 6.06  | 1.42        | 1.33     |
| 4   | 4     | 96  | PRO  | N-CD  | 6.06  | 1.56        | 1.47     |
| 15  | H     | 328 | GLU  | CA-C  | -6.06 | 1.45        | 1.52     |
| 17  | J     | 93  | LYS  | C-N   | 6.06  | 1.41        | 1.33     |
| 21  | N     | 398 | ARG  | N-CA  | -6.06 | 1.38        | 1.46     |
| 30  | W     | 60  | ARG  | N-CA  | -6.05 | 1.38        | 1.46     |
| 2   | 2     | 24  | PRO  | N-CD  | 6.05  | 1.56        | 1.47     |
| 7   | 7     | 179 | ARG  | C-N   | 6.05  | 1.42        | 1.33     |
| 3   | 3     | 138 | PHE  | C-N   | 6.05  | 1.41        | 1.33     |
| 18  | K     | 60  | LEU  | N-CA  | 6.05  | 1.53        | 1.46     |
| 21  | N     | 767 | ALA  | CA-C  | -6.05 | 1.45        | 1.52     |
| 27  | T     | 28  | PRO  | N-CD  | 6.05  | 1.56        | 1.47     |
| 10  | C     | 6   | TYR  | C-N   | 6.04  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | 2     | 13  | VAL  | C-O   | -6.04 | 1.17        | 1.24     |
| 8   | A     | 184 | ASN  | CA-C  | -6.04 | 1.45        | 1.52     |
| 12  | E     | 140 | VAL  | CA-C  | -6.04 | 1.45        | 1.52     |
| 30  | W     | 75  | GLY  | CA-C  | 6.04  | 1.59        | 1.51     |
| 8   | A     | 171 | THR  | C-N   | 6.04  | 1.42        | 1.33     |
| 13  | F     | 144 | LEU  | CA-C  | 6.04  | 1.59        | 1.52     |
| 17  | J     | 119 | SER  | C-N   | 6.04  | 1.42        | 1.33     |
| 22  | O     | 169 | ASN  | CA-C  | 6.04  | 1.60        | 1.52     |
| 25  | R     | 130 | GLN  | C-N   | 6.04  | 1.42        | 1.33     |
| 24  | Q     | 250 | THR  | C-O   | -6.04 | 1.18        | 1.24     |
| 6   | 6     | 116 | PHE  | C-N   | 6.04  | 1.42        | 1.33     |
| 8   | A     | 225 | VAL  | CA-C  | -6.04 | 1.45        | 1.52     |
| 27  | T     | 39  | LEU  | CA-C  | -6.03 | 1.44        | 1.52     |
| 20  | M     | 426 | LYS  | CA-C  | -6.03 | 1.45        | 1.52     |
| 33  | Z     | 848 | THR  | CA-C  | -6.03 | 1.45        | 1.52     |
| 12  | E     | 231 | TYR  | C-N   | 6.03  | 1.41        | 1.33     |
| 22  | O     | 3   | ASN  | N-CA  | 6.03  | 1.54        | 1.46     |
| 29  | V     | 232 | GLU  | C-N   | 6.03  | 1.41        | 1.33     |
| 19  | L     | 208 | GLN  | CA-C  | 6.03  | 1.60        | 1.52     |
| 33  | Z     | 736 | LEU  | C-N   | 6.03  | 1.41        | 1.33     |
| 15  | H     | 312 | ASP  | N-CA  | -6.02 | 1.38        | 1.46     |
| 21  | N     | 111 | GLN  | N-CA  | -6.02 | 1.39        | 1.46     |
| 33  | Z     | 598 | ALA  | CA-C  | -6.02 | 1.45        | 1.52     |
| 2   | 2     | 71  | SER  | C-N   | 6.02  | 1.41        | 1.33     |
| 17  | J     | 284 | THR  | C-O   | -6.02 | 1.16        | 1.23     |
| 23  | P     | 258 | LYS  | C-N   | 6.02  | 1.41        | 1.33     |
| 26  | S     | 473 | ASP  | C-O   | -6.02 | 1.17        | 1.24     |
| 16  | I     | 413 | ALA  | CA-C  | -6.02 | 1.44        | 1.52     |
| 11  | D     | 238 | GLN  | CA-C  | -6.02 | 1.44        | 1.52     |
| 4   | 4     | 37  | LEU  | CA-C  | 6.01  | 1.60        | 1.52     |
| 22  | O     | 353 | VAL  | C-N   | 6.01  | 1.42        | 1.33     |
| 18  | K     | 419 | ASN  | CA-C  | 6.01  | 1.60        | 1.52     |
| 26  | S     | 243 | ASN  | N-CA  | -6.01 | 1.39        | 1.46     |
| 33  | Z     | 616 | LEU  | C-N   | 6.01  | 1.41        | 1.33     |
| 4   | 4     | 189 | ARG  | N-CA  | -6.01 | 1.38        | 1.46     |
| 5   | 5     | 157 | GLY  | N-CA  | -6.01 | 1.38        | 1.45     |
| 6   | 6     | 42  | VAL  | C-N   | 6.01  | 1.41        | 1.33     |
| 10  | C     | 89  | ASN  | N-CA  | -6.01 | 1.38        | 1.46     |
| 21  | N     | 77  | SER  | C-N   | 6.01  | 1.41        | 1.33     |
| 27  | T     | 196 | SER  | N-CA  | -6.01 | 1.39        | 1.46     |
| 27  | T     | 27  | LEU  | N-CA  | -6.00 | 1.41        | 1.46     |
| 1   | 1     | 106 | ASN  | C-N   | 6.00  | 1.39        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | 3     | 182 | LYS  | N-CA  | -6.00 | 1.38        | 1.45     |
| 15  | H     | 141 | GLU  | C-N   | 6.00  | 1.42        | 1.33     |
| 21  | N     | 294 | PRO  | N-CD  | 6.00  | 1.56        | 1.47     |
| 19  | L     | 378 | ALA  | CA-C  | -6.00 | 1.45        | 1.52     |
| 24  | Q     | 228 | GLU  | CA-C  | -6.00 | 1.44        | 1.52     |
| 19  | L     | 298 | ASP  | C-N   | 6.00  | 1.41        | 1.33     |
| 26  | S     | 197 | SER  | CA-C  | -6.00 | 1.44        | 1.52     |
| 7   | 7     | 40  | ASN  | C-N   | 5.99  | 1.41        | 1.33     |
| 1   | 1     | 177 | VAL  | CA-C  | -5.99 | 1.45        | 1.52     |
| 14  | G     | 9   | LEU  | C-N   | 5.99  | 1.41        | 1.33     |
| 21  | N     | 469 | VAL  | C-N   | 5.99  | 1.41        | 1.33     |
| 21  | N     | 655 | ALA  | N-CA  | 5.99  | 1.53        | 1.46     |
| 25  | R     | 225 | LYS  | N-CA  | 5.99  | 1.53        | 1.46     |
| 16  | I     | 161 | GLN  | C-N   | 5.99  | 1.42        | 1.33     |
| 25  | R     | 356 | ALA  | CA-C  | -5.99 | 1.44        | 1.52     |
| 26  | S     | 318 | CYS  | CA-C  | -5.99 | 1.45        | 1.52     |
| 7   | 7     | 167 | GLU  | C-O   | -5.98 | 1.17        | 1.24     |
| 9   | B     | 199 | SER  | C-N   | 5.98  | 1.41        | 1.33     |
| 13  | F     | 13  | PHE  | C-N   | 5.98  | 1.40        | 1.32     |
| 1   | 1     | 61  | TYR  | CA-C  | -5.98 | 1.45        | 1.52     |
| 21  | N     | 919 | THR  | N-CA  | -5.98 | 1.38        | 1.45     |
| 30  | W     | 53  | SER  | C-N   | 5.98  | 1.42        | 1.33     |
| 6   | 6     | 88  | LEU  | C-N   | 5.98  | 1.42        | 1.33     |
| 10  | C     | 210 | ARG  | C-N   | 5.98  | 1.42        | 1.33     |
| 30  | W     | 87  | MET  | C-N   | 5.98  | 1.41        | 1.33     |
| 2   | 2     | 98  | LEU  | CA-C  | -5.98 | 1.45        | 1.52     |
| 11  | D     | 185 | PRO  | N-CA  | -5.97 | 1.40        | 1.47     |
| 12  | E     | 177 | GLU  | C-N   | 5.97  | 1.40        | 1.33     |
| 25  | R     | 312 | TYR  | CA-C  | -5.97 | 1.45        | 1.52     |
| 30  | W     | 84  | LYS  | CA-C  | -5.97 | 1.45        | 1.52     |
| 20  | M     | 323 | VAL  | CA-C  | -5.97 | 1.45        | 1.52     |
| 21  | N     | 647 | ASP  | CA-C  | 5.97  | 1.60        | 1.53     |
| 8   | A     | 240 | ASN  | C-N   | 5.96  | 1.41        | 1.33     |
| 22  | O     | 321 | LYS  | CA-C  | -5.96 | 1.45        | 1.52     |
| 33  | Z     | 233 | LEU  | N-CA  | 5.96  | 1.52        | 1.46     |
| 21  | N     | 595 | LEU  | C-N   | 5.96  | 1.42        | 1.33     |
| 24  | Q     | 81  | SER  | C-N   | 5.95  | 1.41        | 1.33     |
| 25  | R     | 359 | VAL  | C-N   | 5.95  | 1.41        | 1.33     |
| 26  | S     | 387 | VAL  | CA-C  | -5.95 | 1.45        | 1.52     |
| 24  | Q     | 358 | GLU  | C-N   | 5.95  | 1.41        | 1.34     |
| 7   | 7     | 7   | LYS  | CA-C  | -5.95 | 1.45        | 1.52     |
| 17  | J     | 167 | PRO  | C-N   | 5.95  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 22  | O     | 355 | PRO  | N-CA  | -5.94 | 1.39        | 1.47     |
| 23  | P     | 331 | GLY  | CA-C  | -5.94 | 1.45        | 1.51     |
| 27  | T     | 185 | ILE  | C-N   | 5.94  | 1.42        | 1.34     |
| 11  | D     | 187 | THR  | C-O   | -5.94 | 1.17        | 1.24     |
| 27  | T     | 49  | ASP  | CA-C  | -5.94 | 1.45        | 1.52     |
| 16  | I     | 223 | GLY  | C-N   | 5.93  | 1.42        | 1.33     |
| 31  | X     | 125 | MET  | CA-C  | -5.93 | 1.45        | 1.52     |
| 16  | I     | 168 | VAL  | C-N   | 5.93  | 1.41        | 1.33     |
| 21  | N     | 282 | TYR  | CA-C  | -5.93 | 1.45        | 1.52     |
| 25  | R     | 41  | GLU  | C-N   | 5.93  | 1.41        | 1.33     |
| 29  | V     | 296 | LEU  | C-N   | 5.93  | 1.41        | 1.33     |
| 15  | H     | 256 | LYS  | N-CA  | -5.93 | 1.39        | 1.46     |
| 21  | N     | 533 | ASP  | N-CA  | 5.93  | 1.53        | 1.46     |
| 20  | M     | 325 | ALA  | C-N   | 5.93  | 1.41        | 1.33     |
| 31  | X     | 71  | GLY  | CA-C  | -5.93 | 1.43        | 1.51     |
| 30  | W     | 176 | PRO  | N-CD  | 5.92  | 1.56        | 1.47     |
| 28  | U     | 12  | PRO  | N-CD  | 5.92  | 1.56        | 1.47     |
| 3   | 3     | 124 | ALA  | N-CA  | -5.92 | 1.38        | 1.45     |
| 13  | F     | 76  | GLY  | N-CA  | -5.92 | 1.36        | 1.45     |
| 33  | Z     | 58  | GLU  | CA-C  | -5.92 | 1.45        | 1.52     |
| 8   | A     | 102 | ALA  | C-N   | 5.92  | 1.41        | 1.33     |
| 11  | D     | 192 | VAL  | C-N   | 5.92  | 1.41        | 1.33     |
| 18  | K     | 377 | SER  | CA-C  | -5.92 | 1.45        | 1.53     |
| 19  | L     | 251 | ILE  | CA-C  | 5.92  | 1.60        | 1.52     |
| 21  | N     | 343 | THR  | C-N   | 5.92  | 1.42        | 1.33     |
| 26  | S     | 165 | PRO  | N-CD  | 5.92  | 1.56        | 1.47     |
| 29  | V     | 149 | GLY  | C-N   | 5.92  | 1.41        | 1.33     |
| 33  | Z     | 58  | GLU  | N-CA  | -5.91 | 1.39        | 1.45     |
| 23  | P     | 434 | THR  | N-CA  | -5.91 | 1.39        | 1.46     |
| 9   | B     | 245 | ASP  | CA-C  | -5.91 | 1.45        | 1.52     |
| 10  | C     | 232 | PRO  | N-CD  | 5.91  | 1.56        | 1.47     |
| 29  | V     | 216 | LEU  | CA-C  | -5.91 | 1.45        | 1.52     |
| 12  | E     | 20  | ARG  | CA-C  | -5.91 | 1.45        | 1.52     |
| 31  | X     | 14  | VAL  | N-CA  | -5.91 | 1.37        | 1.46     |
| 8   | A     | 85  | GLY  | C-N   | -5.91 | 1.25        | 1.33     |
| 18  | K     | 417 | THR  | N-CA  | -5.91 | 1.37        | 1.46     |
| 22  | O     | 91  | ASP  | CA-C  | -5.91 | 1.45        | 1.52     |
| 33  | Z     | 251 | ALA  | CA-C  | 5.90  | 1.60        | 1.52     |
| 5   | 5     | 95  | LEU  | C-N   | 5.90  | 1.41        | 1.33     |
| 16  | I     | 303 | GLN  | N-CA  | -5.90 | 1.39        | 1.46     |
| 9   | B     | 190 | HIS  | C-N   | 5.90  | 1.41        | 1.33     |
| 26  | S     | 169 | CYS  | C-N   | 5.90  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 29  | V     | 123 | VAL  | C-N   | 5.90  | 1.42        | 1.34     |
| 7   | 7     | 165 | ALA  | C-N   | 5.90  | 1.42        | 1.34     |
| 15  | H     | 324 | GLY  | N-CA  | -5.90 | 1.36        | 1.45     |
| 20  | M     | 146 | VAL  | N-CA  | -5.90 | 1.39        | 1.46     |
| 24  | Q     | 139 | ILE  | CA-C  | -5.90 | 1.45        | 1.52     |
| 18  | K     | 338 | ILE  | N-CA  | -5.90 | 1.39        | 1.46     |
| 30  | W     | 25  | ARG  | C-N   | 5.90  | 1.41        | 1.33     |
| 9   | B     | 132 | VAL  | N-CA  | -5.89 | 1.40        | 1.46     |
| 22  | O     | 52  | ALA  | N-CA  | -5.89 | 1.38        | 1.46     |
| 25  | R     | 341 | LEU  | C-O   | -5.89 | 1.17        | 1.24     |
| 20  | M     | 83  | VAL  | CA-C  | -5.89 | 1.45        | 1.52     |
| 1   | 1     | 121 | LYS  | C-N   | 5.89  | 1.40        | 1.33     |
| 25  | R     | 175 | ALA  | N-CA  | -5.89 | 1.39        | 1.46     |
| 26  | S     | 319 | CYS  | C-N   | 5.89  | 1.41        | 1.33     |
| 17  | J     | 118 | ASP  | CA-C  | -5.89 | 1.44        | 1.52     |
| 19  | L     | 360 | ILE  | CA-C  | 5.89  | 1.60        | 1.52     |
| 28  | U     | 200 | LEU  | N-CA  | -5.89 | 1.39        | 1.46     |
| 30  | W     | 131 | THR  | CA-C  | -5.89 | 1.44        | 1.52     |
| 6   | 6     | 84  | ILE  | C-N   | 5.89  | 1.41        | 1.33     |
| 19  | L     | 87  | LEU  | N-CA  | -5.89 | 1.39        | 1.46     |
| 30  | W     | 146 | GLU  | CA-C  | -5.88 | 1.44        | 1.52     |
| 8   | A     | 182 | LEU  | C-O   | -5.88 | 1.17        | 1.24     |
| 12  | E     | 219 | LEU  | N-CA  | -5.88 | 1.38        | 1.45     |
| 13  | F     | 157 | TYR  | C-N   | 5.88  | 1.41        | 1.33     |
| 21  | N     | 369 | ALA  | CA-C  | -5.88 | 1.44        | 1.52     |
| 6   | 6     | 166 | LEU  | CA-C  | -5.88 | 1.45        | 1.52     |
| 9   | B     | 219 | PRO  | N-CD  | 5.88  | 1.55        | 1.47     |
| 1   | 1     | 162 | ALA  | C-N   | 5.88  | 1.41        | 1.33     |
| 19  | L     | 68  | ARG  | N-CA  | 5.88  | 1.53        | 1.46     |
| 28  | U     | 129 | GLY  | C-N   | 5.88  | 1.41        | 1.33     |
| 19  | L     | 285 | ALA  | CA-C  | -5.88 | 1.45        | 1.52     |
| 14  | G     | 36  | SER  | CA-C  | -5.87 | 1.45        | 1.52     |
| 21  | N     | 553 | PHE  | C-O   | -5.87 | 1.16        | 1.24     |
| 25  | R     | 111 | LYS  | CA-C  | 5.87  | 1.60        | 1.52     |
| 3   | 3     | 109 | LYS  | CA-C  | -5.87 | 1.45        | 1.52     |
| 29  | V     | 251 | TYR  | N-CA  | -5.87 | 1.39        | 1.46     |
| 21  | N     | 182 | ASN  | CA-C  | -5.87 | 1.44        | 1.52     |
| 4   | 4     | 51  | ASP  | C-N   | 5.87  | 1.41        | 1.33     |
| 7   | 7     | 128 | THR  | CA-C  | -5.87 | 1.45        | 1.52     |
| 22  | O     | 117 | ASN  | N-CA  | 5.87  | 1.53        | 1.46     |
| 24  | Q     | 330 | LEU  | CA-C  | -5.87 | 1.45        | 1.52     |
| 19  | L     | 325 | MET  | CA-C  | -5.87 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 25  | R     | 87  | SER  | C-N   | 5.87  | 1.41        | 1.33     |
| 20  | M     | 304 | THR  | C-N   | 5.87  | 1.41        | 1.33     |
| 13  | F     | 28  | ALA  | C-N   | 5.86  | 1.41        | 1.33     |
| 19  | L     | 326 | ALA  | CA-C  | -5.86 | 1.45        | 1.52     |
| 20  | M     | 275 | PRO  | N-CD  | 5.86  | 1.56        | 1.47     |
| 23  | P     | 163 | LEU  | C-N   | 5.86  | 1.42        | 1.33     |
| 21  | N     | 690 | HIS  | C-N   | 5.86  | 1.41        | 1.33     |
| 23  | P     | 417 | HIS  | C-N   | 5.86  | 1.41        | 1.33     |
| 16  | I     | 147 | VAL  | CA-C  | -5.86 | 1.46        | 1.52     |
| 33  | Z     | 383 | SER  | N-CA  | -5.86 | 1.39        | 1.46     |
| 27  | T     | 59  | LYS  | C-O   | -5.86 | 1.17        | 1.24     |
| 33  | Z     | 260 | GLU  | CA-CB | 5.86  | 1.62        | 1.53     |
| 20  | M     | 120 | LYS  | CA-C  | -5.85 | 1.45        | 1.52     |
| 25  | R     | 80  | GLU  | C-O   | 5.85  | 1.29        | 1.24     |
| 33  | Z     | 530 | LEU  | CA-C  | -5.85 | 1.45        | 1.52     |
| 26  | S     | 128 | ILE  | N-CA  | -5.85 | 1.39        | 1.46     |
| 26  | S     | 235 | ASN  | CA-C  | -5.85 | 1.45        | 1.52     |
| 12  | E     | 90  | GLU  | N-CA  | -5.85 | 1.39        | 1.46     |
| 19  | L     | 218 | VAL  | C-N   | 5.85  | 1.42        | 1.33     |
| 12  | E     | 35  | SER  | N-CA  | -5.84 | 1.39        | 1.45     |
| 15  | H     | 203 | LYS  | C-N   | 5.84  | 1.41        | 1.33     |
| 16  | I     | 337 | ALA  | CA-C  | -5.84 | 1.45        | 1.52     |
| 17  | J     | 265 | ASP  | C-N   | 5.84  | 1.41        | 1.33     |
| 26  | S     | 185 | PHE  | CA-C  | -5.84 | 1.45        | 1.52     |
| 27  | T     | 147 | LYS  | C-N   | 5.84  | 1.41        | 1.33     |
| 24  | Q     | 259 | CYS  | C-N   | 5.84  | 1.41        | 1.33     |
| 20  | M     | 243 | PHE  | N-CA  | 5.84  | 1.53        | 1.46     |
| 23  | P     | 314 | VAL  | CA-C  | -5.84 | 1.45        | 1.52     |
| 26  | S     | 425 | ARG  | CA-C  | -5.84 | 1.45        | 1.52     |
| 31  | X     | 112 | ASN  | N-CA  | -5.84 | 1.38        | 1.46     |
| 6   | 6     | 173 | LYS  | C-N   | 5.84  | 1.41        | 1.33     |
| 11  | D     | 77  | GLY  | CA-C  | -5.84 | 1.43        | 1.51     |
| 16  | I     | 90  | GLU  | CA-C  | -5.84 | 1.45        | 1.52     |
| 12  | E     | 43  | LYS  | CA-C  | -5.84 | 1.45        | 1.52     |
| 19  | L     | 346 | LYS  | N-CA  | -5.84 | 1.39        | 1.46     |
| 15  | H     | 201 | GLU  | CA-C  | -5.83 | 1.46        | 1.53     |
| 3   | 3     | 47  | LEU  | C-O   | -5.83 | 1.17        | 1.23     |
| 33  | Z     | 132 | HIS  | C-N   | 5.83  | 1.41        | 1.33     |
| 7   | 7     | 33  | ARG  | N-CA  | -5.83 | 1.38        | 1.45     |
| 12  | E     | 246 | LYS  | C-O   | -5.83 | 1.17        | 1.24     |
| 25  | R     | 151 | GLU  | N-CA  | -5.83 | 1.39        | 1.46     |
| 5   | 5     | 176 | ASN  | N-CA  | -5.83 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 14  | G     | 163 | ALA  | C-N   | 5.83  | 1.40        | 1.33     |
| 25  | R     | 58  | GLU  | N-CA  | -5.83 | 1.38        | 1.46     |
| 33  | Z     | 981 | VAL  | N-CA  | -5.83 | 1.39        | 1.46     |
| 28  | U     | 198 | LYS  | C-N   | 5.83  | 1.41        | 1.33     |
| 16  | I     | 93  | LYS  | CA-C  | -5.83 | 1.45        | 1.52     |
| 17  | J     | 93  | LYS  | CA-C  | -5.83 | 1.45        | 1.52     |
| 23  | P     | 203 | ILE  | C-N   | 5.83  | 1.41        | 1.33     |
| 30  | W     | 69  | PHE  | C-N   | 5.83  | 1.42        | 1.33     |
| 17  | J     | 59  | LYS  | CA-C  | 5.82  | 1.60        | 1.52     |
| 6   | 6     | 136 | LEU  | CA-C  | -5.82 | 1.44        | 1.52     |
| 21  | N     | 38  | GLU  | C-O   | -5.82 | 1.16        | 1.24     |
| 29  | V     | 161 | THR  | C-N   | 5.82  | 1.41        | 1.33     |
| 31  | X     | 21  | SER  | C-O   | -5.82 | 1.18        | 1.24     |
| 13  | F     | 185 | ASN  | C-O   | -5.82 | 1.19        | 1.25     |
| 16  | I     | 390 | ALA  | C-N   | 5.82  | 1.42        | 1.34     |
| 24  | Q     | 397 | LEU  | CA-C  | -5.82 | 1.45        | 1.52     |
| 11  | D     | 49  | ARG  | CA-C  | -5.82 | 1.45        | 1.52     |
| 23  | P     | 252 | SER  | CA-C  | -5.82 | 1.45        | 1.52     |
| 33  | Z     | 262 | VAL  | CA-C  | -5.82 | 1.46        | 1.53     |
| 33  | Z     | 772 | ILE  | N-CA  | -5.82 | 1.39        | 1.46     |
| 1   | 1     | 171 | GLY  | CA-C  | -5.81 | 1.43        | 1.52     |
| 8   | A     | 133 | TYR  | CA-C  | -5.81 | 1.45        | 1.52     |
| 33  | Z     | 987 | PRO  | C-N   | 5.81  | 1.42        | 1.33     |
| 9   | B     | 138 | GLY  | CA-C  | -5.81 | 1.45        | 1.51     |
| 9   | B     | 187 | ASP  | N-CA  | -5.81 | 1.38        | 1.46     |
| 30  | W     | 174 | VAL  | C-N   | 5.81  | 1.42        | 1.33     |
| 7   | 7     | 206 | VAL  | CA-C  | 5.81  | 1.59        | 1.52     |
| 16  | I     | 371 | LEU  | CA-C  | -5.81 | 1.45        | 1.52     |
| 33  | Z     | 299 | ASP  | CA-C  | -5.80 | 1.45        | 1.52     |
| 29  | V     | 27  | VAL  | N-CA  | -5.80 | 1.39        | 1.46     |
| 32  | Y     | 83  | ARG  | N-CA  | 5.80  | 1.53        | 1.46     |
| 23  | P     | 175 | GLU  | C-N   | 5.80  | 1.41        | 1.33     |
| 2   | 2     | 46  | ALA  | CA-C  | -5.80 | 1.45        | 1.52     |
| 20  | M     | 420 | SER  | C-N   | 5.80  | 1.41        | 1.33     |
| 21  | N     | 761 | ILE  | CA-C  | -5.80 | 1.45        | 1.52     |
| 18  | K     | 303 | MET  | C-N   | 5.79  | 1.42        | 1.33     |
| 18  | K     | 227 | ALA  | C-N   | 5.79  | 1.41        | 1.33     |
| 25  | R     | 416 | LYS  | C-N   | 5.79  | 1.41        | 1.33     |
| 28  | U     | 90  | ILE  | CA-C  | 5.79  | 1.60        | 1.52     |
| 17  | J     | 213 | VAL  | CA-C  | 5.79  | 1.60        | 1.52     |
| 28  | U     | 200 | LEU  | CA-C  | -5.79 | 1.45        | 1.52     |
| 3   | 3     | 160 | GLN  | CA-C  | -5.79 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 5     | 79  | ALA  | CA-C  | -5.79 | 1.45        | 1.52     |
| 9   | B     | 55  | LEU  | CA-C  | -5.79 | 1.44        | 1.52     |
| 19  | L     | 169 | ASN  | C-N   | 5.79  | 1.40        | 1.33     |
| 25  | R     | 228 | ALA  | N-CA  | -5.78 | 1.39        | 1.46     |
| 20  | M     | 158 | THR  | CA-C  | -5.78 | 1.45        | 1.52     |
| 21  | N     | 578 | ASP  | C-O   | -5.78 | 1.16        | 1.24     |
| 26  | S     | 225 | HIS  | CA-C  | -5.78 | 1.45        | 1.52     |
| 7   | 7     | 164 | VAL  | N-CA  | -5.78 | 1.39        | 1.46     |
| 9   | B     | 60  | THR  | C-N   | 5.78  | 1.41        | 1.33     |
| 16  | I     | 247 | ILE  | CA-C  | -5.78 | 1.45        | 1.52     |
| 25  | R     | 91  | TRP  | C-N   | 5.78  | 1.41        | 1.33     |
| 25  | R     | 248 | SER  | CA-C  | 5.78  | 1.60        | 1.52     |
| 28  | U     | 303 | GLU  | C-N   | 5.78  | 1.41        | 1.33     |
| 16  | I     | 266 | GLN  | N-CA  | -5.78 | 1.39        | 1.46     |
| 25  | R     | 411 | LEU  | N-CA  | -5.78 | 1.39        | 1.46     |
| 8   | A     | 108 | TYR  | C-N   | 5.77  | 1.41        | 1.33     |
| 10  | C     | 12  | ILE  | C-N   | 5.77  | 1.41        | 1.33     |
| 11  | D     | 185 | PRO  | N-CD  | 5.77  | 1.55        | 1.47     |
| 21  | N     | 736 | PHE  | N-CA  | -5.77 | 1.39        | 1.46     |
| 29  | V     | 154 | ASP  | N-CA  | -5.77 | 1.38        | 1.45     |
| 6   | 6     | 164 | LYS  | CA-C  | -5.77 | 1.45        | 1.52     |
| 23  | P     | 288 | ASN  | CA-C  | -5.77 | 1.45        | 1.52     |
| 5   | 5     | 212 | GLY  | N-CA  | -5.77 | 1.36        | 1.45     |
| 7   | 7     | 175 | VAL  | CA-C  | -5.77 | 1.45        | 1.52     |
| 2   | 2     | 135 | MET  | C-N   | 5.76  | 1.41        | 1.33     |
| 11  | D     | 18  | PHE  | C-O   | -5.76 | 1.17        | 1.24     |
| 8   | A     | 123 | ASN  | C-N   | 5.76  | 1.41        | 1.33     |
| 21  | N     | 609 | LEU  | C-N   | 5.76  | 1.41        | 1.33     |
| 20  | M     | 203 | ARG  | CA-C  | 5.76  | 1.60        | 1.52     |
| 28  | U     | 140 | ILE  | C-N   | 5.75  | 1.41        | 1.33     |
| 3   | 3     | 52  | THR  | N-CA  | -5.75 | 1.39        | 1.46     |
| 4   | 4     | 163 | CYS  | N-CA  | -5.75 | 1.39        | 1.46     |
| 15  | H     | 255 | GLY  | C-N   | 5.75  | 1.41        | 1.33     |
| 17  | J     | 27  | ILE  | CA-C  | -5.75 | 1.45        | 1.52     |
| 19  | L     | 129 | VAL  | CA-C  | -5.75 | 1.45        | 1.52     |
| 8   | A     | 36  | ASN  | N-CA  | -5.75 | 1.38        | 1.46     |
| 30  | W     | 147 | ILE  | C-N   | 5.75  | 1.41        | 1.33     |
| 11  | D     | 228 | GLU  | CA-C  | -5.75 | 1.45        | 1.52     |
| 18  | K     | 71  | GLU  | C-N   | 5.75  | 1.41        | 1.33     |
| 25  | R     | 311 | THR  | C-N   | 5.75  | 1.41        | 1.33     |
| 31  | X     | 46  | TRP  | CA-C  | -5.74 | 1.45        | 1.52     |
| 33  | Z     | 771 | HIS  | CA-C  | -5.74 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9   | B     | 156 | TYR  | CA-C  | -5.74 | 1.45        | 1.52     |
| 3   | 3     | 3   | VAL  | CA-C  | -5.74 | 1.45        | 1.52     |
| 3   | 3     | 154 | LEU  | C-N   | 5.74  | 1.41        | 1.33     |
| 7   | 7     | 90  | THR  | N-CA  | -5.74 | 1.39        | 1.46     |
| 14  | G     | 88  | VAL  | N-CA  | -5.74 | 1.39        | 1.46     |
| 21  | N     | 35  | LEU  | N-CA  | -5.74 | 1.39        | 1.46     |
| 33  | Z     | 778 | LEU  | CA-C  | -5.74 | 1.45        | 1.52     |
| 25  | R     | 44  | LYS  | C-O   | 5.74  | 1.30        | 1.24     |
| 22  | O     | 297 | ILE  | C-O   | -5.73 | 1.17        | 1.24     |
| 27  | T     | 186 | ARG  | CA-C  | -5.73 | 1.45        | 1.52     |
| 2   | 2     | 94  | ILE  | CA-C  | -5.73 | 1.45        | 1.52     |
| 20  | M     | 300 | GLU  | C-N   | 5.73  | 1.41        | 1.33     |
| 23  | P     | 119 | ILE  | C-N   | 5.73  | 1.41        | 1.34     |
| 25  | R     | 230 | LEU  | C-N   | 5.73  | 1.41        | 1.33     |
| 26  | S     | 236 | LEU  | CA-C  | -5.73 | 1.45        | 1.52     |
| 6   | 6     | 53  | ASP  | C-N   | 5.73  | 1.41        | 1.33     |
| 17  | J     | 34  | ILE  | N-CA  | -5.73 | 1.39        | 1.46     |
| 20  | M     | 369 | THR  | CA-C  | -5.73 | 1.45        | 1.52     |
| 9   | B     | 20  | GLN  | CA-C  | -5.73 | 1.45        | 1.52     |
| 21  | N     | 697 | PHE  | CA-C  | -5.73 | 1.45        | 1.52     |
| 23  | P     | 379 | TYR  | CA-C  | -5.72 | 1.45        | 1.52     |
| 12  | E     | 240 | ILE  | N-CA  | -5.72 | 1.39        | 1.46     |
| 18  | K     | 165 | GLU  | CA-C  | -5.72 | 1.45        | 1.53     |
| 6   | 6     | 187 | ILE  | N-CA  | -5.72 | 1.40        | 1.46     |
| 15  | H     | 297 | MET  | CA-C  | -5.72 | 1.45        | 1.52     |
| 18  | K     | 134 | SER  | C-N   | 5.72  | 1.41        | 1.33     |
| 30  | W     | 141 | ILE  | C-N   | 5.72  | 1.41        | 1.33     |
| 1   | 1     | 100 | ALA  | CA-C  | -5.72 | 1.45        | 1.52     |
| 33  | Z     | 361 | HIS  | N-CA  | -5.72 | 1.39        | 1.46     |
| 12  | E     | 137 | PRO  | CA-CB | -5.72 | 1.46        | 1.53     |
| 20  | M     | 322 | LYS  | CA-C  | -5.72 | 1.45        | 1.52     |
| 29  | V     | 255 | ILE  | CA-C  | -5.71 | 1.45        | 1.52     |
| 21  | N     | 535 | LEU  | C-N   | 5.71  | 1.41        | 1.33     |
| 22  | O     | 297 | ILE  | N-CA  | -5.71 | 1.39        | 1.46     |
| 18  | K     | 362 | LEU  | N-CA  | 5.71  | 1.53        | 1.45     |
| 21  | N     | 208 | ARG  | C-N   | 5.71  | 1.42        | 1.33     |
| 18  | K     | 387 | MET  | CA-C  | -5.71 | 1.45        | 1.52     |
| 20  | M     | 327 | THR  | CA-C  | -5.71 | 1.45        | 1.52     |
| 23  | P     | 137 | ALA  | N-CA  | -5.71 | 1.39        | 1.46     |
| 27  | T     | 74  | ASN  | CA-C  | -5.71 | 1.45        | 1.53     |
| 5   | 5     | 185 | TRP  | N-CA  | 5.70  | 1.53        | 1.45     |
| 25  | R     | 228 | ALA  | CA-C  | -5.70 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 31  | X     | 82  | LYS  | C-N   | 5.70  | 1.41        | 1.33     |
| 13  | F     | 206 | LEU  | CA-C  | -5.70 | 1.45        | 1.52     |
| 24  | Q     | 350 | ILE  | CA-C  | -5.70 | 1.45        | 1.52     |
| 26  | S     | 373 | LYS  | C-N   | 5.70  | 1.41        | 1.33     |
| 2   | 2     | 189 | ASN  | C-N   | 5.70  | 1.41        | 1.34     |
| 11  | D     | 76  | SER  | N-CA  | -5.70 | 1.39        | 1.46     |
| 16  | I     | 251 | GLU  | N-CA  | 5.70  | 1.53        | 1.46     |
| 33  | Z     | 810 | ASN  | C-N   | 5.70  | 1.41        | 1.33     |
| 19  | L     | 82  | ARG  | N-CA  | -5.69 | 1.39        | 1.46     |
| 26  | S     | 434 | ALA  | CA-C  | -5.69 | 1.45        | 1.52     |
| 17  | J     | 58  | ILE  | CA-C  | -5.69 | 1.45        | 1.52     |
| 3   | 3     | 87  | TYR  | C-N   | 5.69  | 1.41        | 1.33     |
| 22  | O     | 214 | ALA  | CA-C  | -5.69 | 1.45        | 1.52     |
| 29  | V     | 254 | ARG  | C-N   | 5.69  | 1.41        | 1.33     |
| 25  | R     | 84  | LYS  | N-CA  | -5.69 | 1.38        | 1.46     |
| 33  | Z     | 809 | MET  | C-N   | 5.69  | 1.41        | 1.34     |
| 12  | E     | 151 | ASP  | N-CA  | 5.69  | 1.52        | 1.47     |
| 18  | K     | 130 | LEU  | CA-C  | -5.69 | 1.45        | 1.52     |
| 24  | Q     | 98  | LYS  | CA-C  | 5.69  | 1.60        | 1.52     |
| 6   | 6     | 188 | GLN  | C-N   | 5.68  | 1.41        | 1.33     |
| 30  | W     | 184 | ASN  | CA-C  | -5.68 | 1.45        | 1.52     |
| 2   | 2     | 28  | ASP  | C-N   | 5.68  | 1.42        | 1.33     |
| 5   | 5     | 194 | GLY  | N-CA  | -5.68 | 1.38        | 1.45     |
| 33  | Z     | 775 | MET  | C-N   | 5.68  | 1.39        | 1.33     |
| 8   | A     | 198 | SER  | C-N   | 5.68  | 1.41        | 1.34     |
| 2   | 2     | 141 | HIS  | C-N   | 5.68  | 1.41        | 1.33     |
| 9   | B     | 5   | TYR  | C-N   | 5.68  | 1.41        | 1.33     |
| 9   | B     | 8   | SER  | CA-C  | -5.68 | 1.45        | 1.53     |
| 21  | N     | 174 | LEU  | CA-C  | -5.68 | 1.45        | 1.52     |
| 23  | P     | 388 | ILE  | CA-C  | -5.68 | 1.45        | 1.53     |
| 33  | Z     | 601 | VAL  | N-CA  | -5.68 | 1.39        | 1.46     |
| 2   | 2     | 81  | GLN  | C-N   | 5.67  | 1.41        | 1.33     |
| 29  | V     | 38  | LEU  | CA-C  | -5.67 | 1.45        | 1.52     |
| 12  | E     | 146 | GLY  | CA-C  | -5.67 | 1.45        | 1.51     |
| 8   | A     | 209 | HIS  | N-CA  | 5.67  | 1.53        | 1.46     |
| 21  | N     | 730 | VAL  | N-CA  | -5.67 | 1.39        | 1.46     |
| 16  | I     | 216 | PRO  | N-CD  | 5.67  | 1.55        | 1.47     |
| 26  | S     | 134 | ILE  | C-N   | 5.67  | 1.41        | 1.33     |
| 33  | Z     | 203 | LEU  | C-N   | 5.67  | 1.41        | 1.33     |
| 2   | 2     | 119 | THR  | CA-C  | -5.66 | 1.46        | 1.52     |
| 8   | A     | 136 | PRO  | C-N   | 5.66  | 1.41        | 1.33     |
| 8   | A     | 164 | VAL  | N-CA  | -5.66 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | M     | 358 | ALA  | C-N   | 5.66  | 1.41        | 1.33     |
| 24  | Q     | 275 | ILE  | N-CA  | -5.66 | 1.39        | 1.46     |
| 20  | M     | 67  | GLU  | C-N   | 5.66  | 1.41        | 1.33     |
| 15  | H     | 252 | PRO  | CA-C  | -5.66 | 1.46        | 1.52     |
| 22  | O     | 278 | PRO  | CA-C  | -5.66 | 1.42        | 1.52     |
| 33  | Z     | 97  | PRO  | N-CD  | 5.66  | 1.55        | 1.47     |
| 14  | G     | 196 | ALA  | C-N   | 5.66  | 1.41        | 1.33     |
| 21  | N     | 240 | GLN  | CA-C  | -5.66 | 1.45        | 1.52     |
| 1   | 1     | 169 | SER  | N-CA  | -5.66 | 1.38        | 1.45     |
| 33  | Z     | 598 | ALA  | N-CA  | -5.66 | 1.39        | 1.46     |
| 33  | Z     | 228 | GLU  | N-CA  | -5.65 | 1.38        | 1.46     |
| 5   | 5     | 164 | ALA  | C-O   | -5.65 | 1.17        | 1.24     |
| 16  | I     | 317 | ASP  | N-CA  | -5.65 | 1.39        | 1.45     |
| 17  | J     | 293 | ALA  | CA-C  | -5.65 | 1.45        | 1.52     |
| 22  | O     | 306 | ARG  | CA-C  | 5.65  | 1.61        | 1.52     |
| 30  | W     | 133 | LYS  | C-N   | 5.65  | 1.41        | 1.34     |
| 26  | S     | 419 | VAL  | N-CA  | -5.65 | 1.39        | 1.46     |
| 3   | 3     | 158 | ILE  | CA-C  | -5.65 | 1.45        | 1.52     |
| 11  | D     | 238 | GLN  | N-CA  | 5.65  | 1.53        | 1.46     |
| 15  | H     | 304 | CYS  | N-CA  | -5.65 | 1.39        | 1.46     |
| 3   | 3     | 53  | THR  | C-N   | 5.64  | 1.41        | 1.33     |
| 10  | C     | 157 | TYR  | N-CA  | -5.64 | 1.38        | 1.45     |
| 15  | H     | 355 | THR  | CA-C  | -5.64 | 1.45        | 1.52     |
| 21  | N     | 57  | ASP  | C-N   | 5.64  | 1.41        | 1.33     |
| 5   | 5     | 142 | SER  | CA-C  | -5.64 | 1.45        | 1.52     |
| 7   | 7     | 200 | PHE  | CA-C  | -5.64 | 1.46        | 1.52     |
| 12  | E     | 208 | MET  | CA-C  | -5.64 | 1.45        | 1.52     |
| 19  | L     | 350 | PRO  | N-CD  | 5.64  | 1.55        | 1.47     |
| 8   | A     | 66  | PRO  | N-CD  | 5.64  | 1.55        | 1.47     |
| 15  | H     | 156 | VAL  | CA-C  | -5.64 | 1.45        | 1.52     |
| 30  | W     | 30  | ILE  | N-CA  | -5.64 | 1.39        | 1.46     |
| 18  | K     | 423 | LYS  | N-CA  | -5.64 | 1.38        | 1.45     |
| 21  | N     | 917 | ILE  | CA-C  | -5.64 | 1.45        | 1.52     |
| 27  | T     | 228 | ILE  | N-CA  | -5.64 | 1.39        | 1.46     |
| 1   | 1     | 58  | ILE  | N-CA  | -5.63 | 1.39        | 1.46     |
| 2   | 2     | 6   | VAL  | N-CA  | -5.63 | 1.39        | 1.46     |
| 16  | I     | 244 | PHE  | C-N   | 5.63  | 1.41        | 1.33     |
| 21  | N     | 277 | LEU  | CA-C  | -5.63 | 1.45        | 1.52     |
| 21  | N     | 592 | GLY  | CA-C  | -5.63 | 1.45        | 1.52     |
| 29  | V     | 35  | LEU  | N-CA  | -5.63 | 1.39        | 1.46     |
| 32  | Y     | 79  | ALA  | C-O   | -5.63 | 1.17        | 1.24     |
| 33  | Z     | 530 | LEU  | C-N   | 5.63  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 33  | Z     | 786 | SER  | C-O   | -5.63 | 1.17        | 1.24     |
| 10  | C     | 204 | SER  | C-N   | 5.62  | 1.41        | 1.33     |
| 12  | E     | 132 | ARG  | CA-C  | -5.62 | 1.45        | 1.52     |
| 16  | I     | 219 | VAL  | C-N   | 5.62  | 1.41        | 1.33     |
| 22  | O     | 239 | MET  | C-O   | -5.62 | 1.19        | 1.23     |
| 5   | 5     | 205 | GLY  | CA-C  | -5.62 | 1.44        | 1.51     |
| 29  | V     | 56  | GLU  | C-N   | 5.62  | 1.41        | 1.33     |
| 26  | S     | 254 | ILE  | CA-C  | -5.62 | 1.45        | 1.52     |
| 8   | A     | 126 | GLN  | C-N   | 5.61  | 1.41        | 1.33     |
| 17  | J     | 252 | SER  | C-N   | 5.61  | 1.40        | 1.34     |
| 22  | O     | 162 | SER  | C-N   | 5.61  | 1.39        | 1.33     |
| 33  | Z     | 270 | SER  | CA-C  | -5.61 | 1.45        | 1.52     |
| 3   | 3     | 77  | THR  | N-CA  | -5.61 | 1.39        | 1.46     |
| 4   | 4     | 42  | LEU  | C-N   | 5.61  | 1.41        | 1.33     |
| 33  | Z     | 747 | ALA  | C-O   | -5.61 | 1.16        | 1.24     |
| 4   | 4     | 144 | ASP  | C-N   | 5.61  | 1.41        | 1.33     |
| 12  | E     | 171 | ALA  | CA-C  | -5.61 | 1.46        | 1.52     |
| 8   | A     | 211 | ILE  | C-N   | 5.61  | 1.41        | 1.33     |
| 23  | P     | 208 | PHE  | C-N   | 5.61  | 1.41        | 1.33     |
| 30  | W     | 139 | VAL  | C-N   | 5.61  | 1.41        | 1.33     |
| 33  | Z     | 141 | SER  | CA-C  | 5.61  | 1.60        | 1.52     |
| 14  | G     | 97  | SER  | CA-C  | -5.61 | 1.45        | 1.52     |
| 4   | 4     | 131 | ALA  | CA-C  | 5.60  | 1.59        | 1.52     |
| 8   | A     | 81  | MET  | C-N   | 5.60  | 1.40        | 1.33     |
| 29  | V     | 276 | PRO  | N-CD  | 5.60  | 1.55        | 1.47     |
| 13  | F     | 145 | LEU  | CA-C  | -5.60 | 1.45        | 1.52     |
| 22  | O     | 332 | ILE  | C-N   | 5.60  | 1.41        | 1.33     |
| 24  | Q     | 85  | MET  | N-CA  | -5.60 | 1.39        | 1.46     |
| 21  | N     | 142 | GLU  | CA-C  | -5.60 | 1.45        | 1.52     |
| 9   | B     | 226 | GLY  | N-CA  | -5.60 | 1.38        | 1.45     |
| 19  | L     | 73  | GLN  | N-CA  | 5.60  | 1.53        | 1.46     |
| 20  | M     | 294 | GLU  | CA-C  | 5.60  | 1.60        | 1.52     |
| 23  | P     | 84  | LYS  | C-O   | -5.60 | 1.17        | 1.24     |
| 26  | S     | 378 | GLN  | N-CA  | -5.60 | 1.39        | 1.46     |
| 18  | K     | 219 | LYS  | N-CA  | -5.60 | 1.39        | 1.46     |
| 26  | S     | 235 | ASN  | C-N   | 5.59  | 1.41        | 1.33     |
| 29  | V     | 99  | GLY  | CA-C  | -5.59 | 1.43        | 1.51     |
| 31  | X     | 57  | VAL  | N-CA  | -5.59 | 1.39        | 1.46     |
| 3   | 3     | 82  | VAL  | N-CA  | -5.59 | 1.40        | 1.46     |
| 10  | C     | 236 | LYS  | N-CA  | 5.59  | 1.53        | 1.46     |
| 21  | N     | 678 | ILE  | N-CA  | -5.59 | 1.40        | 1.46     |
| 3   | 3     | 27  | VAL  | N-CA  | -5.59 | 1.39        | 1.45     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | 7     | 62  | LEU  | C-N   | 5.59  | 1.40        | 1.33     |
| 15  | H     | 305 | ILE  | C-N   | 5.59  | 1.40        | 1.33     |
| 33  | Z     | 785 | VAL  | N-CA  | -5.59 | 1.39        | 1.46     |
| 15  | H     | 288 | ALA  | C-N   | 5.59  | 1.41        | 1.33     |
| 21  | N     | 215 | MET  | N-CA  | -5.59 | 1.39        | 1.46     |
| 7   | 7     | 158 | PRO  | C-N   | 5.58  | 1.41        | 1.33     |
| 20  | M     | 371 | ASP  | C-N   | 5.58  | 1.41        | 1.33     |
| 22  | O     | 104 | ALA  | CA-C  | -5.58 | 1.45        | 1.52     |
| 23  | P     | 383 | LEU  | N-CA  | -5.58 | 1.39        | 1.46     |
| 21  | N     | 330 | THR  | CA-C  | -5.58 | 1.45        | 1.52     |
| 13  | F     | 85  | SER  | CA-C  | -5.58 | 1.45        | 1.52     |
| 28  | U     | 9   | THR  | C-N   | 5.58  | 1.40        | 1.33     |
| 11  | D     | 155 | ILE  | CA-C  | -5.58 | 1.45        | 1.52     |
| 19  | L     | 415 | LEU  | N-CA  | -5.58 | 1.39        | 1.46     |
| 20  | M     | 412 | HIS  | N-CA  | -5.58 | 1.39        | 1.46     |
| 9   | B     | 13  | SER  | C-N   | 5.58  | 1.40        | 1.34     |
| 14  | G     | 30  | VAL  | CA-C  | 5.58  | 1.59        | 1.52     |
| 8   | A     | 92  | ASN  | C-N   | 5.57  | 1.41        | 1.33     |
| 17  | J     | 96  | VAL  | CA-C  | -5.57 | 1.46        | 1.52     |
| 31  | X     | 109 | LEU  | CA-C  | -5.57 | 1.46        | 1.52     |
| 11  | D     | 198 | SER  | N-CA  | -5.57 | 1.39        | 1.46     |
| 27  | T     | 2   | PRO  | N-CA  | -5.57 | 1.40        | 1.47     |
| 24  | Q     | 357 | VAL  | N-CA  | -5.57 | 1.40        | 1.46     |
| 18  | K     | 205 | PRO  | CA-C  | -5.56 | 1.47        | 1.52     |
| 5   | 5     | 87  | VAL  | N-CA  | -5.56 | 1.40        | 1.46     |
| 11  | D     | 118 | GLN  | CA-C  | -5.56 | 1.45        | 1.52     |
| 25  | R     | 131 | ALA  | C-N   | 5.56  | 1.41        | 1.33     |
| 23  | P     | 437 | GLU  | CA-C  | -5.56 | 1.45        | 1.52     |
| 27  | T     | 269 | SER  | C-O   | -5.56 | 1.16        | 1.24     |
| 7   | 7     | 136 | THR  | C-N   | 5.56  | 1.40        | 1.33     |
| 16  | I     | 289 | THR  | CA-C  | -5.56 | 1.45        | 1.52     |
| 19  | L     | 400 | PHE  | CA-C  | -5.56 | 1.45        | 1.52     |
| 31  | X     | 52  | PRO  | N-CA  | -5.56 | 1.40        | 1.46     |
| 20  | M     | 333 | LEU  | C-N   | 5.56  | 1.39        | 1.33     |
| 23  | P     | 372 | THR  | C-N   | 5.56  | 1.41        | 1.33     |
| 28  | U     | 63  | SER  | CA-C  | 5.56  | 1.60        | 1.52     |
| 7   | 7     | 67  | ALA  | N-CA  | -5.55 | 1.38        | 1.46     |
| 10  | C     | 133 | VAL  | N-CA  | -5.55 | 1.39        | 1.46     |
| 17  | J     | 359 | LYS  | CA-C  | -5.55 | 1.45        | 1.52     |
| 5   | 5     | 156 | LEU  | CA-C  | -5.55 | 1.45        | 1.52     |
| 12  | E     | 149 | ALA  | CA-C  | -5.55 | 1.44        | 1.52     |
| 11  | D     | 177 | LYS  | CA-C  | -5.55 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9   | B     | 147 | LEU  | C-N   | 5.55  | 1.41        | 1.33     |
| 21  | N     | 253 | LEU  | N-CA  | -5.55 | 1.39        | 1.46     |
| 27  | T     | 35  | ILE  | C-N   | 5.55  | 1.41        | 1.33     |
| 33  | Z     | 758 | LEU  | CA-C  | -5.55 | 1.45        | 1.52     |
| 33  | Z     | 767 | TYR  | C-N   | 5.55  | 1.41        | 1.33     |
| 18  | K     | 384 | ALA  | CA-C  | -5.55 | 1.45        | 1.52     |
| 3   | 3     | 187 | VAL  | CA-C  | -5.54 | 1.46        | 1.52     |
| 20  | M     | 134 | LEU  | N-CA  | -5.54 | 1.39        | 1.46     |
| 23  | P     | 396 | PRO  | N-CD  | 5.54  | 1.55        | 1.47     |
| 1   | 1     | 116 | GLY  | C-N   | 5.54  | 1.41        | 1.33     |
| 6   | 6     | 35  | PHE  | CA-C  | -5.54 | 1.45        | 1.52     |
| 7   | 7     | 183 | SER  | N-CA  | -5.54 | 1.39        | 1.46     |
| 11  | D     | 241 | GLN  | CA-C  | -5.54 | 1.45        | 1.53     |
| 16  | I     | 111 | GLU  | N-CA  | -5.54 | 1.39        | 1.46     |
| 25  | R     | 233 | ASP  | CA-C  | -5.54 | 1.45        | 1.52     |
| 26  | S     | 286 | TYR  | C-O   | -5.54 | 1.17        | 1.24     |
| 28  | U     | 17  | SER  | C-N   | 5.54  | 1.41        | 1.33     |
| 12  | E     | 243 | LEU  | N-CA  | -5.54 | 1.39        | 1.46     |
| 19  | L     | 104 | LEU  | N-CA  | -5.54 | 1.38        | 1.45     |
| 21  | N     | 51  | ASP  | C-N   | 5.54  | 1.41        | 1.33     |
| 9   | B     | 25  | LEU  | CA-C  | -5.54 | 1.45        | 1.52     |
| 11  | D     | 122 | GLN  | CA-C  | 5.54  | 1.60        | 1.52     |
| 24  | Q     | 27  | TYR  | N-CA  | -5.54 | 1.39        | 1.46     |
| 12  | E     | 247 | GLU  | N-CA  | -5.53 | 1.39        | 1.46     |
| 19  | L     | 386 | PHE  | N-CA  | 5.53  | 1.52        | 1.45     |
| 7   | 7     | 219 | GLY  | CA-C  | -5.53 | 1.45        | 1.52     |
| 2   | 2     | 170 | GLY  | C-N   | 5.53  | 1.41        | 1.33     |
| 16  | I     | 148 | LEU  | CA-C  | 5.53  | 1.59        | 1.52     |
| 22  | O     | 205 | ILE  | N-CA  | 5.53  | 1.53        | 1.46     |
| 27  | T     | 194 | GLU  | N-CA  | -5.53 | 1.39        | 1.46     |
| 15  | H     | 98  | GLN  | CA-C  | 5.53  | 1.60        | 1.52     |
| 25  | R     | 386 | GLY  | C-N   | 5.52  | 1.41        | 1.33     |
| 27  | T     | 206 | LYS  | C-N   | 5.52  | 1.41        | 1.33     |
| 4   | 4     | 47  | GLY  | C-O   | 5.52  | 1.27        | 1.23     |
| 7   | 7     | 135 | ALA  | C-N   | 5.52  | 1.40        | 1.33     |
| 19  | L     | 127 | TYR  | CA-C  | -5.52 | 1.45        | 1.52     |
| 33  | Z     | 152 | GLU  | C-N   | 5.52  | 1.40        | 1.33     |
| 33  | Z     | 975 | SER  | C-N   | 5.52  | 1.40        | 1.33     |
| 16  | I     | 285 | ASP  | CA-C  | -5.52 | 1.45        | 1.52     |
| 16  | I     | 257 | LEU  | C-N   | 5.52  | 1.40        | 1.33     |
| 17  | J     | 264 | GLY  | CA-C  | -5.52 | 1.44        | 1.51     |
| 20  | M     | 393 | ALA  | C-N   | 5.52  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 24  | Q     | 181 | GLU  | CA-C  | -5.52 | 1.45        | 1.52     |
| 26  | S     | 132 | ALA  | N-CA  | -5.52 | 1.39        | 1.46     |
| 5   | 5     | 29  | GLN  | N-CA  | -5.51 | 1.40        | 1.46     |
| 25  | R     | 90  | GLU  | C-N   | 5.51  | 1.40        | 1.33     |
| 27  | T     | 228 | ILE  | C-O   | -5.51 | 1.18        | 1.24     |
| 19  | L     | 376 | PHE  | C-N   | 5.51  | 1.41        | 1.33     |
| 24  | Q     | 26  | VAL  | CA-C  | -5.51 | 1.45        | 1.52     |
| 16  | I     | 173 | MET  | C-O   | -5.51 | 1.17        | 1.24     |
| 17  | J     | 382 | PHE  | C-N   | 5.51  | 1.40        | 1.33     |
| 29  | V     | 237 | ASN  | C-N   | 5.51  | 1.40        | 1.33     |
| 2   | 2     | 194 | ASN  | C-N   | 5.51  | 1.40        | 1.33     |
| 3   | 3     | 1   | GLY  | C-O   | -5.51 | 1.19        | 1.23     |
| 18  | K     | 90  | GLN  | C-N   | 5.51  | 1.41        | 1.33     |
| 20  | M     | 399 | GLY  | N-CA  | -5.51 | 1.39        | 1.45     |
| 4   | 4     | 31  | ASP  | C-N   | 5.51  | 1.41        | 1.33     |
| 21  | N     | 768 | ILE  | CA-C  | 5.51  | 1.57        | 1.52     |
| 14  | G     | 170 | SER  | CA-C  | -5.51 | 1.45        | 1.52     |
| 27  | T     | 176 | SER  | N-CA  | -5.51 | 1.39        | 1.46     |
| 15  | H     | 351 | VAL  | N-CA  | -5.50 | 1.39        | 1.46     |
| 18  | K     | 255 | ARG  | CA-C  | -5.50 | 1.45        | 1.52     |
| 19  | L     | 196 | VAL  | CA-C  | 5.50  | 1.61        | 1.52     |
| 7   | 7     | 46  | SER  | N-CA  | -5.50 | 1.39        | 1.45     |
| 13  | F     | 67  | ASP  | C-O   | -5.50 | 1.18        | 1.24     |
| 21  | N     | 904 | VAL  | N-CA  | -5.50 | 1.39        | 1.46     |
| 27  | T     | 177 | PHE  | C-N   | 5.50  | 1.40        | 1.33     |
| 13  | F     | 75  | ALA  | CA-C  | -5.50 | 1.46        | 1.52     |
| 23  | P     | 115 | ARG  | CA-C  | -5.50 | 1.45        | 1.52     |
| 25  | R     | 290 | SER  | C-O   | -5.50 | 1.17        | 1.24     |
| 22  | O     | 345 | ASN  | CA-C  | -5.49 | 1.45        | 1.52     |
| 31  | X     | 43  | LEU  | CA-C  | -5.49 | 1.45        | 1.52     |
| 4   | 4     | 33  | LYS  | N-CA  | -5.49 | 1.40        | 1.46     |
| 21  | N     | 253 | LEU  | C-N   | 5.49  | 1.41        | 1.34     |
| 11  | D     | 193 | LYS  | CA-C  | -5.49 | 1.45        | 1.52     |
| 15  | H     | 209 | SER  | CA-C  | -5.48 | 1.46        | 1.52     |
| 33  | Z     | 114 | SER  | N-CA  | -5.48 | 1.39        | 1.46     |
| 7   | 7     | 155 | SER  | C-N   | 5.48  | 1.42        | 1.33     |
| 22  | O     | 353 | VAL  | CA-C  | -5.48 | 1.45        | 1.52     |
| 14  | G     | 51  | LYS  | CA-C  | 5.48  | 1.59        | 1.52     |
| 16  | I     | 79  | SER  | C-N   | 5.48  | 1.41        | 1.33     |
| 17  | J     | 75  | VAL  | C-N   | 5.48  | 1.39        | 1.33     |
| 21  | N     | 642 | ASP  | N-CA  | -5.48 | 1.42        | 1.46     |
| 24  | Q     | 14  | LEU  | CA-C  | -5.48 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | 2     | 40  | LYS  | N-CA  | -5.47 | 1.40        | 1.46     |
| 13  | F     | 90  | GLN  | N-CA  | -5.47 | 1.39        | 1.46     |
| 16  | I     | 363 | GLY  | C-N   | 5.47  | 1.40        | 1.33     |
| 18  | K     | 410 | ALA  | C-N   | -5.47 | 1.26        | 1.33     |
| 21  | N     | 24  | ALA  | N-CA  | -5.47 | 1.39        | 1.46     |
| 25  | R     | 104 | LYS  | C-N   | 5.47  | 1.41        | 1.33     |
| 25  | R     | 116 | LYS  | CA-C  | -5.47 | 1.45        | 1.52     |
| 26  | S     | 228 | GLU  | N-CA  | -5.47 | 1.39        | 1.46     |
| 21  | N     | 183 | VAL  | N-CA  | -5.47 | 1.39        | 1.46     |
| 33  | Z     | 411 | LYS  | C-N   | 5.47  | 1.41        | 1.33     |
| 1   | 1     | 105 | LYS  | N-CA  | -5.47 | 1.39        | 1.46     |
| 9   | B     | 59  | GLU  | CA-C  | -5.47 | 1.45        | 1.52     |
| 22  | O     | 100 | ASP  | C-N   | 5.47  | 1.40        | 1.33     |
| 9   | B     | 134 | LEU  | N-CA  | 5.47  | 1.52        | 1.45     |
| 19  | L     | 247 | PRO  | N-CA  | -5.47 | 1.40        | 1.47     |
| 23  | P     | 424 | GLU  | CA-C  | -5.47 | 1.45        | 1.52     |
| 10  | C     | 96  | GLN  | CA-C  | -5.46 | 1.45        | 1.52     |
| 24  | Q     | 415 | LEU  | N-CA  | -5.46 | 1.39        | 1.46     |
| 26  | S     | 350 | LYS  | CA-C  | -5.46 | 1.45        | 1.52     |
| 28  | U     | 33  | CYS  | CA-C  | -5.46 | 1.46        | 1.52     |
| 33  | Z     | 991 | GLU  | CA-C  | -5.46 | 1.45        | 1.52     |
| 4   | 4     | 73  | GLU  | CA-C  | -5.46 | 1.46        | 1.52     |
| 14  | G     | 81  | ILE  | C-O   | -5.46 | 1.20        | 1.24     |
| 15  | H     | 212 | GLY  | CA-C  | -5.46 | 1.44        | 1.51     |
| 21  | N     | 112 | GLU  | N-CA  | -5.46 | 1.39        | 1.46     |
| 24  | Q     | 10  | GLU  | CA-C  | -5.46 | 1.45        | 1.52     |
| 33  | Z     | 209 | PRO  | N-CA  | -5.46 | 1.40        | 1.47     |
| 33  | Z     | 262 | VAL  | C-N   | 5.46  | 1.41        | 1.33     |
| 3   | 3     | 84  | SER  | N-CA  | -5.46 | 1.39        | 1.46     |
| 21  | N     | 694 | LEU  | CA-C  | -5.46 | 1.45        | 1.52     |
| 23  | P     | 98  | GLN  | CA-C  | 5.46  | 1.59        | 1.52     |
| 10  | C     | 210 | ARG  | N-CA  | -5.46 | 1.39        | 1.46     |
| 25  | R     | 46  | ALA  | N-CA  | -5.46 | 1.39        | 1.46     |
| 27  | T     | 213 | ASN  | CA-C  | -5.46 | 1.45        | 1.52     |
| 11  | D     | 64  | VAL  | N-CA  | -5.45 | 1.39        | 1.46     |
| 33  | Z     | 86  | PRO  | C-N   | 5.45  | 1.40        | 1.33     |
| 21  | N     | 642 | ASP  | CA-C  | -5.45 | 1.46        | 1.52     |
| 5   | 5     | 102 | CYS  | CA-C  | -5.45 | 1.46        | 1.52     |
| 20  | M     | 147 | GLY  | CA-C  | -5.45 | 1.44        | 1.51     |
| 25  | R     | 128 | LEU  | C-N   | 5.45  | 1.41        | 1.33     |
| 24  | Q     | 284 | ALA  | N-CA  | -5.45 | 1.39        | 1.45     |
| 27  | T     | 127 | GLN  | C-N   | 5.45  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23  | P     | 199 | LEU  | N-CA  | -5.45 | 1.39        | 1.46     |
| 26  | S     | 417 | GLN  | CA-C  | 5.45  | 1.58        | 1.52     |
| 33  | Z     | 971 | ILE  | N-CA  | -5.45 | 1.39        | 1.46     |
| 13  | F     | 37  | GLY  | C-N   | 5.44  | 1.40        | 1.33     |
| 7   | 7     | 158 | PRO  | CA-C  | -5.44 | 1.42        | 1.52     |
| 21  | N     | 438 | ASP  | C-N   | 5.44  | 1.40        | 1.33     |
| 21  | N     | 657 | MET  | C-N   | 5.44  | 1.40        | 1.34     |
| 22  | O     | 205 | ILE  | C-N   | 5.44  | 1.40        | 1.33     |
| 24  | Q     | 127 | ARG  | C-O   | -5.44 | 1.17        | 1.24     |
| 2   | 2     | 28  | ASP  | N-CA  | -5.44 | 1.39        | 1.46     |
| 13  | F     | 50  | LYS  | CA-C  | -5.44 | 1.46        | 1.52     |
| 17  | J     | 310 | ILE  | CA-C  | -5.44 | 1.45        | 1.52     |
| 2   | 2     | 132 | LEU  | CA-C  | -5.44 | 1.45        | 1.52     |
| 7   | 7     | -6  | GLN  | N-CA  | -5.44 | 1.40        | 1.46     |
| 24  | Q     | 429 | LYS  | CA-C  | -5.44 | 1.46        | 1.52     |
| 11  | D     | 29  | ARG  | CA-C  | -5.44 | 1.45        | 1.52     |
| 16  | I     | 155 | SER  | C-N   | 5.44  | 1.39        | 1.33     |
| 29  | V     | 132 | LEU  | C-N   | 5.44  | 1.41        | 1.33     |
| 21  | N     | 155 | GLY  | CA-C  | 5.44  | 1.58        | 1.51     |
| 12  | E     | 62  | ASP  | CA-C  | -5.43 | 1.46        | 1.53     |
| 21  | N     | 707 | ASN  | C-N   | 5.43  | 1.40        | 1.33     |
| 23  | P     | 138 | ARG  | N-CA  | -5.43 | 1.39        | 1.46     |
| 24  | Q     | 204 | ALA  | CA-C  | -5.43 | 1.45        | 1.52     |
| 7   | 7     | 94  | GLN  | N-CA  | -5.43 | 1.39        | 1.46     |
| 16  | I     | 143 | PRO  | CA-C  | -5.43 | 1.46        | 1.52     |
| 15  | H     | 275 | ILE  | CA-C  | -5.43 | 1.46        | 1.52     |
| 12  | E     | 188 | HIS  | C-N   | 5.43  | 1.39        | 1.33     |
| 24  | Q     | 205 | ALA  | CA-C  | -5.43 | 1.45        | 1.52     |
| 25  | R     | 388 | VAL  | N-CA  | -5.43 | 1.39        | 1.46     |
| 27  | T     | 221 | ALA  | C-N   | 5.43  | 1.41        | 1.33     |
| 17  | J     | 191 | PRO  | C-N   | 5.42  | 1.41        | 1.33     |
| 24  | Q     | 165 | PHE  | CA-C  | 5.42  | 1.60        | 1.52     |
| 24  | Q     | 430 | ALA  | CA-C  | -5.42 | 1.45        | 1.52     |
| 7   | 7     | 27  | ARG  | N-CA  | -5.42 | 1.40        | 1.46     |
| 14  | G     | 175 | LEU  | C-O   | -5.42 | 1.17        | 1.24     |
| 19  | L     | 391 | ILE  | C-N   | 5.42  | 1.41        | 1.33     |
| 19  | L     | 412 | PRO  | N-CD  | 5.42  | 1.55        | 1.47     |
| 21  | N     | 435 | GLY  | C-O   | -5.42 | 1.16        | 1.23     |
| 33  | Z     | 138 | ARG  | N-CA  | -5.42 | 1.39        | 1.46     |
| 18  | K     | 183 | GLU  | N-CA  | -5.42 | 1.40        | 1.46     |
| 21  | N     | 544 | GLU  | C-N   | 5.42  | 1.40        | 1.33     |
| 17  | J     | 207 | ASP  | CA-C  | -5.42 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23  | P     | 211 | PRO  | C-N   | 5.42  | 1.41        | 1.33     |
| 8   | A     | 87  | ILE  | N-CA  | -5.42 | 1.40        | 1.46     |
| 8   | A     | 145 | SER  | CA-C  | -5.42 | 1.46        | 1.52     |
| 23  | P     | 110 | LEU  | C-N   | 5.41  | 1.41        | 1.34     |
| 25  | R     | 65  | TYR  | C-N   | 5.41  | 1.41        | 1.33     |
| 25  | R     | 176 | ARG  | C-N   | 5.41  | 1.40        | 1.33     |
| 33  | Z     | 230 | ILE  | C-N   | 5.41  | 1.41        | 1.33     |
| 14  | G     | 175 | LEU  | N-CA  | -5.41 | 1.39        | 1.46     |
| 15  | H     | 96  | PRO  | N-CD  | 5.41  | 1.55        | 1.47     |
| 18  | K     | 212 | TYR  | N-CA  | -5.41 | 1.39        | 1.46     |
| 21  | N     | 675 | VAL  | C-N   | 5.41  | 1.41        | 1.33     |
| 27  | T     | 178 | THR  | C-N   | 5.41  | 1.41        | 1.33     |
| 30  | W     | 166 | GLU  | C-N   | 5.41  | 1.41        | 1.33     |
| 17  | J     | 97  | ASP  | C-N   | 5.41  | 1.41        | 1.33     |
| 33  | Z     | 975 | SER  | N-CA  | -5.41 | 1.39        | 1.46     |
| 6   | 6     | 181 | SER  | N-CA  | 5.41  | 1.53        | 1.46     |
| 15  | H     | 368 | PRO  | N-CD  | 5.41  | 1.55        | 1.47     |
| 19  | L     | 362 | LYS  | C-N   | 5.41  | 1.40        | 1.33     |
| 21  | N     | 606 | VAL  | N-CA  | -5.41 | 1.38        | 1.46     |
| 26  | S     | 377 | TYR  | C-N   | 5.41  | 1.41        | 1.34     |
| 10  | C     | 99  | LEU  | N-CA  | -5.41 | 1.40        | 1.46     |
| 13  | F     | 11  | VAL  | CA-C  | -5.41 | 1.45        | 1.52     |
| 14  | G     | 144 | GLY  | C-O   | 5.41  | 1.30        | 1.23     |
| 12  | E     | 180 | GLN  | N-CA  | 5.40  | 1.53        | 1.46     |
| 28  | U     | 265 | LEU  | CA-C  | 5.40  | 1.60        | 1.52     |
| 33  | Z     | 305 | VAL  | CA-C  | -5.40 | 1.46        | 1.52     |
| 16  | I     | 121 | THR  | CA-C  | -5.40 | 1.46        | 1.52     |
| 11  | D     | 208 | LYS  | C-N   | 5.40  | 1.40        | 1.33     |
| 26  | S     | 270 | ALA  | N-CA  | -5.40 | 1.39        | 1.46     |
| 27  | T     | 40  | LEU  | CA-C  | -5.40 | 1.45        | 1.52     |
| 2   | 2     | 37  | ILE  | CA-C  | -5.40 | 1.47        | 1.52     |
| 5   | 5     | 28  | SER  | N-CA  | -5.40 | 1.39        | 1.46     |
| 12  | E     | 154 | GLN  | CA-C  | -5.40 | 1.46        | 1.52     |
| 21  | N     | 290 | LEU  | N-CA  | 5.40  | 1.53        | 1.46     |
| 1   | 1     | 32  | ASP  | C-N   | 5.40  | 1.41        | 1.33     |
| 20  | M     | 129 | LEU  | CA-C  | -5.40 | 1.46        | 1.52     |
| 21  | N     | 541 | ALA  | CA-C  | -5.40 | 1.45        | 1.52     |
| 29  | V     | 278 | LYS  | N-CA  | 5.40  | 1.52        | 1.46     |
| 21  | N     | 373 | VAL  | C-N   | 5.39  | 1.40        | 1.33     |
| 4   | 4     | 92  | ARG  | N-CA  | -5.39 | 1.39        | 1.46     |
| 6   | 6     | 89  | TYR  | C-N   | 5.39  | 1.40        | 1.33     |
| 8   | A     | 70  | SER  | CA-C  | 5.39  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 17  | J     | 342 | ASN  | CA-C  | -5.39 | 1.46        | 1.52     |
| 22  | O     | 3   | ASN  | CA-C  | -5.39 | 1.45        | 1.52     |
| 24  | Q     | 200 | ALA  | C-N   | 5.39  | 1.41        | 1.33     |
| 26  | S     | 154 | GLN  | CA-C  | -5.39 | 1.45        | 1.52     |
| 16  | I     | 422 | ARG  | N-CA  | -5.39 | 1.40        | 1.46     |
| 5   | 5     | 115 | VAL  | CA-C  | -5.38 | 1.46        | 1.52     |
| 25  | R     | 125 | GLU  | C-O   | 5.38  | 1.30        | 1.24     |
| 29  | V     | 67  | ASP  | CA-C  | 5.38  | 1.59        | 1.52     |
| 22  | O     | 164 | PRO  | CA-C  | -5.38 | 1.44        | 1.52     |
| 1   | 1     | 62  | HIS  | N-CA  | 5.38  | 1.53        | 1.46     |
| 6   | 6     | 2   | THR  | N-CA  | 5.38  | 1.52        | 1.46     |
| 7   | 7     | 152 | ASP  | C-N   | 5.38  | 1.40        | 1.33     |
| 14  | G     | 45  | VAL  | C-N   | 5.38  | 1.41        | 1.33     |
| 1   | 1     | 7   | THR  | CA-C  | -5.38 | 1.45        | 1.52     |
| 3   | 3     | 168 | ARG  | N-CA  | -5.38 | 1.39        | 1.46     |
| 14  | G     | 55  | SER  | N-CA  | -5.38 | 1.39        | 1.45     |
| 28  | U     | 15  | LEU  | N-CA  | -5.38 | 1.39        | 1.46     |
| 9   | B     | 99  | ARG  | N-CA  | -5.38 | 1.38        | 1.45     |
| 18  | K     | 97  | GLY  | N-CA  | 5.38  | 1.50        | 1.45     |
| 26  | S     | 353 | LYS  | N-CA  | 5.38  | 1.52        | 1.46     |
| 17  | J     | 235 | VAL  | C-N   | 5.38  | 1.41        | 1.33     |
| 3   | 3     | 2   | ILE  | C-N   | 5.37  | 1.40        | 1.33     |
| 3   | 3     | 188 | LYS  | CA-C  | -5.37 | 1.46        | 1.52     |
| 7   | 7     | 63  | VAL  | N-CA  | -5.37 | 1.40        | 1.46     |
| 14  | G     | 89  | ASN  | CA-C  | 5.37  | 1.59        | 1.52     |
| 22  | O     | 326 | HIS  | N-CA  | -5.37 | 1.39        | 1.46     |
| 30  | W     | 86  | HIS  | N-CA  | -5.37 | 1.37        | 1.46     |
| 33  | Z     | 778 | LEU  | N-CA  | 5.37  | 1.52        | 1.46     |
| 8   | A     | 210 | MET  | N-CA  | -5.37 | 1.39        | 1.46     |
| 27  | T     | 118 | ASN  | CA-C  | -5.37 | 1.46        | 1.52     |
| 24  | Q     | 7   | LYS  | N-CA  | -5.37 | 1.39        | 1.46     |
| 12  | E     | 50  | VAL  | C-N   | 5.37  | 1.41        | 1.33     |
| 18  | K     | 319 | ASN  | CA-C  | 5.37  | 1.59        | 1.52     |
| 25  | R     | 132 | GLN  | C-N   | 5.37  | 1.41        | 1.34     |
| 28  | U     | 204 | LEU  | N-CA  | -5.37 | 1.40        | 1.46     |
| 6   | 6     | 75  | LEU  | CA-C  | 5.37  | 1.59        | 1.52     |
| 22  | O     | 36  | LYS  | N-CA  | 5.37  | 1.52        | 1.45     |
| 16  | I     | 97  | GLU  | C-N   | 5.37  | 1.41        | 1.33     |
| 17  | J     | 297 | LEU  | C-N   | 5.36  | 1.41        | 1.33     |
| 21  | N     | 895 | LYS  | C-N   | 5.36  | 1.41        | 1.33     |
| 24  | Q     | 199 | THR  | CA-C  | -5.36 | 1.45        | 1.52     |
| 14  | G     | 29  | ALA  | CA-C  | -5.36 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | 6     | 209 | GLU  | CA-C  | -5.36 | 1.45        | 1.52     |
| 20  | M     | 115 | LYS  | N-CA  | -5.36 | 1.39        | 1.46     |
| 25  | R     | 320 | LYS  | N-CA  | -5.36 | 1.39        | 1.46     |
| 27  | T     | 173 | GLU  | N-CA  | -5.36 | 1.40        | 1.46     |
| 30  | W     | 3   | LEU  | C-N   | 5.36  | 1.40        | 1.33     |
| 28  | U     | 190 | LEU  | C-N   | 5.36  | 1.41        | 1.33     |
| 20  | M     | 398 | ALA  | CA-C  | -5.35 | 1.45        | 1.52     |
| 24  | Q     | 298 | ALA  | C-N   | 5.35  | 1.41        | 1.34     |
| 26  | S     | 213 | THR  | N-CA  | 5.35  | 1.52        | 1.46     |
| 9   | B     | 37  | ILE  | C-N   | 5.35  | 1.41        | 1.33     |
| 9   | B     | 119 | GLN  | C-N   | 5.35  | 1.41        | 1.33     |
| 21  | N     | 679 | ASN  | N-CA  | -5.35 | 1.39        | 1.46     |
| 22  | O     | 22  | LEU  | C-N   | 5.35  | 1.40        | 1.33     |
| 22  | O     | 307 | MET  | C-N   | -5.35 | 1.25        | 1.33     |
| 21  | N     | 568 | VAL  | C-N   | -5.35 | 1.26        | 1.33     |
| 22  | O     | 218 | SER  | N-CA  | -5.35 | 1.39        | 1.46     |
| 13  | F     | 147 | PHE  | N-CA  | -5.35 | 1.39        | 1.46     |
| 19  | L     | 412 | PRO  | C-N   | 5.35  | 1.41        | 1.33     |
| 31  | X     | 23  | LEU  | C-N   | 5.35  | 1.40        | 1.33     |
| 24  | Q     | 341 | THR  | N-CA  | -5.34 | 1.39        | 1.46     |
| 1   | 1     | 151 | THR  | C-N   | 5.34  | 1.40        | 1.33     |
| 10  | C     | 200 | THR  | CA-C  | 5.34  | 1.59        | 1.52     |
| 23  | P     | 361 | THR  | C-N   | 5.34  | 1.41        | 1.33     |
| 5   | 5     | 55  | TRP  | CA-C  | -5.34 | 1.45        | 1.52     |
| 22  | O     | 336 | LEU  | N-CA  | -5.34 | 1.39        | 1.46     |
| 21  | N     | 60  | MET  | C-N   | 5.34  | 1.40        | 1.33     |
| 30  | W     | 190 | ILE  | CA-C  | -5.34 | 1.46        | 1.52     |
| 33  | Z     | 976 | HIS  | N-CA  | -5.34 | 1.39        | 1.46     |
| 1   | 1     | 30  | VAL  | C-N   | 5.33  | 1.39        | 1.33     |
| 7   | 7     | 65  | GLU  | CA-C  | -5.33 | 1.45        | 1.52     |
| 9   | B     | 164 | ILE  | CA-C  | -5.33 | 1.46        | 1.52     |
| 24  | Q     | 381 | ILE  | N-CA  | -5.33 | 1.40        | 1.46     |
| 15  | H     | 448 | ASP  | N-CA  | -5.33 | 1.40        | 1.46     |
| 18  | K     | 241 | GLU  | N-CA  | -5.33 | 1.40        | 1.46     |
| 18  | K     | 347 | ARG  | C-N   | 5.33  | 1.41        | 1.33     |
| 20  | M     | 338 | LEU  | CA-C  | -5.33 | 1.46        | 1.52     |
| 4   | 4     | 22  | ARG  | N-CA  | -5.33 | 1.39        | 1.46     |
| 12  | E     | 139 | GLY  | C-N   | 5.33  | 1.40        | 1.33     |
| 25  | R     | 242 | GLU  | N-CA  | -5.33 | 1.38        | 1.46     |
| 33  | Z     | 473 | LEU  | C-N   | 5.33  | 1.41        | 1.33     |
| 33  | Z     | 776 | VAL  | CA-C  | -5.33 | 1.47        | 1.52     |
| 21  | N     | 298 | TYR  | N-CA  | 5.33  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | 1     | 11  | GLY  | CA-C  | -5.33 | 1.44        | 1.51     |
| 21  | N     | 588 | VAL  | C-N   | 5.33  | 1.40        | 1.33     |
| 24  | Q     | 118 | CYS  | C-N   | 5.33  | 1.41        | 1.33     |
| 29  | V     | 23  | THR  | N-CA  | 5.33  | 1.56        | 1.46     |
| 33  | Z     | 424 | SER  | CA-C  | -5.33 | 1.46        | 1.52     |
| 4   | 4     | 72  | TYR  | N-CA  | -5.33 | 1.39        | 1.46     |
| 17  | J     | 227 | SER  | CA-C  | -5.33 | 1.45        | 1.52     |
| 18  | K     | 195 | ALA  | N-CA  | -5.33 | 1.39        | 1.46     |
| 28  | U     | 120 | LEU  | N-CA  | -5.33 | 1.39        | 1.46     |
| 31  | X     | 87  | PHE  | CA-C  | -5.33 | 1.46        | 1.52     |
| 11  | D     | 200 | LEU  | CA-C  | -5.32 | 1.45        | 1.52     |
| 12  | E     | 189 | SER  | CA-C  | -5.32 | 1.47        | 1.53     |
| 21  | N     | 736 | PHE  | C-N   | 5.32  | 1.41        | 1.33     |
| 29  | V     | 157 | ARG  | N-CA  | -5.32 | 1.39        | 1.46     |
| 26  | S     | 404 | LEU  | C-N   | 5.32  | 1.41        | 1.33     |
| 33  | Z     | 123 | ALA  | N-CA  | 5.32  | 1.52        | 1.46     |
| 21  | N     | 471 | TYR  | CA-C  | -5.32 | 1.45        | 1.52     |
| 21  | N     | 503 | THR  | C-N   | 5.32  | 1.41        | 1.34     |
| 9   | B     | 95  | THR  | N-CA  | -5.32 | 1.39        | 1.46     |
| 9   | B     | 15  | SER  | C-N   | 5.31  | 1.40        | 1.33     |
| 33  | Z     | 868 | ASN  | CA-C  | -5.31 | 1.46        | 1.52     |
| 20  | M     | 403 | LEU  | CA-C  | -5.31 | 1.46        | 1.52     |
| 21  | N     | 153 | ALA  | C-O   | 5.31  | 1.30        | 1.24     |
| 25  | R     | 413 | LYS  | CA-C  | -5.31 | 1.45        | 1.52     |
| 13  | F     | 225 | TYR  | N-CA  | -5.31 | 1.39        | 1.46     |
| 26  | S     | 257 | LEU  | C-N   | 5.31  | 1.41        | 1.33     |
| 4   | 4     | 24  | ILE  | N-CA  | -5.31 | 1.40        | 1.46     |
| 9   | B     | 3   | ASP  | CA-C  | -5.31 | 1.45        | 1.52     |
| 14  | G     | 176 | GLU  | CA-C  | -5.31 | 1.45        | 1.52     |
| 2   | 2     | 88  | PHE  | N-CA  | -5.31 | 1.40        | 1.46     |
| 15  | H     | 296 | GLU  | CA-C  | -5.31 | 1.45        | 1.52     |
| 19  | L     | 176 | GLY  | N-CA  | -5.31 | 1.40        | 1.44     |
| 33  | Z     | 424 | SER  | C-O   | -5.31 | 1.17        | 1.24     |
| 33  | Z     | 894 | MET  | C-N   | 5.31  | 1.40        | 1.33     |
| 21  | N     | 230 | VAL  | N-CA  | -5.31 | 1.40        | 1.46     |
| 6   | 6     | 25  | SER  | C-N   | 5.30  | 1.41        | 1.33     |
| 20  | M     | 120 | LYS  | N-CA  | -5.30 | 1.39        | 1.46     |
| 24  | Q     | 304 | GLU  | CA-C  | -5.30 | 1.46        | 1.52     |
| 27  | T     | 181 | LEU  | N-CA  | -5.30 | 1.40        | 1.46     |
| 6   | 6     | 76  | SER  | N-CA  | -5.30 | 1.39        | 1.45     |
| 20  | M     | 118 | VAL  | C-O   | -5.30 | 1.18        | 1.24     |
| 24  | Q     | 176 | ASP  | C-N   | 5.30  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | 1     | 124 | TYR  | N-CA  | -5.30 | 1.39        | 1.46     |
| 16  | I     | 247 | ILE  | C-N   | 5.30  | 1.40        | 1.33     |
| 33  | Z     | 915 | ALA  | N-CA  | -5.30 | 1.39        | 1.46     |
| 14  | G     | 119 | VAL  | C-N   | 5.30  | 1.41        | 1.34     |
| 25  | R     | 291 | SER  | N-CA  | -5.30 | 1.40        | 1.46     |
| 11  | D     | 27  | VAL  | C-N   | 5.30  | 1.41        | 1.34     |
| 18  | K     | 295 | ILE  | N-CA  | -5.30 | 1.40        | 1.46     |
| 21  | N     | 763 | GLY  | CA-C  | -5.30 | 1.42        | 1.51     |
| 23  | P     | 431 | HIS  | C-N   | 5.29  | 1.40        | 1.33     |
| 31  | X     | 103 | GLU  | CA-C  | 5.29  | 1.60        | 1.53     |
| 13  | F     | 118 | LYS  | CA-C  | -5.29 | 1.45        | 1.52     |
| 21  | N     | 90  | ASP  | C-N   | 5.29  | 1.39        | 1.34     |
| 29  | V     | 194 | ARG  | CA-C  | -5.29 | 1.45        | 1.52     |
| 8   | A     | 88  | PRO  | N-CD  | 5.29  | 1.55        | 1.47     |
| 22  | O     | 121 | ASP  | C-N   | 5.29  | 1.40        | 1.33     |
| 26  | S     | 442 | PHE  | CA-C  | -5.29 | 1.46        | 1.52     |
| 33  | Z     | 486 | SER  | C-O   | -5.29 | 1.17        | 1.24     |
| 24  | Q     | 149 | LYS  | N-CA  | 5.29  | 1.53        | 1.46     |
| 28  | U     | 53  | ALA  | CA-C  | -5.29 | 1.46        | 1.52     |
| 33  | Z     | 886 | VAL  | C-N   | 5.29  | 1.41        | 1.33     |
| 3   | 3     | 127 | PHE  | N-CA  | -5.29 | 1.39        | 1.45     |
| 33  | Z     | 52  | LEU  | CA-C  | -5.29 | 1.45        | 1.52     |
| 1   | 1     | 187 | ILE  | N-CA  | -5.28 | 1.40        | 1.46     |
| 11  | D     | 165 | GLY  | C-N   | 5.28  | 1.40        | 1.33     |
| 24  | Q     | 395 | GLY  | CA-C  | -5.28 | 1.44        | 1.51     |
| 19  | L     | 98  | LEU  | CA-C  | 5.28  | 1.60        | 1.52     |
| 21  | N     | 660 | LEU  | CA-C  | -5.28 | 1.45        | 1.52     |
| 22  | O     | 47  | LYS  | N-CA  | 5.28  | 1.52        | 1.46     |
| 23  | P     | 315 | GLN  | CA-C  | -5.28 | 1.46        | 1.52     |
| 26  | S     | 243 | ASN  | C-N   | 5.28  | 1.41        | 1.33     |
| 16  | I     | 359 | LYS  | C-N   | 5.28  | 1.41        | 1.33     |
| 9   | B     | 172 | LYS  | C-N   | 5.28  | 1.40        | 1.33     |
| 11  | D     | 169 | LYS  | CA-C  | -5.28 | 1.46        | 1.52     |
| 21  | N     | 731 | VAL  | CA-C  | -5.28 | 1.46        | 1.52     |
| 31  | X     | 101 | LEU  | C-N   | 5.28  | 1.40        | 1.33     |
| 33  | Z     | 265 | LEU  | C-N   | 5.28  | 1.41        | 1.33     |
| 12  | E     | 42  | THR  | CA-C  | -5.28 | 1.45        | 1.52     |
| 17  | J     | 231 | ARG  | C-O   | 5.28  | 1.30        | 1.24     |
| 25  | R     | 161 | ALA  | N-CA  | -5.28 | 1.39        | 1.46     |
| 30  | W     | 61  | VAL  | CA-C  | -5.28 | 1.46        | 1.52     |
| 8   | A     | 224 | GLU  | N-CA  | -5.27 | 1.39        | 1.46     |
| 1   | 1     | 56  | ALA  | N-CA  | 5.27  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15  | H     | 265 | ASN  | N-CA  | -5.27 | 1.40        | 1.46     |
| 24  | Q     | 249 | LEU  | C-N   | 5.27  | 1.40        | 1.33     |
| 9   | B     | 215 | GLY  | CA-C  | -5.27 | 1.44        | 1.51     |
| 9   | B     | 51  | SER  | CA-C  | -5.27 | 1.46        | 1.52     |
| 12  | E     | 83  | ALA  | C-N   | 5.27  | 1.41        | 1.34     |
| 25  | R     | 77  | SER  | CA-C  | 5.27  | 1.59        | 1.52     |
| 5   | 5     | 31  | VAL  | C-N   | 5.27  | 1.40        | 1.33     |
| 21  | N     | 658 | ILE  | C-N   | 5.27  | 1.41        | 1.33     |
| 13  | F     | 64  | ILE  | CA-C  | -5.26 | 1.45        | 1.52     |
| 24  | Q     | 422 | VAL  | CA-C  | 5.26  | 1.59        | 1.52     |
| 1   | 1     | 79  | ALA  | N-CA  | -5.26 | 1.39        | 1.46     |
| 6   | 6     | 58  | ARG  | CA-C  | -5.26 | 1.46        | 1.52     |
| 1   | 1     | 132 | THR  | C-N   | 5.26  | 1.41        | 1.33     |
| 8   | A     | 244 | ARG  | C-N   | 5.26  | 1.40        | 1.33     |
| 14  | G     | 228 | LYS  | CA-C  | -5.26 | 1.46        | 1.52     |
| 15  | H     | 245 | GLY  | C-O   | -5.26 | 1.17        | 1.23     |
| 17  | J     | 153 | LEU  | C-N   | 5.26  | 1.40        | 1.33     |
| 17  | J     | 208 | CYS  | CA-C  | -5.26 | 1.46        | 1.52     |
| 19  | L     | 300 | GLU  | N-CA  | -5.26 | 1.39        | 1.46     |
| 21  | N     | 311 | ILE  | N-CA  | -5.26 | 1.39        | 1.46     |
| 33  | Z     | 845 | LEU  | CA-C  | -5.26 | 1.46        | 1.52     |
| 19  | L     | 280 | MET  | CA-C  | -5.26 | 1.46        | 1.52     |
| 20  | M     | 163 | PHE  | N-CA  | -5.26 | 1.39        | 1.45     |
| 22  | O     | 26  | PHE  | C-O   | -5.26 | 1.18        | 1.24     |
| 24  | Q     | 351 | ILE  | CA-C  | -5.25 | 1.46        | 1.52     |
| 17  | J     | 230 | VAL  | N-CA  | -5.25 | 1.40        | 1.46     |
| 20  | M     | 211 | GLY  | CA-C  | 5.25  | 1.59        | 1.51     |
| 5   | 5     | 202 | GLU  | N-CA  | -5.25 | 1.40        | 1.46     |
| 7   | 7     | 154 | GLU  | CA-C  | 5.25  | 1.59        | 1.52     |
| 8   | A     | 153 | SER  | C-N   | 5.25  | 1.40        | 1.33     |
| 22  | O     | 118 | GLY  | N-CA  | 5.25  | 1.52        | 1.45     |
| 31  | X     | 79  | LYS  | C-N   | 5.25  | 1.41        | 1.33     |
| 8   | A     | 228 | ALA  | C-N   | 5.25  | 1.40        | 1.33     |
| 22  | O     | 80  | LYS  | C-N   | 5.25  | 1.40        | 1.33     |
| 1   | 1     | 91  | ASP  | CA-C  | -5.25 | 1.45        | 1.52     |
| 7   | 7     | 144 | ASN  | C-O   | -5.25 | 1.19        | 1.24     |
| 10  | C     | 29  | ILE  | C-N   | 5.25  | 1.41        | 1.33     |
| 8   | A     | 72  | ILE  | N-CA  | -5.24 | 1.40        | 1.46     |
| 14  | G     | 247 | ASN  | N-CA  | -5.24 | 1.40        | 1.46     |
| 16  | I     | 293 | ASP  | C-N   | 5.24  | 1.40        | 1.33     |
| 18  | K     | 132 | LYS  | C-N   | 5.24  | 1.39        | 1.34     |
| 23  | P     | 414 | GLU  | C-N   | 5.24  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | 1     | 186 | LEU  | C-O   | -5.24 | 1.17        | 1.24     |
| 1   | 1     | 190 | PRO  | C-N   | 5.24  | 1.40        | 1.33     |
| 8   | A     | 79  | ILE  | N-CA  | -5.24 | 1.39        | 1.46     |
| 12  | E     | 26  | TYR  | CA-C  | -5.24 | 1.45        | 1.52     |
| 17  | J     | 244 | ILE  | CA-C  | -5.24 | 1.46        | 1.52     |
| 18  | K     | 299 | LEU  | N-CA  | -5.24 | 1.40        | 1.46     |
| 21  | N     | 384 | LYS  | CA-C  | -5.24 | 1.46        | 1.52     |
| 27  | T     | 170 | ASN  | C-N   | 5.24  | 1.40        | 1.33     |
| 17  | J     | 373 | ARG  | N-CA  | -5.24 | 1.39        | 1.46     |
| 20  | M     | 303 | ARG  | CA-C  | -5.24 | 1.46        | 1.52     |
| 21  | N     | 587 | ALA  | CA-C  | -5.24 | 1.46        | 1.52     |
| 1   | 1     | 100 | ALA  | N-CA  | -5.24 | 1.39        | 1.46     |
| 25  | R     | 123 | ASP  | N-CA  | -5.24 | 1.40        | 1.46     |
| 33  | Z     | 244 | ARG  | CA-C  | -5.24 | 1.46        | 1.52     |
| 4   | 4     | 96  | PRO  | C-N   | 5.24  | 1.40        | 1.33     |
| 21  | N     | 203 | ARG  | C-O   | -5.24 | 1.18        | 1.24     |
| 22  | O     | 171 | PHE  | CA-C  | 5.24  | 1.59        | 1.52     |
| 30  | W     | 140 | ASP  | C-O   | 5.24  | 1.29        | 1.24     |
| 7   | 7     | -1  | GLY  | C-N   | 5.23  | 1.41        | 1.33     |
| 23  | P     | 376 | THR  | C-O   | -5.23 | 1.18        | 1.24     |
| 19  | L     | 251 | ILE  | C-N   | 5.23  | 1.38        | 1.33     |
| 15  | H     | 415 | THR  | C-N   | 5.23  | 1.41        | 1.33     |
| 16  | I     | 353 | PRO  | N-CD  | 5.23  | 1.55        | 1.47     |
| 22  | O     | 18  | ALA  | CA-C  | -5.23 | 1.46        | 1.52     |
| 5   | 5     | 83  | LEU  | N-CA  | -5.23 | 1.40        | 1.46     |
| 26  | S     | 408 | CYS  | C-O   | -5.23 | 1.18        | 1.24     |
| 29  | V     | 57  | PHE  | N-CA  | -5.23 | 1.39        | 1.46     |
| 32  | Y     | 82  | ASP  | CA-C  | -5.23 | 1.46        | 1.52     |
| 7   | 7     | 116 | ASP  | C-N   | 5.23  | 1.40        | 1.33     |
| 21  | N     | 31  | VAL  | N-CA  | -5.23 | 1.40        | 1.46     |
| 24  | Q     | 52  | ASN  | C-N   | 5.23  | 1.41        | 1.34     |
| 18  | K     | 211 | LEU  | N-CA  | 5.23  | 1.52        | 1.46     |
| 11  | D     | 119 | ARG  | C-O   | -5.22 | 1.18        | 1.24     |
| 15  | H     | 194 | SER  | CA-C  | -5.22 | 1.48        | 1.53     |
| 21  | N     | 102 | VAL  | C-N   | 5.22  | 1.40        | 1.33     |
| 22  | O     | 267 | ASP  | N-CA  | 5.22  | 1.52        | 1.46     |
| 33  | Z     | 115 | LEU  | C-N   | 5.22  | 1.40        | 1.33     |
| 4   | 4     | 42  | LEU  | N-CA  | -5.22 | 1.39        | 1.45     |
| 11  | D     | 23  | ALA  | CA-C  | -5.22 | 1.46        | 1.52     |
| 18  | K     | 179 | MET  | N-CA  | -5.22 | 1.40        | 1.46     |
| 20  | M     | 384 | ASP  | N-CA  | 5.22  | 1.52        | 1.46     |
| 15  | H     | 280 | VAL  | CA-C  | 5.22  | 1.58        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 17  | J     | 28  | GLN  | N-CA  | 5.22  | 1.52        | 1.46     |
| 33  | Z     | 89  | LEU  | C-N   | 5.22  | 1.40        | 1.33     |
| 22  | O     | 334 | LEU  | N-CA  | -5.22 | 1.40        | 1.46     |
| 27  | T     | 141 | LEU  | C-O   | -5.22 | 1.18        | 1.24     |
| 31  | X     | 35  | ILE  | N-CA  | -5.22 | 1.39        | 1.46     |
| 10  | C     | 136 | ILE  | C-O   | -5.22 | 1.18        | 1.24     |
| 33  | Z     | 74  | SER  | N-CA  | -5.22 | 1.39        | 1.46     |
| 15  | H     | 410 | LEU  | N-CA  | 5.21  | 1.53        | 1.46     |
| 18  | K     | 221 | MET  | CA-C  | -5.21 | 1.46        | 1.52     |
| 8   | A     | 169 | THR  | C-N   | 5.21  | 1.40        | 1.33     |
| 18  | K     | 275 | ASP  | C-N   | -5.21 | 1.27        | 1.33     |
| 26  | S     | 382 | ARG  | N-CA  | -5.21 | 1.40        | 1.46     |
| 33  | Z     | 486 | SER  | N-CA  | -5.21 | 1.39        | 1.46     |
| 5   | 5     | 117 | SER  | C-O   | 5.21  | 1.30        | 1.24     |
| 16  | I     | 314 | ASP  | CA-C  | -5.21 | 1.45        | 1.52     |
| 17  | J     | 26  | LYS  | C-O   | -5.21 | 1.18        | 1.24     |
| 18  | K     | 312 | VAL  | CA-C  | -5.21 | 1.46        | 1.52     |
| 19  | L     | 382 | MET  | N-CA  | -5.21 | 1.39        | 1.46     |
| 7   | 7     | 23  | GLY  | CA-C  | -5.21 | 1.44        | 1.51     |
| 18  | K     | 164 | ASN  | C-N   | 5.21  | 1.40        | 1.33     |
| 33  | Z     | 839 | SER  | C-N   | 5.21  | 1.41        | 1.33     |
| 13  | F     | 49  | LEU  | N-CA  | -5.21 | 1.39        | 1.46     |
| 28  | U     | 172 | GLU  | C-N   | 5.21  | 1.41        | 1.33     |
| 2   | 2     | 70  | THR  | N-CA  | -5.21 | 1.39        | 1.46     |
| 11  | D     | 131 | VAL  | CA-C  | -5.21 | 1.46        | 1.52     |
| 21  | N     | 902 | VAL  | N-CA  | -5.21 | 1.39        | 1.46     |
| 17  | J     | 131 | ASP  | N-CA  | 5.21  | 1.51        | 1.46     |
| 18  | K     | 329 | LEU  | CA-C  | -5.21 | 1.45        | 1.52     |
| 1   | 1     | 172 | VAL  | N-CA  | -5.20 | 1.39        | 1.46     |
| 4   | 4     | 34  | THR  | CA-C  | -5.20 | 1.46        | 1.52     |
| 19  | L     | 188 | GLU  | N-CA  | -5.20 | 1.40        | 1.46     |
| 21  | N     | 916 | LEU  | C-N   | 5.20  | 1.40        | 1.33     |
| 22  | O     | 255 | LEU  | N-CA  | -5.20 | 1.40        | 1.46     |
| 33  | Z     | 109 | PRO  | CA-C  | 5.20  | 1.59        | 1.52     |
| 4   | 4     | 120 | TYR  | N-CA  | 5.20  | 1.53        | 1.46     |
| 16  | I     | 391 | ASP  | N-CA  | -5.20 | 1.39        | 1.46     |
| 29  | V     | 255 | ILE  | N-CA  | 5.20  | 1.52        | 1.46     |
| 33  | Z     | 89  | LEU  | C-O   | -5.20 | 1.18        | 1.24     |
| 21  | N     | 273 | LEU  | C-N   | 5.20  | 1.40        | 1.33     |
| 22  | O     | 23  | HIS  | N-CA  | -5.20 | 1.39        | 1.46     |
| 26  | S     | 414 | ASP  | C-N   | 5.20  | 1.40        | 1.33     |
| 18  | K     | 149 | ILE  | N-CA  | -5.20 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 18  | K     | 424 | PHE  | C-N   | 5.20  | 1.40        | 1.33     |
| 27  | T     | 270 | ILE  | C-N   | 5.19  | 1.41        | 1.33     |
| 9   | B     | 135 | LEU  | C-N   | 5.19  | 1.40        | 1.33     |
| 11  | D     | 151 | GLU  | CA-C  | 5.19  | 1.57        | 1.52     |
| 11  | D     | 184 | PRO  | N-CD  | 5.19  | 1.55        | 1.47     |
| 19  | L     | 369 | LYS  | C-N   | 5.19  | 1.39        | 1.33     |
| 28  | U     | 305 | ARG  | N-CA  | -5.19 | 1.40        | 1.46     |
| 7   | 7     | 177 | TYR  | CA-C  | -5.19 | 1.45        | 1.52     |
| 15  | H     | 346 | ARG  | C-O   | 5.19  | 1.30        | 1.23     |
| 19  | L     | 426 | LYS  | N-CA  | -5.19 | 1.39        | 1.46     |
| 6   | 6     | 206 | GLU  | CA-C  | -5.19 | 1.46        | 1.52     |
| 19  | L     | 308 | LEU  | CA-C  | -5.19 | 1.46        | 1.52     |
| 33  | Z     | 406 | TRP  | C-O   | -5.19 | 1.18        | 1.24     |
| 33  | Z     | 422 | ILE  | N-CA  | -5.19 | 1.40        | 1.46     |
| 15  | H     | 209 | SER  | N-CA  | 5.19  | 1.51        | 1.46     |
| 18  | K     | 239 | GLY  | CA-C  | -5.19 | 1.44        | 1.51     |
| 28  | U     | 168 | GLU  | N-CA  | -5.19 | 1.40        | 1.46     |
| 8   | A     | 238 | ALA  | N-CA  | 5.19  | 1.52        | 1.46     |
| 14  | G     | 27  | VAL  | CA-C  | 5.19  | 1.59        | 1.52     |
| 16  | I     | 101 | GLY  | CA-C  | -5.19 | 1.44        | 1.51     |
| 16  | I     | 166 | PRO  | N-CD  | 5.19  | 1.55        | 1.47     |
| 26  | S     | 245 | GLY  | N-CA  | -5.19 | 1.39        | 1.45     |
| 12  | E     | 223 | THR  | C-O   | -5.18 | 1.17        | 1.23     |
| 14  | G     | 178 | LEU  | N-CA  | -5.18 | 1.40        | 1.46     |
| 33  | Z     | 284 | LEU  | C-N   | -5.18 | 1.26        | 1.33     |
| 33  | Z     | 748 | LEU  | N-CA  | -5.18 | 1.39        | 1.46     |
| 33  | Z     | 845 | LEU  | C-N   | 5.18  | 1.40        | 1.33     |
| 24  | Q     | 46  | VAL  | CA-C  | -5.18 | 1.46        | 1.52     |
| 16  | I     | 306 | MET  | C-O   | -5.18 | 1.18        | 1.24     |
| 17  | J     | 251 | ASP  | N-CA  | -5.18 | 1.40        | 1.46     |
| 21  | N     | 425 | ASN  | N-CA  | 5.18  | 1.52        | 1.46     |
| 21  | N     | 491 | GLY  | CA-C  | -5.18 | 1.44        | 1.51     |
| 26  | S     | 173 | LEU  | CA-C  | -5.18 | 1.48        | 1.53     |
| 29  | V     | 188 | LEU  | N-CA  | -5.18 | 1.40        | 1.46     |
| 27  | T     | 210 | PHE  | CA-C  | -5.17 | 1.45        | 1.52     |
| 24  | Q     | 309 | ARG  | CA-C  | -5.17 | 1.47        | 1.53     |
| 5   | 5     | 110 | PRO  | CA-C  | -5.17 | 1.46        | 1.52     |
| 24  | Q     | 257 | LYS  | CA-C  | -5.17 | 1.46        | 1.52     |
| 24  | Q     | 282 | LEU  | C-N   | 5.17  | 1.41        | 1.34     |
| 33  | Z     | 826 | ARG  | C-N   | 5.17  | 1.40        | 1.34     |
| 21  | N     | 268 | GLN  | N-CA  | -5.17 | 1.39        | 1.46     |
| 27  | T     | 125 | GLU  | N-CA  | -5.17 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | M     | 430 | VAL  | CA-C  | -5.16 | 1.48        | 1.52     |
| 26  | S     | 353 | LYS  | C-O   | -5.16 | 1.18        | 1.24     |
| 31  | X     | 80  | SER  | CA-C  | -5.16 | 1.46        | 1.53     |
| 17  | J     | 391 | ASN  | C-N   | 5.16  | 1.41        | 1.34     |
| 21  | N     | 408 | LEU  | C-N   | 5.16  | 1.40        | 1.33     |
| 2   | 2     | 55  | VAL  | CA-C  | -5.16 | 1.46        | 1.52     |
| 6   | 6     | 86  | HIS  | C-N   | 5.16  | 1.40        | 1.33     |
| 21  | N     | 561 | GLY  | C-N   | 5.16  | 1.40        | 1.33     |
| 29  | V     | 143 | PRO  | C-N   | 5.16  | 1.40        | 1.33     |
| 16  | I     | 92  | GLU  | C-N   | 5.16  | 1.41        | 1.33     |
| 19  | L     | 347 | VAL  | N-CA  | -5.16 | 1.39        | 1.46     |
| 23  | P     | 104 | LEU  | CA-C  | -5.16 | 1.46        | 1.52     |
| 24  | Q     | 391 | ASP  | CA-C  | -5.16 | 1.46        | 1.53     |
| 25  | R     | 187 | VAL  | C-N   | 5.16  | 1.40        | 1.33     |
| 4   | 4     | 44  | SER  | N-CA  | 5.16  | 1.51        | 1.45     |
| 18  | K     | 372 | ILE  | C-N   | 5.16  | 1.40        | 1.33     |
| 22  | O     | 314 | SER  | CA-C  | -5.16 | 1.46        | 1.52     |
| 6   | 6     | 32  | PRO  | N-CA  | -5.16 | 1.41        | 1.47     |
| 16  | I     | 164 | ALA  | C-O   | 5.16  | 1.31        | 1.23     |
| 31  | X     | 52  | PRO  | CA-C  | -5.16 | 1.47        | 1.52     |
| 18  | K     | 329 | LEU  | C-N   | 5.15  | 1.40        | 1.33     |
| 4   | 4     | 172 | PRO  | N-CA  | 5.15  | 1.52        | 1.47     |
| 11  | D     | 158 | SER  | C-N   | -5.15 | 1.26        | 1.33     |
| 12  | E     | 188 | HIS  | N-CA  | -5.15 | 1.39        | 1.45     |
| 13  | F     | 128 | TYR  | N-CA  | -5.15 | 1.40        | 1.46     |
| 25  | R     | 283 | THR  | CA-C  | -5.15 | 1.46        | 1.52     |
| 26  | S     | 293 | ILE  | C-O   | -5.15 | 1.18        | 1.24     |
| 30  | W     | 161 | VAL  | C-N   | 5.15  | 1.41        | 1.33     |
| 6   | 6     | 7   | ALA  | N-CA  | -5.15 | 1.39        | 1.46     |
| 29  | V     | 138 | ALA  | CA-C  | -5.15 | 1.46        | 1.52     |
| 30  | W     | 181 | LEU  | CA-C  | -5.15 | 1.46        | 1.52     |
| 10  | C     | 148 | LEU  | C-N   | 5.15  | 1.40        | 1.33     |
| 17  | J     | 273 | LEU  | CA-C  | -5.15 | 1.45        | 1.52     |
| 21  | N     | 905 | LEU  | CA-C  | -5.15 | 1.46        | 1.52     |
| 25  | R     | 54  | ILE  | CA-C  | -5.15 | 1.46        | 1.52     |
| 13  | F     | 126 | ARG  | C-N   | 5.14  | 1.40        | 1.33     |
| 14  | G     | 6   | GLY  | CA-C  | -5.14 | 1.44        | 1.51     |
| 22  | O     | 357 | ILE  | C-N   | 5.14  | 1.40        | 1.33     |
| 25  | R     | 251 | THR  | N-CA  | -5.14 | 1.40        | 1.46     |
| 30  | W     | 91  | LEU  | N-CA  | -5.14 | 1.40        | 1.46     |
| 33  | Z     | 114 | SER  | C-N   | 5.14  | 1.40        | 1.33     |
| 17  | J     | 51  | LEU  | C-O   | 5.14  | 1.30        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 5     | 168 | ASP  | C-N   | -5.14 | 1.26        | 1.33     |
| 4   | 4     | 47  | GLY  | CA-C  | 5.14  | 1.59        | 1.52     |
| 7   | 7     | 101 | PRO  | CA-C  | -5.14 | 1.46        | 1.52     |
| 25  | R     | 29  | LYS  | N-CA  | -5.14 | 1.39        | 1.46     |
| 27  | T     | 127 | GLN  | CA-C  | -5.14 | 1.46        | 1.52     |
| 29  | V     | 59  | ASP  | C-N   | 5.14  | 1.42        | 1.34     |
| 13  | F     | 162 | GLY  | C-N   | 5.14  | 1.40        | 1.33     |
| 28  | U     | 36  | VAL  | C-N   | 5.14  | 1.41        | 1.33     |
| 30  | W     | 160 | ALA  | C-N   | 5.14  | 1.40        | 1.34     |
| 7   | 7     | 173 | MET  | CA-C  | -5.14 | 1.45        | 1.52     |
| 10  | C     | 158 | THR  | C-N   | 5.14  | 1.38        | 1.33     |
| 11  | D     | 150 | THR  | C-O   | -5.14 | 1.17        | 1.23     |
| 15  | H     | 288 | ALA  | N-CA  | -5.14 | 1.39        | 1.46     |
| 26  | S     | 170 | TYR  | CA-C  | 5.14  | 1.59        | 1.52     |
| 26  | S     | 324 | MET  | C-N   | 5.14  | 1.41        | 1.33     |
| 27  | T     | 65  | GLY  | C-N   | 5.14  | 1.40        | 1.33     |
| 29  | V     | 210 | THR  | CA-C  | 5.14  | 1.59        | 1.52     |
| 4   | 4     | 20  | VAL  | CA-C  | -5.13 | 1.46        | 1.52     |
| 16  | I     | 385 | ASP  | N-CA  | -5.13 | 1.40        | 1.46     |
| 21  | N     | 413 | ALA  | C-N   | 5.13  | 1.39        | 1.33     |
| 33  | Z     | 486 | SER  | C-N   | 5.13  | 1.40        | 1.33     |
| 25  | R     | 408 | ASP  | C-N   | 5.13  | 1.40        | 1.33     |
| 28  | U     | 56  | PHE  | N-CA  | -5.13 | 1.39        | 1.46     |
| 33  | Z     | 981 | VAL  | CA-C  | -5.13 | 1.46        | 1.52     |
| 7   | 7     | 143 | ALA  | CA-C  | -5.13 | 1.46        | 1.52     |
| 11  | D     | 76  | SER  | CA-C  | -5.13 | 1.46        | 1.52     |
| 13  | F     | 118 | LYS  | N-CA  | -5.13 | 1.40        | 1.46     |
| 25  | R     | 337 | VAL  | C-N   | 5.13  | 1.40        | 1.33     |
| 26  | S     | 128 | ILE  | C-N   | 5.13  | 1.40        | 1.33     |
| 12  | E     | 108 | ASN  | C-N   | 5.13  | 1.40        | 1.33     |
| 19  | L     | 96  | LYS  | N-CA  | 5.13  | 1.52        | 1.46     |
| 25  | R     | 362 | ALA  | CA-C  | -5.13 | 1.45        | 1.52     |
| 27  | T     | 171 | ILE  | CA-C  | -5.13 | 1.46        | 1.52     |
| 7   | 7     | 81  | PRO  | N-CD  | 5.12  | 1.54        | 1.47     |
| 10  | C     | 174 | THR  | CA-C  | 5.12  | 1.59        | 1.52     |
| 17  | J     | 64  | LEU  | CA-C  | -5.12 | 1.46        | 1.52     |
| 33  | Z     | 812 | ILE  | C-N   | 5.12  | 1.40        | 1.33     |
| 12  | E     | 86  | ARG  | N-CA  | -5.12 | 1.40        | 1.46     |
| 21  | N     | 399 | PHE  | CA-C  | -5.12 | 1.45        | 1.52     |
| 33  | Z     | 105 | LYS  | CA-C  | -5.12 | 1.46        | 1.53     |
| 9   | B     | 56  | ALA  | CA-C  | -5.12 | 1.46        | 1.53     |
| 19  | L     | 379 | ALA  | N-CA  | -5.12 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | M     | 345 | ARG  | C-N   | 5.12  | 1.40        | 1.33     |
| 24  | Q     | 121 | SER  | N-CA  | -5.12 | 1.40        | 1.46     |
| 24  | Q     | 321 | TYR  | C-N   | 5.12  | 1.40        | 1.33     |
| 10  | C     | 27  | GLU  | C-N   | 5.12  | 1.40        | 1.33     |
| 12  | E     | 55  | THR  | C-N   | 5.12  | 1.39        | 1.33     |
| 12  | E     | 57  | PRO  | N-CD  | 5.12  | 1.54        | 1.47     |
| 14  | G     | 124 | LEU  | C-N   | 5.12  | 1.41        | 1.33     |
| 24  | Q     | 16  | ASN  | CA-C  | -5.12 | 1.46        | 1.52     |
| 26  | S     | 158 | PHE  | N-CA  | -5.12 | 1.40        | 1.46     |
| 18  | K     | 175 | GLY  | C-N   | 5.11  | 1.40        | 1.33     |
| 19  | L     | 92  | GLU  | C-N   | 5.11  | 1.40        | 1.33     |
| 22  | O     | 9   | THR  | CA-C  | -5.11 | 1.46        | 1.52     |
| 19  | L     | 344 | ASP  | CA-C  | -5.11 | 1.48        | 1.52     |
| 10  | C     | 54  | SER  | CA-C  | -5.11 | 1.46        | 1.53     |
| 21  | N     | 352 | ASN  | N-CA  | -5.11 | 1.40        | 1.46     |
| 20  | M     | 429 | SER  | N-CA  | -5.11 | 1.40        | 1.46     |
| 25  | R     | 162 | ILE  | CA-C  | 5.11  | 1.59        | 1.52     |
| 19  | L     | 201 | LEU  | C-N   | 5.10  | 1.40        | 1.33     |
| 23  | P     | 170 | SER  | C-N   | 5.10  | 1.40        | 1.33     |
| 13  | F     | 70  | MET  | CA-C  | -5.10 | 1.46        | 1.52     |
| 18  | K     | 96  | ILE  | C-N   | 5.10  | 1.41        | 1.33     |
| 22  | O     | 156 | THR  | C-N   | 5.10  | 1.40        | 1.33     |
| 26  | S     | 444 | GLU  | CA-C  | -5.10 | 1.46        | 1.52     |
| 29  | V     | 111 | HIS  | C-O   | -5.10 | 1.21        | 1.25     |
| 14  | G     | 206 | ASN  | CA-C  | -5.10 | 1.47        | 1.52     |
| 15  | H     | 235 | PHE  | C-O   | -5.10 | 1.18        | 1.24     |
| 17  | J     | 77  | LYS  | CA-C  | -5.10 | 1.45        | 1.52     |
| 4   | 4     | 76  | PRO  | N-CA  | -5.10 | 1.40        | 1.47     |
| 13  | F     | 153 | VAL  | N-CA  | -5.10 | 1.39        | 1.46     |
| 31  | X     | 99  | PHE  | C-N   | 5.10  | 1.40        | 1.33     |
| 3   | 3     | 93  | PRO  | N-CD  | 5.10  | 1.54        | 1.47     |
| 13  | F     | 215 | ILE  | C-N   | 5.10  | 1.39        | 1.33     |
| 18  | K     | 378 | LEU  | CA-C  | -5.10 | 1.46        | 1.52     |
| 21  | N     | 369 | ALA  | C-N   | 5.10  | 1.41        | 1.33     |
| 24  | Q     | 417 | GLY  | CA-C  | 5.10  | 1.57        | 1.52     |
| 33  | Z     | 403 | ASN  | CA-C  | -5.10 | 1.46        | 1.52     |
| 19  | L     | 184 | GLY  | CA-C  | 5.10  | 1.57        | 1.52     |
| 21  | N     | 142 | GLU  | C-N   | 5.10  | 1.40        | 1.33     |
| 12  | E     | 155 | LEU  | N-CA  | -5.09 | 1.39        | 1.46     |
| 14  | G     | 101 | LEU  | C-N   | 5.09  | 1.40        | 1.33     |
| 15  | H     | 52  | THR  | C-N   | 5.09  | 1.40        | 1.33     |
| 16  | I     | 232 | LEU  | N-CA  | -5.09 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | E     | 120 | ALA  | CA-C    | -5.09 | 1.45        | 1.52     |
| 25  | R     | 47  | ALA  | CA-C    | -5.09 | 1.46        | 1.52     |
| 24  | Q     | 133 | LEU  | CA-C    | -5.09 | 1.45        | 1.52     |
| 26  | S     | 366 | LYS  | N-CA    | -5.09 | 1.40        | 1.46     |
| 27  | T     | 27  | LEU  | C-O     | -5.09 | 1.19        | 1.24     |
| 20  | M     | 364 | HIS  | CD2-NE2 | -5.09 | 1.32        | 1.37     |
| 28  | U     | 264 | ALA  | CA-C    | -5.09 | 1.46        | 1.52     |
| 15  | H     | 411 | CYS  | CA-C    | -5.09 | 1.48        | 1.53     |
| 24  | Q     | 198 | LEU  | CA-C    | 5.09  | 1.59        | 1.52     |
| 29  | V     | 190 | HIS  | CD2-NE2 | -5.09 | 1.32        | 1.37     |
| 4   | 4     | 193 | ASP  | CA-C    | 5.09  | 1.59        | 1.52     |
| 23  | P     | 334 | ASN  | C-N     | 5.09  | 1.40        | 1.33     |
| 27  | T     | 231 | SER  | N-CA    | -5.09 | 1.39        | 1.46     |
| 32  | Y     | 82  | ASP  | C-N     | 5.09  | 1.40        | 1.33     |
| 26  | S     | 131 | THR  | C-N     | 5.08  | 1.40        | 1.33     |
| 33  | Z     | 902 | TYR  | CA-C    | -5.08 | 1.45        | 1.52     |
| 1   | 1     | 165 | TRP  | C-N     | 5.08  | 1.40        | 1.33     |
| 1   | 1     | 195 | GLN  | N-CA    | -5.08 | 1.40        | 1.46     |
| 11  | D     | 148 | TYR  | N-CA    | -5.08 | 1.39        | 1.45     |
| 14  | G     | 185 | GLY  | CA-C    | -5.08 | 1.44        | 1.51     |
| 21  | N     | 714 | THR  | C-N     | 5.08  | 1.39        | 1.33     |
| 23  | P     | 318 | TYR  | CA-C    | -5.08 | 1.46        | 1.52     |
| 27  | T     | 147 | LYS  | N-CA    | -5.08 | 1.40        | 1.46     |
| 13  | F     | 154 | THR  | C-N     | 5.08  | 1.40        | 1.33     |
| 19  | L     | 149 | ASP  | CA-C    | -5.08 | 1.46        | 1.52     |
| 19  | L     | 414 | ASP  | CA-C    | -5.08 | 1.46        | 1.52     |
| 25  | R     | 110 | ILE  | C-O     | -5.08 | 1.18        | 1.24     |
| 25  | R     | 325 | HIS  | CD2-NE2 | -5.08 | 1.32        | 1.37     |
| 21  | N     | 383 | LYS  | CA-C    | -5.08 | 1.46        | 1.52     |
| 33  | Z     | 291 | GLU  | CA-C    | -5.08 | 1.46        | 1.52     |
| 33  | Z     | 871 | HIS  | CD2-NE2 | -5.08 | 1.32        | 1.37     |
| 12  | E     | 62  | ASP  | C-N     | 5.08  | 1.40        | 1.33     |
| 19  | L     | 180 | PHE  | N-CA    | -5.08 | 1.39        | 1.46     |
| 24  | Q     | 311 | LEU  | N-CA    | -5.08 | 1.40        | 1.46     |
| 19  | L     | 196 | VAL  | C-N     | 5.08  | 1.40        | 1.33     |
| 21  | N     | 329 | HIS  | CD2-NE2 | -5.08 | 1.32        | 1.37     |
| 23  | P     | 438 | ILE  | C-N     | 5.08  | 1.40        | 1.33     |
| 12  | E     | 105 | GLU  | N-CA    | 5.08  | 1.52        | 1.45     |
| 14  | G     | 8   | ASP  | CA-C    | -5.08 | 1.45        | 1.52     |
| 14  | G     | 240 | ASP  | C-N     | 5.08  | 1.40        | 1.34     |
| 23  | P     | 77  | GLU  | C-N     | 5.08  | 1.40        | 1.33     |
| 28  | U     | 223 | HIS  | CD2-NE2 | -5.08 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | U     | 230 | GLN  | CA-C    | 5.08  | 1.59        | 1.52     |
| 33  | Z     | 415 | MET  | N-CA    | 5.08  | 1.52        | 1.46     |
| 15  | H     | 381 | ASP  | CA-C    | -5.07 | 1.46        | 1.53     |
| 21  | N     | 447 | SER  | C-N     | 5.07  | 1.40        | 1.33     |
| 27  | T     | 123 | HIS  | CD2-NE2 | -5.07 | 1.32        | 1.37     |
| 10  | C     | 125 | HIS  | CD2-NE2 | -5.07 | 1.32        | 1.37     |
| 15  | H     | 348 | ASN  | CA-C    | -5.07 | 1.49        | 1.52     |
| 18  | K     | 331 | PRO  | N-CD    | 5.07  | 1.54        | 1.47     |
| 26  | S     | 372 | LEU  | N-CA    | -5.07 | 1.40        | 1.46     |
| 29  | V     | 43  | ALA  | N-CA    | -5.07 | 1.39        | 1.46     |
| 33  | Z     | 760 | HIS  | CD2-NE2 | -5.07 | 1.32        | 1.37     |
| 12  | E     | 188 | HIS  | CA-C    | -5.07 | 1.46        | 1.52     |
| 6   | 6     | 23  | ASP  | C-N     | 5.07  | 1.40        | 1.33     |
| 10  | C     | 83  | ASP  | C-N     | 5.07  | 1.40        | 1.33     |
| 12  | E     | 184 | LEU  | CA-C    | 5.07  | 1.59        | 1.52     |
| 29  | V     | 80  | VAL  | CA-C    | 5.07  | 1.59        | 1.52     |
| 33  | Z     | 506 | LEU  | C-N     | 5.07  | 1.40        | 1.33     |
| 16  | I     | 365 | HIS  | CD2-NE2 | -5.06 | 1.32        | 1.37     |
| 26  | S     | 355 | GLY  | C-O     | -5.06 | 1.17        | 1.24     |
| 6   | 6     | 43  | MET  | C-N     | 5.06  | 1.40        | 1.33     |
| 7   | 7     | 66  | ASN  | N-CA    | -5.06 | 1.39        | 1.46     |
| 9   | B     | 52  | SER  | CA-C    | -5.06 | 1.46        | 1.52     |
| 14  | G     | 86  | HIS  | CD2-NE2 | -5.06 | 1.32        | 1.37     |
| 33  | Z     | 207 | ILE  | C-N     | 5.06  | 1.41        | 1.33     |
| 9   | B     | 80  | PRO  | N-CD    | 5.06  | 1.54        | 1.47     |
| 17  | J     | 204 | HIS  | CD2-NE2 | -5.06 | 1.32        | 1.37     |
| 19  | L     | 195 | GLU  | N-CA    | -5.06 | 1.39        | 1.46     |
| 19  | L     | 373 | GLU  | N-CA    | -5.06 | 1.40        | 1.46     |
| 20  | M     | 224 | PRO  | C-O     | 5.06  | 1.28        | 1.23     |
| 33  | Z     | 959 | HIS  | CD2-NE2 | -5.06 | 1.32        | 1.37     |
| 2   | 2     | 38  | SER  | N-CA    | -5.06 | 1.39        | 1.46     |
| 17  | J     | 357 | ASP  | C-N     | 5.06  | 1.40        | 1.33     |
| 19  | L     | 346 | LYS  | CA-C    | -5.05 | 1.47        | 1.53     |
| 20  | M     | 239 | THR  | CA-C    | -5.05 | 1.45        | 1.52     |
| 28  | U     | 75  | ASN  | CA-C    | -5.05 | 1.46        | 1.52     |
| 33  | Z     | 295 | ARG  | C-N     | 5.05  | 1.40        | 1.33     |
| 21  | N     | 444 | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 21  | N     | 743 | PHE  | N-CA    | -5.05 | 1.42        | 1.46     |
| 33  | Z     | 897 | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 13  | F     | 174 | ARG  | CA-C    | -5.05 | 1.47        | 1.53     |
| 26  | S     | 472 | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 27  | T     | 44  | LEU  | N-CA    | -5.05 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 1     | 157 | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 5   | 5     | 66  | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 23  | P     | 375 | GLN  | C-N     | 5.05  | 1.40        | 1.33     |
| 30  | W     | 47  | ASN  | N-CA    | -5.05 | 1.39        | 1.46     |
| 30  | W     | 66  | THR  | CA-C    | 5.05  | 1.58        | 1.52     |
| 5   | 5     | 85  | ASN  | CA-C    | 5.05  | 1.59        | 1.52     |
| 24  | Q     | 145 | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 2   | 2     | 114 | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 11  | D     | 59  | ILE  | CA-C    | -5.05 | 1.46        | 1.52     |
| 14  | G     | 104 | THR  | C-O     | -5.05 | 1.18        | 1.24     |
| 14  | G     | 227 | HIS  | CD2-NE2 | -5.05 | 1.32        | 1.37     |
| 15  | H     | 251 | PRO  | N-CD    | 5.05  | 1.54        | 1.47     |
| 16  | I     | 281 | ILE  | C-N     | 5.05  | 1.40        | 1.33     |
| 21  | N     | 378 | ASN  | N-CA    | -5.05 | 1.40        | 1.46     |
| 21  | N     | 754 | THR  | CA-C    | -5.05 | 1.47        | 1.52     |
| 22  | O     | 280 | LEU  | C-O     | -5.05 | 1.18        | 1.24     |
| 23  | P     | 187 | SER  | C-N     | 5.05  | 1.40        | 1.33     |
| 25  | R     | 275 | GLU  | C-N     | 5.05  | 1.40        | 1.34     |
| 21  | N     | 567 | ALA  | C-O     | -5.04 | 1.18        | 1.24     |
| 26  | S     | 159 | ASN  | N-CA    | 5.04  | 1.52        | 1.46     |
| 29  | V     | 195 | HIS  | CD2-NE2 | -5.04 | 1.32        | 1.37     |
| 24  | Q     | 342 | LEU  | CA-C    | -5.04 | 1.46        | 1.52     |
| 25  | R     | 170 | VAL  | CA-C    | -5.04 | 1.46        | 1.52     |
| 29  | V     | 201 | ILE  | N-CA    | -5.04 | 1.40        | 1.46     |
| 33  | Z     | 136 | ARG  | C-N     | 5.04  | 1.40        | 1.33     |
| 23  | P     | 336 | HIS  | CD2-NE2 | -5.04 | 1.32        | 1.37     |
| 2   | 2     | 141 | HIS  | CD2-NE2 | -5.04 | 1.32        | 1.37     |
| 16  | I     | 117 | HIS  | CD2-NE2 | -5.04 | 1.32        | 1.37     |
| 18  | K     | 161 | MET  | C-N     | 5.04  | 1.37        | 1.33     |
| 21  | N     | 304 | LEU  | CA-C    | -5.04 | 1.46        | 1.52     |
| 1   | 1     | 131 | SER  | CA-C    | -5.04 | 1.46        | 1.52     |
| 21  | N     | 270 | LEU  | N-CA    | -5.04 | 1.40        | 1.46     |
| 29  | V     | 191 | GLY  | CA-C    | -5.04 | 1.44        | 1.51     |
| 3   | 3     | 191 | LEU  | C-O     | -5.04 | 1.17        | 1.23     |
| 4   | 4     | 77  | GLN  | CA-C    | 5.04  | 1.59        | 1.52     |
| 21  | N     | 653 | ARG  | C-N     | 5.04  | 1.40        | 1.33     |
| 22  | O     | 283 | HIS  | C-N     | 5.04  | 1.40        | 1.33     |
| 21  | N     | 568 | VAL  | CA-C    | 5.03  | 1.59        | 1.52     |
| 23  | P     | 282 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 27  | T     | 90  | PHE  | N-CA    | -5.03 | 1.39        | 1.46     |
| 29  | V     | 217 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 33  | Z     | 856 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | D     | 198 | SER  | C-N     | 5.03  | 1.41        | 1.33     |
| 12  | E     | 157 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 14  | G     | 229 | PHE  | C-N     | 5.03  | 1.40        | 1.33     |
| 21  | N     | 636 | SER  | C-N     | 5.03  | 1.40        | 1.33     |
| 26  | S     | 139 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 33  | Z     | 532 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 33  | Z     | 593 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 1   | 1     | 86  | CYS  | CA-C    | -5.03 | 1.46        | 1.52     |
| 2   | 2     | 63  | ILE  | C-O     | -5.03 | 1.17        | 1.24     |
| 2   | 2     | 66  | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 24  | Q     | 269 | LYS  | C-N     | 5.03  | 1.40        | 1.33     |
| 33  | Z     | 761 | PHE  | N-CA    | 5.03  | 1.52        | 1.46     |
| 14  | G     | 182 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 22  | O     | 235 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 25  | R     | 81  | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 8   | A     | 15  | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 8   | A     | 229 | THR  | C-N     | 5.03  | 1.40        | 1.33     |
| 9   | B     | 55  | LEU  | C-N     | 5.03  | 1.40        | 1.33     |
| 11  | D     | 209 | ASN  | C-N     | 5.03  | 1.40        | 1.33     |
| 17  | J     | 388 | LYS  | CA-C    | -5.03 | 1.46        | 1.52     |
| 21  | N     | 375 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 22  | O     | 184 | ASP  | N-CA    | -5.03 | 1.40        | 1.46     |
| 22  | O     | 326 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 29  | V     | 111 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 33  | Z     | 487 | SER  | C-N     | 5.03  | 1.40        | 1.33     |
| 3   | 3     | 95  | PHE  | C-N     | 5.03  | 1.40        | 1.33     |
| 7   | 7     | 209 | MET  | N-CA    | 5.03  | 1.52        | 1.46     |
| 9   | B     | 94  | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 9   | B     | 190 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 17  | J     | 205 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 21  | N     | 573 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 27  | T     | 94  | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 27  | T     | 122 | PHE  | CA-C    | 5.03  | 1.59        | 1.52     |
| 30  | W     | 170 | HIS  | CD2-NE2 | -5.03 | 1.32        | 1.37     |
| 6   | 6     | 186 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 7   | 7     | 172 | ALA  | C-O     | -5.02 | 1.18        | 1.24     |
| 10  | C     | 94  | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 27  | T     | 165 | GLN  | C-N     | 5.02  | 1.41        | 1.33     |
| 30  | W     | 100 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 1   | 1     | 104 | ASP  | N-CA    | 5.02  | 1.52        | 1.46     |
| 7   | 7     | 184 | SER  | C-N     | 5.02  | 1.40        | 1.34     |
| 14  | G     | 74  | GLY  | N-CA    | -5.02 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | I     | 427 | LYS  | N-CA    | -5.02 | 1.40        | 1.46     |
| 26  | S     | 237 | ILE  | C-N     | 5.02  | 1.40        | 1.33     |
| 26  | S     | 376 | THR  | CA-C    | -5.02 | 1.45        | 1.52     |
| 4   | 4     | 145 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 11  | D     | 167 | ASN  | CA-C    | -5.02 | 1.47        | 1.53     |
| 12  | E     | 73  | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 20  | M     | 69  | ILE  | C-N     | 5.02  | 1.40        | 1.33     |
| 24  | Q     | 80  | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 3   | 3     | 39  | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 17  | J     | 376 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 21  | N     | 510 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 24  | Q     | 178 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 26  | S     | 407 | ILE  | C-N     | 5.02  | 1.40        | 1.33     |
| 33  | Z     | 151 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 33  | Z     | 156 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 33  | Z     | 503 | ASP  | CA-C    | -5.02 | 1.46        | 1.52     |
| 33  | Z     | 590 | ALA  | C-N     | 5.02  | 1.37        | 1.33     |
| 6   | 6     | 86  | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 17  | J     | 123 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 17  | J     | 214 | SER  | C-N     | 5.02  | 1.40        | 1.33     |
| 18  | K     | 270 | PHE  | N-CA    | 5.02  | 1.52        | 1.46     |
| 33  | Z     | 763 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 33  | Z     | 976 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 5   | 5     | 188 | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 6   | 6     | 70  | HIS  | CD2-NE2 | -5.02 | 1.32        | 1.37     |
| 1   | 1     | 38  | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 11  | D     | 96  | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 12  | E     | 188 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 14  | G     | 203 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 15  | H     | 412 | PRO  | CA-C    | -5.01 | 1.46        | 1.52     |
| 16  | I     | 234 | LYS  | CA-C    | 5.01  | 1.59        | 1.52     |
| 21  | N     | 499 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 26  | S     | 438 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 18  | K     | 244 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 23  | P     | 147 | LYS  | CA-C    | 5.01  | 1.59        | 1.52     |
| 9   | B     | 73  | ALA  | CA-C    | -5.01 | 1.46        | 1.52     |
| 20  | M     | 340 | SER  | C-N     | 5.01  | 1.40        | 1.33     |
| 21  | N     | 190 | LEU  | C-N     | 5.01  | 1.40        | 1.33     |
| 21  | N     | 589 | ILE  | CA-C    | 5.01  | 1.59        | 1.52     |
| 25  | R     | 259 | PHE  | N-CA    | -5.01 | 1.40        | 1.46     |
| 26  | S     | 334 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 31  | X     | 53  | THR  | CA-C    | 5.01  | 1.58        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33  | Z     | 259 | PRO  | CA-CB   | 5.01  | 1.60        | 1.53     |
| 8   | A     | 193 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 19  | L     | 273 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 19  | L     | 414 | ASP  | C-O     | -5.01 | 1.18        | 1.24     |
| 20  | M     | 410 | VAL  | C-N     | 5.01  | 1.40        | 1.33     |
| 21  | N     | 430 | ASN  | CA-C    | 5.01  | 1.59        | 1.52     |
| 21  | N     | 643 | PRO  | C-O     | -5.01 | 1.17        | 1.24     |
| 16  | I     | 107 | GLY  | CA-C    | -5.01 | 1.44        | 1.51     |
| 21  | N     | 923 | MET  | C-N     | 5.01  | 1.40        | 1.33     |
| 29  | V     | 279 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 3   | 3     | 97  | GLY  | C-N     | -5.01 | 1.26        | 1.33     |
| 11  | D     | 34  | VAL  | N-CA    | -5.01 | 1.40        | 1.46     |
| 21  | N     | 340 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 21  | N     | 616 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 33  | Z     | 463 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 6   | 6     | 99  | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 9   | B     | 55  | LEU  | N-CA    | -5.00 | 1.39        | 1.46     |
| 22  | O     | 12  | SER  | CA-C    | -5.00 | 1.46        | 1.52     |
| 4   | 4     | 132 | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 5   | 5     | 159 | ARG  | CA-C    | -5.00 | 1.46        | 1.52     |
| 7   | 7     | 141 | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 16  | I     | 204 | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 25  | R     | 313 | ALA  | C-N     | 5.00  | 1.41        | 1.33     |
| 25  | R     | 317 | ILE  | CA-C    | 5.00  | 1.58        | 1.52     |
| 2   | 2     | 206 | PRO  | N-CA    | -5.00 | 1.41        | 1.47     |
| 11  | D     | 140 | PRO  | N-CD    | 5.00  | 1.54        | 1.47     |
| 13  | F     | 94  | TYR  | N-CA    | -5.00 | 1.40        | 1.46     |
| 14  | G     | 72  | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 16  | I     | 405 | ARG  | C-N     | 5.00  | 1.40        | 1.33     |
| 18  | K     | 74  | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 21  | N     | 747 | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 23  | P     | 230 | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 24  | Q     | 334 | HIS  | CD2-NE2 | -5.00 | 1.32        | 1.37     |
| 33  | Z     | 844 | ALA  | C-N     | 5.00  | 1.40        | 1.33     |

All (4314) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 19  | L     | 257 | GLY  | O-C-N  | -28.79 | 88.64       | 122.33   |
| 19  | L     | 257 | GLY  | CA-C-N | 18.94  | 152.97      | 120.58   |
| 19  | L     | 257 | GLY  | C-N-CA | 18.94  | 152.97      | 120.58   |
| 20  | M     | 251 | LEU  | O-C-N  | -13.34 | 104.89      | 122.23   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 33  | Z     | 486 | SER  | CA-C-N | 12.47  | 137.40      | 120.44   |
| 33  | Z     | 486 | SER  | C-N-CA | 12.47  | 137.40      | 120.44   |
| 20  | M     | 251 | LEU  | CA-C-N | 12.39  | 144.27      | 121.97   |
| 20  | M     | 251 | LEU  | C-N-CA | 12.39  | 144.27      | 121.97   |
| 24  | Q     | 294 | ARG  | CA-C-N | 12.17  | 133.38      | 120.00   |
| 24  | Q     | 294 | ARG  | C-N-CA | 12.17  | 133.38      | 120.00   |
| 31  | X     | 53  | THR  | N-CA-C | -12.12 | 98.97       | 113.88   |
| 13  | F     | 189 | LEU  | N-CA-C | 11.74  | 124.07      | 111.28   |
| 16  | I     | 338 | LEU  | CA-C-N | 11.65  | 135.47      | 120.56   |
| 16  | I     | 338 | LEU  | C-N-CA | 11.65  | 135.47      | 120.56   |
| 21  | N     | 914 | VAL  | N-CA-C | -11.45 | 101.99      | 113.10   |
| 30  | W     | 163 | ASN  | N-CA-C | -11.19 | 95.27       | 108.25   |
| 27  | T     | 270 | ILE  | N-CA-C | 11.18  | 120.93      | 110.42   |
| 15  | H     | 275 | ILE  | CA-C-N | 10.84  | 132.17      | 120.03   |
| 15  | H     | 275 | ILE  | C-N-CA | 10.84  | 132.17      | 120.03   |
| 15  | H     | 383 | GLU  | CA-C-N | 10.74  | 131.65      | 119.94   |
| 15  | H     | 383 | GLU  | C-N-CA | 10.74  | 131.65      | 119.94   |
| 25  | R     | 328 | PHE  | CA-C-N | 10.60  | 134.22      | 120.44   |
| 25  | R     | 328 | PHE  | C-N-CA | 10.60  | 134.22      | 120.44   |
| 33  | Z     | 61  | SER  | N-CA-C | 10.55  | 122.86      | 111.36   |
| 18  | K     | 103 | ILE  | N-CA-C | -10.47 | 100.67      | 110.82   |
| 27  | T     | 168 | SER  | CA-C-N | 10.45  | 136.19      | 120.31   |
| 27  | T     | 168 | SER  | C-N-CA | 10.45  | 136.19      | 120.31   |
| 21  | N     | 408 | LEU  | N-CA-C | -10.44 | 99.98       | 111.36   |
| 16  | I     | 362 | LEU  | CA-C-N | 10.41  | 131.53      | 119.98   |
| 16  | I     | 362 | LEU  | C-N-CA | 10.41  | 131.53      | 119.98   |
| 19  | L     | 299 | ARG  | N-CA-C | -10.40 | 100.72      | 113.41   |
| 21  | N     | 602 | VAL  | CA-C-N | 10.38  | 130.70      | 119.28   |
| 21  | N     | 602 | VAL  | C-N-CA | 10.38  | 130.70      | 119.28   |
| 10  | C     | 210 | ARG  | N-CA-C | -10.33 | 99.99       | 112.59   |
| 19  | L     | 229 | THR  | CA-C-N | 10.28  | 134.06      | 120.28   |
| 19  | L     | 229 | THR  | C-N-CA | 10.28  | 134.06      | 120.28   |
| 24  | Q     | 44  | ALA  | N-CA-C | -10.27 | 102.91      | 114.62   |
| 22  | O     | 291 | ILE  | N-CA-C | 10.19  | 121.01      | 110.72   |
| 14  | G     | 209 | LYS  | N-CA-C | -10.07 | 94.03       | 109.24   |
| 12  | E     | 178 | GLY  | CA-C-N | 10.06  | 133.76      | 120.28   |
| 12  | E     | 178 | GLY  | C-N-CA | 10.06  | 133.76      | 120.28   |
| 19  | L     | 376 | PHE  | CA-C-N | 10.05  | 133.75      | 120.28   |
| 19  | L     | 376 | PHE  | C-N-CA | 10.05  | 133.75      | 120.28   |
| 27  | T     | 167 | GLY  | CA-C-N | 10.01  | 134.06      | 120.44   |
| 27  | T     | 167 | GLY  | C-N-CA | 10.01  | 134.06      | 120.44   |
| 22  | O     | 147 | ARG  | N-CA-C | 9.99   | 122.17      | 111.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | S     | 403 | SER  | CA-C-N  | 9.99  | 133.66      | 120.28   |
| 26  | S     | 403 | SER  | C-N-CA  | 9.99  | 133.66      | 120.28   |
| 13  | F     | 199 | GLN  | N-CA-C  | -9.96 | 101.22      | 113.97   |
| 21  | N     | 483 | LEU  | CA-C-N  | 9.94  | 131.22      | 119.99   |
| 21  | N     | 483 | LEU  | C-N-CA  | 9.94  | 131.22      | 119.99   |
| 29  | V     | 261 | LEU  | CA-C-N  | 9.91  | 133.32      | 120.44   |
| 29  | V     | 261 | LEU  | C-N-CA  | 9.91  | 133.32      | 120.44   |
| 33  | Z     | 752 | ILE  | CA-C-N  | 9.89  | 130.96      | 119.98   |
| 33  | Z     | 752 | ILE  | C-N-CA  | 9.89  | 130.96      | 119.98   |
| 28  | U     | 110 | PHE  | CA-C-N  | 9.89  | 134.81      | 120.38   |
| 28  | U     | 110 | PHE  | C-N-CA  | 9.89  | 134.81      | 120.38   |
| 33  | Z     | 253 | VAL  | N-CA-CB | 9.88  | 117.14      | 110.52   |
| 18  | K     | 173 | ASP  | N-CA-C  | -9.86 | 101.38      | 113.41   |
| 20  | M     | 233 | ARG  | CA-C-O  | 9.85  | 130.99      | 120.55   |
| 30  | W     | 163 | ASN  | CA-C-O  | -9.82 | 111.30      | 120.34   |
| 19  | L     | 123 | SER  | N-CA-C  | -9.82 | 100.47      | 114.12   |
| 14  | G     | 93  | GLU  | N-CA-C  | 9.80  | 121.96      | 111.28   |
| 21  | N     | 591 | LEU  | CA-C-N  | 9.79  | 130.85      | 119.98   |
| 21  | N     | 591 | LEU  | C-N-CA  | 9.79  | 130.85      | 119.98   |
| 25  | R     | 115 | GLU  | CA-C-N  | 9.76  | 133.13      | 120.44   |
| 25  | R     | 115 | GLU  | C-N-CA  | 9.76  | 133.13      | 120.44   |
| 20  | M     | 417 | GLU  | CA-C-N  | 9.76  | 130.58      | 119.94   |
| 20  | M     | 417 | GLU  | C-N-CA  | 9.76  | 130.58      | 119.94   |
| 3   | 3     | 107 | SER  | N-CA-C  | -9.74 | 102.19      | 114.56   |
| 19  | L     | 222 | GLY  | CA-C-N  | 9.73  | 126.76      | 119.66   |
| 19  | L     | 222 | GLY  | C-N-CA  | 9.73  | 126.76      | 119.66   |
| 19  | L     | 115 | GLU  | N-CA-C  | -9.72 | 102.50      | 114.75   |
| 10  | C     | 190 | ILE  | CA-C-O  | -9.70 | 110.89      | 121.17   |
| 19  | L     | 142 | LYS  | N-CA-C  | 9.68  | 122.83      | 110.24   |
| 25  | R     | 289 | ILE  | N-CA-C  | -9.66 | 103.92      | 113.20   |
| 4   | 4     | 66  | TYR  | CA-C-N  | 9.65  | 133.21      | 120.28   |
| 4   | 4     | 66  | TYR  | C-N-CA  | 9.65  | 133.21      | 120.28   |
| 21  | N     | 76  | GLU  | CA-C-N  | 9.63  | 133.54      | 120.44   |
| 21  | N     | 76  | GLU  | C-N-CA  | 9.63  | 133.54      | 120.44   |
| 17  | J     | 131 | ASP  | CA-C-O  | -9.58 | 109.34      | 118.73   |
| 33  | Z     | 489 | ALA  | CA-C-N  | 9.57  | 134.00      | 120.42   |
| 33  | Z     | 489 | ALA  | C-N-CA  | 9.57  | 134.00      | 120.42   |
| 11  | D     | 50  | SER  | N-CA-C  | -9.53 | 92.65       | 108.76   |
| 25  | R     | 278 | SER  | CA-C-N  | 9.53  | 133.82      | 120.29   |
| 25  | R     | 278 | SER  | C-N-CA  | 9.53  | 133.82      | 120.29   |
| 22  | O     | 74  | ASN  | CA-C-N  | 9.51  | 133.79      | 120.29   |
| 22  | O     | 74  | ASN  | C-N-CA  | 9.51  | 133.79      | 120.29   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | N     | 179 | THR  | CA-C-N  | 9.51  | 133.02      | 120.28   |
| 21  | N     | 179 | THR  | C-N-CA  | 9.51  | 133.02      | 120.28   |
| 21  | N     | 230 | VAL  | O-C-N   | 9.50  | 131.09      | 121.87   |
| 33  | Z     | 898 | HIS  | CA-C-N  | 9.48  | 133.93      | 120.28   |
| 33  | Z     | 898 | HIS  | C-N-CA  | 9.48  | 133.93      | 120.28   |
| 14  | G     | 106 | ILE  | CA-C-N  | 9.47  | 129.55      | 119.89   |
| 14  | G     | 106 | ILE  | C-N-CA  | 9.47  | 129.55      | 119.89   |
| 20  | M     | 139 | LYS  | N-CA-C  | -9.47 | 101.41      | 113.72   |
| 12  | E     | 222 | ILE  | N-CA-C  | -9.46 | 94.35       | 108.17   |
| 27  | T     | 103 | SER  | CA-C-N  | 9.46  | 133.73      | 120.29   |
| 27  | T     | 103 | SER  | C-N-CA  | 9.46  | 133.73      | 120.29   |
| 33  | Z     | 124 | MET  | N-CA-C  | 9.46  | 121.67      | 111.36   |
| 5   | 5     | 9   | GLN  | CA-C-O  | -9.45 | 110.78      | 120.90   |
| 28  | U     | 213 | LYS  | CA-C-N  | 9.45  | 132.78      | 120.60   |
| 28  | U     | 213 | LYS  | C-N-CA  | 9.45  | 132.78      | 120.60   |
| 16  | I     | 160 | LEU  | N-CA-C  | -9.41 | 94.94       | 108.96   |
| 15  | H     | 188 | PRO  | N-CA-C  | 9.38  | 122.14      | 110.70   |
| 20  | M     | 277 | ILE  | N-CA-C  | -9.38 | 94.98       | 108.11   |
| 12  | E     | 168 | ASN  | N-CA-C  | -9.37 | 103.94      | 114.62   |
| 10  | C     | 110 | ILE  | N-CA-C  | 9.35  | 119.39      | 110.42   |
| 21  | N     | 217 | MET  | CA-C-O  | -9.35 | 111.01      | 120.64   |
| 33  | Z     | 502 | ASN  | CA-C-N  | 9.35  | 134.52      | 120.31   |
| 33  | Z     | 502 | ASN  | C-N-CA  | 9.35  | 134.52      | 120.31   |
| 27  | T     | 253 | GLU  | N-CA-C  | 9.32  | 123.03      | 110.35   |
| 24  | Q     | 408 | THR  | CA-C-N  | 9.31  | 132.54      | 120.44   |
| 24  | Q     | 408 | THR  | C-N-CA  | 9.31  | 132.54      | 120.44   |
| 21  | N     | 895 | LYS  | CB-CA-C | -9.31 | 105.83      | 116.54   |
| 24  | Q     | 19  | GLN  | CA-C-N  | 9.31  | 132.75      | 120.28   |
| 24  | Q     | 19  | GLN  | C-N-CA  | 9.31  | 132.75      | 120.28   |
| 29  | V     | 235 | GLU  | N-CA-C  | 9.30  | 121.11      | 110.97   |
| 14  | G     | 81  | ILE  | CA-C-O  | -9.29 | 112.46      | 118.69   |
| 26  | S     | 177 | ASN  | N-CA-C  | -9.29 | 102.77      | 114.56   |
| 28  | U     | 54  | LEU  | CA-C-N  | 9.27  | 129.84      | 119.83   |
| 28  | U     | 54  | LEU  | C-N-CA  | 9.27  | 129.84      | 119.83   |
| 21  | N     | 754 | THR  | CA-C-N  | 9.25  | 129.01      | 119.76   |
| 21  | N     | 754 | THR  | C-N-CA  | 9.25  | 129.01      | 119.76   |
| 24  | Q     | 89  | ALA  | CA-C-N  | 9.25  | 132.67      | 120.28   |
| 24  | Q     | 89  | ALA  | C-N-CA  | 9.25  | 132.67      | 120.28   |
| 15  | H     | 346 | ARG  | N-CA-C  | -9.23 | 102.15      | 113.97   |
| 24  | Q     | 218 | LEU  | N-CA-C  | 9.23  | 121.34      | 111.28   |
| 21  | N     | 692 | GLU  | CA-C-N  | 9.22  | 130.22      | 119.98   |
| 21  | N     | 692 | GLU  | C-N-CA  | 9.22  | 130.22      | 119.98   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 30  | W     | 24  | THR  | N-CA-C | -9.21 | 94.94       | 109.50   |
| 16  | I     | 259 | ASP  | N-CA-C | 9.21  | 120.92      | 111.07   |
| 17  | J     | 317 | PRO  | CA-C-N | 9.20  | 129.86      | 120.38   |
| 17  | J     | 317 | PRO  | C-N-CA | 9.20  | 129.86      | 120.38   |
| 19  | L     | 402 | ALA  | N-CA-C | -9.19 | 99.68       | 112.45   |
| 18  | K     | 49  | PHE  | CA-C-N | 9.18  | 132.93      | 120.54   |
| 18  | K     | 49  | PHE  | C-N-CA | 9.18  | 132.93      | 120.54   |
| 19  | L     | 84  | LEU  | O-C-N  | 9.17  | 132.60      | 122.15   |
| 14  | G     | 99  | LYS  | CA-C-N | 9.15  | 132.55      | 120.28   |
| 14  | G     | 99  | LYS  | C-N-CA | 9.15  | 132.55      | 120.28   |
| 16  | I     | 399 | ALA  | CA-C-N | 9.15  | 131.57      | 120.14   |
| 16  | I     | 399 | ALA  | C-N-CA | 9.15  | 131.57      | 120.14   |
| 21  | N     | 426 | ILE  | CA-C-N | 9.15  | 132.27      | 120.56   |
| 21  | N     | 426 | ILE  | C-N-CA | 9.15  | 132.27      | 120.56   |
| 16  | I     | 305 | THR  | N-CA-C | -9.12 | 101.42      | 111.36   |
| 21  | N     | 387 | ALA  | CA-C-O | -9.12 | 109.94      | 118.33   |
| 33  | Z     | 417 | SER  | CA-C-N | 9.11  | 132.28      | 120.44   |
| 33  | Z     | 417 | SER  | C-N-CA | 9.11  | 132.28      | 120.44   |
| 13  | F     | 170 | THR  | CA-C-N | 9.11  | 132.28      | 120.44   |
| 13  | F     | 170 | THR  | C-N-CA | 9.11  | 132.28      | 120.44   |
| 21  | N     | 128 | ILE  | O-C-N  | 9.11  | 131.21      | 121.83   |
| 17  | J     | 224 | GLY  | CA-C-N | -9.10 | 104.17      | 121.54   |
| 17  | J     | 224 | GLY  | C-N-CA | -9.10 | 104.17      | 121.54   |
| 13  | F     | 27  | GLU  | N-CA-C | -9.09 | 100.52      | 111.69   |
| 16  | I     | 308 | GLU  | CA-C-N | 9.06  | 132.43      | 120.28   |
| 16  | I     | 308 | GLU  | C-N-CA | 9.06  | 132.43      | 120.28   |
| 26  | S     | 439 | GLU  | N-CA-C | -9.04 | 100.36      | 111.40   |
| 8   | A     | 188 | LYS  | N-CA-C | 9.01  | 121.10      | 111.28   |
| 24  | Q     | 247 | HIS  | N-CA-C | 9.01  | 120.71      | 111.07   |
| 30  | W     | 165 | GLN  | CA-C-N | 9.01  | 132.15      | 120.44   |
| 30  | W     | 165 | GLN  | C-N-CA | 9.01  | 132.15      | 120.44   |
| 2   | 2     | 49  | ALA  | N-CA-C | 8.99  | 121.90      | 111.11   |
| 25  | R     | 184 | GLN  | N-CA-C | -8.99 | 102.22      | 113.55   |
| 5   | 5     | 138 | GLY  | CA-C-N | 8.98  | 131.88      | 120.56   |
| 5   | 5     | 138 | GLY  | C-N-CA | 8.98  | 131.88      | 120.56   |
| 19  | L     | 100 | SER  | CA-C-N | 8.94  | 134.46      | 120.34   |
| 19  | L     | 100 | SER  | C-N-CA | 8.94  | 134.46      | 120.34   |
| 6   | 6     | 51  | ASP  | CA-C-N | 8.91  | 129.83      | 119.94   |
| 6   | 6     | 51  | ASP  | C-N-CA | 8.91  | 129.83      | 119.94   |
| 8   | A     | 112 | MET  | CA-C-N | 8.90  | 128.97      | 119.89   |
| 8   | A     | 112 | MET  | C-N-CA | 8.90  | 128.97      | 119.89   |
| 27  | T     | 180 | ILE  | CA-C-N | 8.90  | 132.21      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 27  | T     | 180 | ILE  | C-N-CA | 8.90  | 132.21      | 120.28   |
| 12  | E     | 55  | THR  | N-CA-C | -8.90 | 101.49      | 114.39   |
| 21  | N     | 123 | PHE  | N-CA-C | 8.87  | 122.06      | 111.33   |
| 25  | R     | 52  | ALA  | N-CA-C | 8.86  | 120.55      | 111.07   |
| 33  | Z     | 439 | TYR  | CA-C-N | 8.85  | 131.94      | 120.44   |
| 33  | Z     | 439 | TYR  | C-N-CA | 8.85  | 131.94      | 120.44   |
| 19  | L     | 223 | PRO  | CA-C-O | -8.83 | 114.54      | 120.90   |
| 1   | 1     | 152 | VAL  | CA-C-O | -8.83 | 111.77      | 120.95   |
| 8   | A     | 211 | ILE  | CA-C-O | -8.83 | 111.81      | 121.17   |
| 20  | M     | 159 | LEU  | CA-C-O | -8.82 | 113.23      | 121.08   |
| 28  | U     | 164 | GLU  | N-CA-C | -8.80 | 93.11       | 108.69   |
| 10  | C     | 171 | ALA  | CA-C-N | 8.80  | 132.41      | 120.44   |
| 10  | C     | 171 | ALA  | C-N-CA | 8.80  | 132.41      | 120.44   |
| 19  | L     | 381 | LYS  | N-CA-C | 8.78  | 120.85      | 111.28   |
| 21  | N     | 17  | GLN  | CA-C-N | 8.78  | 132.04      | 120.28   |
| 21  | N     | 17  | GLN  | C-N-CA | 8.78  | 132.04      | 120.28   |
| 9   | B     | 217 | GLU  | N-CA-C | -8.77 | 93.17       | 108.69   |
| 21  | N     | 448 | LEU  | CA-C-N | 8.75  | 129.69      | 119.98   |
| 21  | N     | 448 | LEU  | C-N-CA | 8.75  | 129.69      | 119.98   |
| 6   | 6     | -7  | ASN  | CA-C-O | -8.75 | 110.77      | 119.69   |
| 8   | A     | 158 | ASP  | O-C-N  | 8.74  | 127.31      | 121.71   |
| 27  | T     | 6   | GLU  | CA-C-N | 8.74  | 132.00      | 120.28   |
| 27  | T     | 6   | GLU  | C-N-CA | 8.74  | 132.00      | 120.28   |
| 8   | A     | 20  | SER  | CA-C-N | 8.72  | 130.74      | 119.84   |
| 8   | A     | 20  | SER  | C-N-CA | 8.72  | 130.74      | 119.84   |
| 15  | H     | 280 | VAL  | N-CA-C | 8.71  | 121.14      | 107.98   |
| 12  | E     | 236 | THR  | CA-C-N | 8.70  | 131.93      | 120.28   |
| 12  | E     | 236 | THR  | C-N-CA | 8.70  | 131.93      | 120.28   |
| 8   | A     | 59  | VAL  | CA-C-O | -8.69 | 112.64      | 119.25   |
| 33  | Z     | 91  | PHE  | CA-C-N | 8.68  | 131.91      | 120.28   |
| 33  | Z     | 91  | PHE  | C-N-CA | 8.68  | 131.91      | 120.28   |
| 18  | K     | 48  | TYR  | CA-C-N | 8.67  | 131.90      | 120.28   |
| 18  | K     | 48  | TYR  | C-N-CA | 8.67  | 131.90      | 120.28   |
| 27  | T     | 28  | PRO  | CA-C-O | -8.66 | 108.00      | 120.56   |
| 14  | G     | 239 | ILE  | O-C-N  | 8.66  | 130.27      | 121.87   |
| 22  | O     | 273 | GLN  | N-CA-C | 8.66  | 120.33      | 111.07   |
| 33  | Z     | 866 | VAL  | N-CA-C | -8.65 | 104.59      | 112.90   |
| 23  | P     | 421 | GLU  | N-CA-C | -8.65 | 101.93      | 111.36   |
| 21  | N     | 427 | ILE  | N-CA-C | -8.64 | 102.41      | 110.53   |
| 21  | N     | 269 | LEU  | CA-C-N | 8.63  | 131.67      | 120.44   |
| 21  | N     | 269 | LEU  | C-N-CA | 8.63  | 131.67      | 120.44   |
| 6   | 6     | 31  | GLU  | CA-C-O | -8.63 | 111.86      | 119.72   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | B     | 97  | TYR  | CA-C-O | 8.63  | 128.14      | 119.08   |
| 30  | W     | 101 | ARG  | CA-C-N | 8.63  | 132.20      | 120.38   |
| 30  | W     | 101 | ARG  | C-N-CA | 8.63  | 132.20      | 120.38   |
| 7   | 7     | 27  | ARG  | O-C-N  | 8.62  | 130.95      | 122.07   |
| 12  | E     | 190 | SER  | N-CA-C | -8.62 | 101.15      | 113.21   |
| 19  | L     | 226 | THR  | N-CA-C | -8.61 | 102.15      | 114.12   |
| 20  | M     | 260 | ALA  | CA-C-N | 8.61  | 131.81      | 120.28   |
| 20  | M     | 260 | ALA  | C-N-CA | 8.61  | 131.81      | 120.28   |
| 24  | Q     | 2   | SER  | N-CA-C | -8.61 | 100.25      | 110.41   |
| 2   | 2     | 205 | PHE  | CA-C-N | 8.60  | 128.54      | 119.85   |
| 2   | 2     | 205 | PHE  | C-N-CA | 8.60  | 128.54      | 119.85   |
| 23  | P     | 322 | LEU  | CA-C-N | 8.60  | 137.97      | 121.54   |
| 23  | P     | 322 | LEU  | C-N-CA | 8.60  | 137.97      | 121.54   |
| 19  | L     | 84  | LEU  | CA-C-O | -8.60 | 111.31      | 120.42   |
| 21  | N     | 716 | GLN  | N-CA-C | -8.60 | 96.26       | 109.24   |
| 25  | R     | 341 | LEU  | N-CA-C | 8.58  | 120.72      | 111.36   |
| 22  | O     | 145 | LYS  | CA-C-N | 8.58  | 131.77      | 120.28   |
| 22  | O     | 145 | LYS  | C-N-CA | 8.58  | 131.77      | 120.28   |
| 22  | O     | 110 | ASP  | N-CA-C | -8.57 | 101.75      | 112.72   |
| 24  | Q     | 111 | LEU  | CA-C-O | -8.57 | 111.34      | 120.42   |
| 15  | H     | 401 | GLY  | CA-C-N | 8.57  | 132.31      | 120.49   |
| 15  | H     | 401 | GLY  | C-N-CA | 8.57  | 132.31      | 120.49   |
| 20  | M     | 46  | SER  | CA-C-N | 8.57  | 131.76      | 120.28   |
| 20  | M     | 46  | SER  | C-N-CA | 8.57  | 131.76      | 120.28   |
| 13  | F     | 220 | THR  | CA-C-N | 8.56  | 129.22      | 120.14   |
| 13  | F     | 220 | THR  | C-N-CA | 8.56  | 129.22      | 120.14   |
| 20  | M     | 233 | ARG  | O-C-N  | -8.56 | 113.05      | 122.12   |
| 33  | Z     | 51  | LEU  | CA-C-O | 8.56  | 129.82      | 120.32   |
| 20  | M     | 233 | ARG  | CA-C-N | 8.56  | 131.75      | 120.28   |
| 20  | M     | 233 | ARG  | C-N-CA | 8.56  | 131.75      | 120.28   |
| 20  | M     | 48  | LEU  | N-CA-C | 8.55  | 120.69      | 111.36   |
| 24  | Q     | 134 | LYS  | CA-C-N | 8.55  | 132.43      | 120.29   |
| 24  | Q     | 134 | LYS  | C-N-CA | 8.55  | 132.43      | 120.29   |
| 29  | V     | 281 | SER  | CA-C-N | 8.55  | 131.56      | 120.44   |
| 29  | V     | 281 | SER  | C-N-CA | 8.55  | 131.56      | 120.44   |
| 30  | W     | 26  | PHE  | N-CA-C | -8.55 | 101.96      | 111.28   |
| 27  | T     | 7   | LEU  | CA-C-N | 8.54  | 131.54      | 120.44   |
| 27  | T     | 7   | LEU  | C-N-CA | 8.54  | 131.54      | 120.44   |
| 28  | U     | 259 | ASN  | CA-C-N | 8.53  | 131.91      | 120.65   |
| 28  | U     | 259 | ASN  | C-N-CA | 8.53  | 131.91      | 120.65   |
| 29  | V     | 89  | ALA  | CA-C-N | 8.53  | 132.40      | 120.29   |
| 29  | V     | 89  | ALA  | C-N-CA | 8.53  | 132.40      | 120.29   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 17  | J     | 149 | MET  | N-CA-C | -8.53 | 103.39      | 113.88   |
| 22  | O     | 66  | VAL  | CA-C-O | -8.53 | 112.08      | 120.95   |
| 10  | C     | 187 | ASP  | CA-C-N | 8.52  | 132.39      | 120.29   |
| 10  | C     | 187 | ASP  | C-N-CA | 8.52  | 132.39      | 120.29   |
| 11  | D     | 182 | LYS  | N-CA-C | -8.52 | 101.89      | 113.30   |
| 22  | O     | 271 | LYS  | N-CA-C | -8.52 | 97.42       | 109.69   |
| 10  | C     | 95  | ALA  | N-CA-C | 8.51  | 120.18      | 111.07   |
| 33  | Z     | 396 | ASN  | CA-C-O | 8.50  | 128.99      | 120.32   |
| 21  | N     | 494 | LYS  | CA-C-N | 8.50  | 128.20      | 119.19   |
| 21  | N     | 494 | LYS  | C-N-CA | 8.50  | 128.20      | 119.19   |
| 22  | O     | 99  | LEU  | CA-C-N | 8.49  | 131.66      | 120.28   |
| 22  | O     | 99  | LEU  | C-N-CA | 8.49  | 131.66      | 120.28   |
| 29  | V     | 233 | LYS  | CA-C-N | 8.49  | 131.48      | 120.44   |
| 29  | V     | 233 | LYS  | C-N-CA | 8.49  | 131.48      | 120.44   |
| 17  | J     | 55  | VAL  | CA-C-N | 8.49  | 131.65      | 120.28   |
| 17  | J     | 55  | VAL  | C-N-CA | 8.49  | 131.65      | 120.28   |
| 27  | T     | 156 | SER  | CA-C-N | 8.48  | 131.65      | 120.28   |
| 27  | T     | 156 | SER  | C-N-CA | 8.48  | 131.65      | 120.28   |
| 19  | L     | 351 | LEU  | CA-C-O | -8.48 | 113.07      | 120.19   |
| 17  | J     | 271 | THR  | CA-C-N | 8.47  | 131.63      | 120.28   |
| 17  | J     | 271 | THR  | C-N-CA | 8.47  | 131.63      | 120.28   |
| 20  | M     | 216 | LYS  | N-CA-C | -8.47 | 101.77      | 114.64   |
| 2   | 2     | 41  | ILE  | N-CA-C | -8.46 | 93.83       | 107.28   |
| 22  | O     | 220 | SER  | CA-C-O | -8.45 | 111.47      | 120.42   |
| 2   | 2     | 159 | ILE  | CA-C-N | 8.44  | 131.59      | 120.28   |
| 2   | 2     | 159 | ILE  | C-N-CA | 8.44  | 131.59      | 120.28   |
| 21  | N     | 250 | ASP  | O-C-N  | -8.44 | 113.26      | 123.30   |
| 2   | 2     | 197 | GLU  | CA-C-N | 8.43  | 132.68      | 120.71   |
| 2   | 2     | 197 | GLU  | C-N-CA | 8.43  | 132.68      | 120.71   |
| 13  | F     | 104 | ALA  | CA-C-N | 8.43  | 132.01      | 120.46   |
| 13  | F     | 104 | ALA  | C-N-CA | 8.43  | 132.01      | 120.46   |
| 11  | D     | 24  | LEU  | CA-C-O | 8.42  | 129.65      | 119.97   |
| 24  | Q     | 210 | CYS  | O-C-N  | -8.42 | 115.90      | 121.88   |
| 21  | N     | 652 | VAL  | N-CA-C | -8.41 | 101.83      | 111.00   |
| 33  | Z     | 170 | GLU  | CA-C-N | 8.41  | 131.88      | 120.44   |
| 33  | Z     | 170 | GLU  | C-N-CA | 8.41  | 131.88      | 120.44   |
| 25  | R     | 118 | GLN  | CA-C-O | -8.40 | 112.00      | 120.82   |
| 26  | S     | 412 | ASN  | CA-C-N | 8.39  | 131.34      | 120.44   |
| 26  | S     | 412 | ASN  | C-N-CA | 8.39  | 131.34      | 120.44   |
| 22  | O     | 249 | ASP  | CA-C-N | 8.39  | 132.36      | 120.28   |
| 22  | O     | 249 | ASP  | C-N-CA | 8.39  | 132.36      | 120.28   |
| 33  | Z     | 422 | ILE  | CA-C-N | 8.39  | 130.62      | 120.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 422 | ILE  | C-N-CA | 8.39  | 130.62      | 120.14   |
| 20  | M     | 379 | LEU  | CA-C-N | 8.38  | 131.51      | 120.28   |
| 20  | M     | 379 | LEU  | C-N-CA | 8.38  | 131.51      | 120.28   |
| 17  | J     | 301 | ASP  | N-CA-C | -8.38 | 98.53       | 108.25   |
| 33  | Z     | 493 | LEU  | CA-C-N | 8.38  | 129.28      | 119.98   |
| 33  | Z     | 493 | LEU  | C-N-CA | 8.38  | 129.28      | 119.98   |
| 26  | S     | 248 | ASP  | N-CA-C | -8.37 | 102.83      | 113.72   |
| 21  | N     | 276 | GLU  | CA-C-N | 8.37  | 131.83      | 120.44   |
| 21  | N     | 276 | GLU  | C-N-CA | 8.37  | 131.83      | 120.44   |
| 20  | M     | 58  | MET  | CA-C-N | 8.37  | 132.33      | 120.28   |
| 20  | M     | 58  | MET  | C-N-CA | 8.37  | 132.33      | 120.28   |
| 5   | 5     | 204 | GLU  | N-CA-C | -8.36 | 100.83      | 112.45   |
| 27  | T     | 192 | ASN  | O-C-N  | 8.34  | 130.66      | 122.07   |
| 17  | J     | 142 | VAL  | O-C-N  | -8.32 | 111.62      | 121.10   |
| 8   | A     | 164 | VAL  | CA-C-N | 8.30  | 130.25      | 121.45   |
| 8   | A     | 164 | VAL  | C-N-CA | 8.30  | 130.25      | 121.45   |
| 9   | B     | 222 | LEU  | N-CA-C | -8.30 | 103.67      | 113.88   |
| 18  | K     | 349 | ARG  | CA-C-N | 8.30  | 131.75      | 120.38   |
| 18  | K     | 349 | ARG  | C-N-CA | 8.30  | 131.75      | 120.38   |
| 17  | J     | 142 | VAL  | CA-C-N | 8.29  | 130.20      | 119.84   |
| 17  | J     | 142 | VAL  | C-N-CA | 8.29  | 130.20      | 119.84   |
| 22  | O     | 356 | ARG  | N-CA-C | 8.28  | 122.46      | 111.28   |
| 10  | C     | 174 | THR  | CA-C-N | 8.28  | 132.05      | 120.29   |
| 10  | C     | 174 | THR  | C-N-CA | 8.28  | 132.05      | 120.29   |
| 20  | M     | 319 | ASP  | N-CA-C | -8.28 | 101.19      | 112.03   |
| 30  | W     | 160 | ALA  | N-CA-C | 8.27  | 120.08      | 111.14   |
| 18  | K     | 127 | ASP  | CA-C-N | 8.27  | 131.71      | 120.38   |
| 18  | K     | 127 | ASP  | C-N-CA | 8.27  | 131.71      | 120.38   |
| 23  | P     | 129 | LYS  | N-CA-C | -8.27 | 104.33      | 114.75   |
| 16  | I     | 90  | GLU  | O-C-N  | 8.27  | 130.58      | 122.07   |
| 18  | K     | 230 | THR  | N-CA-C | -8.26 | 102.98      | 113.23   |
| 20  | M     | 426 | LYS  | N-CA-C | -8.26 | 95.03       | 109.06   |
| 8   | A     | 206 | ALA  | CA-C-N | 8.25  | 130.95      | 120.56   |
| 8   | A     | 206 | ALA  | C-N-CA | 8.25  | 130.95      | 120.56   |
| 20  | M     | 186 | LEU  | N-CA-C | -8.25 | 102.24      | 112.88   |
| 24  | Q     | 352 | GLU  | CA-C-N | 8.25  | 127.90      | 119.82   |
| 24  | Q     | 352 | GLU  | C-N-CA | 8.25  | 127.90      | 119.82   |
| 33  | Z     | 166 | ASN  | CA-C-N | 8.24  | 131.15      | 120.44   |
| 33  | Z     | 166 | ASN  | C-N-CA | 8.24  | 131.15      | 120.44   |
| 3   | 3     | 24  | SER  | N-CA-C | -8.22 | 103.25      | 113.28   |
| 9   | B     | 122 | THR  | N-CA-C | -8.22 | 102.84      | 113.12   |
| 33  | Z     | 474 | LEU  | CA-C-N | 8.22  | 131.12      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 474 | LEU  | C-N-CA | 8.22  | 131.12      | 120.44   |
| 21  | N     | 477 | SER  | CA-C-N | 8.21  | 130.41      | 120.14   |
| 21  | N     | 477 | SER  | C-N-CA | 8.21  | 130.41      | 120.14   |
| 19  | L     | 203 | ASN  | CA-C-O | -8.21 | 111.03      | 119.49   |
| 20  | M     | 430 | VAL  | N-CA-C | -8.21 | 98.52       | 108.53   |
| 18  | K     | 211 | LEU  | N-CA-C | -8.21 | 95.52       | 108.90   |
| 6   | 6     | 129 | ALA  | N-CA-C | -8.20 | 96.32       | 109.76   |
| 21  | N     | 885 | ILE  | O-C-N  | -8.20 | 114.33      | 123.18   |
| 19  | L     | 233 | LYS  | N-CA-C | 8.19  | 119.83      | 111.07   |
| 7   | 7     | 29  | ASN  | CA-C-O | 8.19  | 129.00      | 120.40   |
| 17  | J     | 30  | THR  | CA-C-N | 8.19  | 131.60      | 120.38   |
| 17  | J     | 30  | THR  | C-N-CA | 8.19  | 131.60      | 120.38   |
| 33  | Z     | 791 | LYS  | CA-C-N | 8.19  | 131.68      | 120.46   |
| 33  | Z     | 791 | LYS  | C-N-CA | 8.19  | 131.68      | 120.46   |
| 22  | O     | 368 | ASP  | CA-C-N | 8.18  | 131.07      | 120.44   |
| 22  | O     | 368 | ASP  | C-N-CA | 8.18  | 131.07      | 120.44   |
| 24  | Q     | 371 | GLN  | CA-C-N | 8.18  | 131.24      | 120.28   |
| 24  | Q     | 371 | GLN  | C-N-CA | 8.18  | 131.24      | 120.28   |
| 14  | G     | 115 | LEU  | CA-C-N | 8.17  | 128.84      | 119.94   |
| 14  | G     | 115 | LEU  | C-N-CA | 8.17  | 128.84      | 119.94   |
| 23  | P     | 382 | ASP  | CA-C-O | -8.17 | 111.76      | 120.42   |
| 20  | M     | 366 | ARG  | CA-C-N | 8.16  | 131.87      | 120.29   |
| 20  | M     | 366 | ARG  | C-N-CA | 8.16  | 131.87      | 120.29   |
| 21  | N     | 908 | ARG  | N-CA-C | 8.16  | 119.80      | 111.07   |
| 12  | E     | 61  | SER  | CA-C-N | 8.15  | 135.32      | 123.17   |
| 12  | E     | 61  | SER  | C-N-CA | 8.15  | 135.32      | 123.17   |
| 27  | T     | 97  | SER  | CA-C-N | 8.15  | 136.00      | 122.87   |
| 27  | T     | 97  | SER  | C-N-CA | 8.15  | 136.00      | 122.87   |
| 24  | Q     | 286 | TYR  | N-CA-C | -8.15 | 102.38      | 113.30   |
| 27  | T     | 125 | GLU  | CA-C-N | 8.14  | 131.19      | 120.28   |
| 27  | T     | 125 | GLU  | C-N-CA | 8.14  | 131.19      | 120.28   |
| 21  | N     | 715 | ILE  | N-CA-C | -8.14 | 96.78       | 108.17   |
| 28  | U     | 287 | ALA  | CA-C-N | 8.13  | 131.01      | 120.44   |
| 28  | U     | 287 | ALA  | C-N-CA | 8.13  | 131.01      | 120.44   |
| 22  | O     | 69  | PHE  | CA-C-N | 8.13  | 131.98      | 120.28   |
| 22  | O     | 69  | PHE  | C-N-CA | 8.13  | 131.98      | 120.28   |
| 18  | K     | 130 | LEU  | N-CA-C | -8.13 | 101.48      | 112.94   |
| 25  | R     | 129 | GLU  | CA-C-N | 8.12  | 131.51      | 120.38   |
| 25  | R     | 129 | GLU  | C-N-CA | 8.12  | 131.51      | 120.38   |
| 7   | 7     | 60  | LYS  | CA-C-N | 8.12  | 131.82      | 120.29   |
| 7   | 7     | 60  | LYS  | C-N-CA | 8.12  | 131.82      | 120.29   |
| 33  | Z     | 494 | GLY  | CA-C-N | 8.11  | 130.94      | 120.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 494 | GLY  | C-N-CA | 8.11  | 130.94      | 120.56   |
| 23  | P     | 72  | TRP  | N-CA-C | 8.09  | 120.18      | 111.36   |
| 26  | S     | 176 | LEU  | N-CA-C | -8.09 | 104.56      | 114.75   |
| 24  | Q     | 310 | SER  | CA-C-N | 8.08  | 131.77      | 120.29   |
| 24  | Q     | 310 | SER  | C-N-CA | 8.08  | 131.77      | 120.29   |
| 23  | P     | 440 | HIS  | CA-C-N | 8.07  | 128.94      | 119.98   |
| 23  | P     | 440 | HIS  | C-N-CA | 8.07  | 128.94      | 119.98   |
| 23  | P     | 198 | VAL  | CA-C-O | -8.07 | 112.30      | 120.85   |
| 33  | Z     | 489 | ALA  | CA-C-O | 8.06  | 129.09      | 120.55   |
| 16  | I     | 130 | VAL  | N-CA-C | 8.05  | 126.09      | 109.34   |
| 1   | 1     | 147 | SER  | CA-C-N | 8.05  | 131.41      | 120.54   |
| 1   | 1     | 147 | SER  | C-N-CA | 8.05  | 131.41      | 120.54   |
| 26  | S     | 377 | TYR  | CA-C-N | 8.05  | 132.13      | 120.38   |
| 26  | S     | 377 | TYR  | C-N-CA | 8.05  | 132.13      | 120.38   |
| 16  | I     | 249 | GLY  | CA-C-N | 8.05  | 131.06      | 120.28   |
| 16  | I     | 249 | GLY  | C-N-CA | 8.05  | 131.06      | 120.28   |
| 33  | Z     | 63  | LEU  | CA-C-N | 8.04  | 130.89      | 120.44   |
| 33  | Z     | 63  | LEU  | C-N-CA | 8.04  | 130.89      | 120.44   |
| 22  | O     | 153 | LEU  | N-CA-C | -8.03 | 102.61      | 111.36   |
| 23  | P     | 374 | SER  | O-C-N  | 8.03  | 130.63      | 122.12   |
| 19  | L     | 336 | ALA  | O-C-N  | -8.02 | 113.62      | 122.12   |
| 21  | N     | 507 | GLU  | N-CA-C | 8.01  | 120.01      | 111.28   |
| 20  | M     | 134 | LEU  | CA-C-N | 8.00  | 132.99      | 122.51   |
| 20  | M     | 134 | LEU  | C-N-CA | 8.00  | 132.99      | 122.51   |
| 2   | 2     | 15  | ALA  | O-C-N  | -7.99 | 114.87      | 123.42   |
| 15  | H     | 453 | GLY  | CA-C-N | 7.99  | 131.64      | 120.29   |
| 15  | H     | 453 | GLY  | C-N-CA | 7.99  | 131.64      | 120.29   |
| 3   | 3     | 27  | VAL  | N-CA-C | -7.99 | 105.43      | 111.90   |
| 30  | W     | 5   | ALA  | N-CA-C | -7.98 | 96.22       | 109.07   |
| 10  | C     | 65  | LYS  | N-CA-C | -7.97 | 102.37      | 114.16   |
| 8   | A     | 77  | ARG  | N-CA-C | -7.96 | 103.78      | 113.97   |
| 22  | O     | 291 | ILE  | CA-C-N | 7.96  | 131.60      | 120.29   |
| 22  | O     | 291 | ILE  | C-N-CA | 7.96  | 131.60      | 120.29   |
| 6   | 6     | 36  | ASP  | CA-C-O | -7.96 | 112.06      | 120.58   |
| 16  | I     | 329 | ASN  | CA-C-O | 7.96  | 128.91      | 119.60   |
| 6   | 6     | 131 | GLY  | CA-C-N | 7.96  | 130.94      | 120.28   |
| 6   | 6     | 131 | GLY  | C-N-CA | 7.96  | 130.94      | 120.28   |
| 16  | I     | 164 | ALA  | N-CA-C | -7.95 | 102.88      | 112.58   |
| 26  | S     | 200 | GLU  | N-CA-C | -7.95 | 102.56      | 114.64   |
| 21  | N     | 410 | LEU  | O-C-N  | 7.94  | 130.35      | 122.09   |
| 5   | 5     | 199 | LYS  | CA-C-N | 7.94  | 131.33      | 120.46   |
| 5   | 5     | 199 | LYS  | C-N-CA | 7.94  | 131.33      | 120.46   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | P     | 181 | LEU  | CA-C-N  | 7.92  | 130.90      | 120.28   |
| 23  | P     | 181 | LEU  | C-N-CA  | 7.92  | 130.90      | 120.28   |
| 6   | 6     | 182 | ALA  | N-CA-C  | 7.92  | 119.91      | 111.28   |
| 11  | D     | 226 | SER  | N-CA-C  | 7.92  | 120.61      | 111.11   |
| 15  | H     | 280 | VAL  | CB-CA-C | -7.92 | 102.68      | 111.23   |
| 20  | M     | 159 | LEU  | CA-C-N  | 7.91  | 127.95      | 119.89   |
| 20  | M     | 159 | LEU  | C-N-CA  | 7.91  | 127.95      | 119.89   |
| 30  | W     | 153 | LEU  | CA-C-N  | 7.91  | 131.66      | 120.28   |
| 30  | W     | 153 | LEU  | C-N-CA  | 7.91  | 131.66      | 120.28   |
| 21  | N     | 371 | LEU  | CA-C-N  | 7.90  | 130.25      | 120.22   |
| 21  | N     | 371 | LEU  | C-N-CA  | 7.90  | 130.25      | 120.22   |
| 19  | L     | 422 | VAL  | CA-C-N  | 7.90  | 130.86      | 120.28   |
| 19  | L     | 422 | VAL  | C-N-CA  | 7.90  | 130.86      | 120.28   |
| 17  | J     | 259 | GLU  | N-CA-C  | -7.89 | 103.22      | 112.92   |
| 25  | R     | 27  | SER  | CA-C-N  | 7.89  | 130.85      | 120.28   |
| 25  | R     | 27  | SER  | C-N-CA  | 7.89  | 130.85      | 120.28   |
| 15  | H     | 193 | PRO  | CA-C-N  | 7.88  | 136.45      | 122.89   |
| 15  | H     | 193 | PRO  | C-N-CA  | 7.88  | 136.45      | 122.89   |
| 29  | V     | 64  | ASN  | CA-C-O  | -7.87 | 111.85      | 120.43   |
| 23  | P     | 292 | LYS  | CA-C-N  | 7.87  | 130.83      | 120.28   |
| 23  | P     | 292 | LYS  | C-N-CA  | 7.87  | 130.83      | 120.28   |
| 30  | W     | 163 | ASN  | CA-C-N  | 7.87  | 129.68      | 119.84   |
| 30  | W     | 163 | ASN  | C-N-CA  | 7.87  | 129.68      | 119.84   |
| 18  | K     | 242 | PHE  | N-CA-C  | -7.87 | 103.13      | 112.89   |
| 6   | 6     | 48  | PHE  | CA-C-N  | 7.87  | 130.82      | 120.28   |
| 6   | 6     | 48  | PHE  | C-N-CA  | 7.87  | 130.82      | 120.28   |
| 6   | 6     | 132 | ALA  | N-CA-C  | 7.87  | 119.86      | 111.28   |
| 4   | 4     | 186 | ASP  | N-CA-C  | -7.86 | 103.71      | 113.38   |
| 10  | C     | 71  | ASP  | N-CA-C  | -7.86 | 103.26      | 113.17   |
| 28  | U     | 233 | PHE  | O-C-N   | 7.86  | 130.26      | 122.09   |
| 33  | Z     | 241 | THR  | CA-C-N  | 7.86  | 130.81      | 120.28   |
| 33  | Z     | 241 | THR  | C-N-CA  | 7.86  | 130.81      | 120.28   |
| 7   | 7     | 75  | ALA  | N-CA-C  | -7.84 | 100.56      | 113.50   |
| 23  | P     | 300 | VAL  | N-CA-C  | -7.84 | 102.80      | 110.72   |
| 17  | J     | 31  | GLU  | CA-C-N  | 7.83  | 130.77      | 120.28   |
| 17  | J     | 31  | GLU  | C-N-CA  | 7.83  | 130.77      | 120.28   |
| 30  | W     | 162 | ASN  | CA-C-N  | 7.82  | 135.91      | 122.38   |
| 30  | W     | 162 | ASN  | C-N-CA  | 7.82  | 135.91      | 122.38   |
| 21  | N     | 205 | SER  | CA-C-O  | -7.82 | 112.26      | 120.55   |
| 21  | N     | 375 | HIS  | N-CA-C  | -7.82 | 103.30      | 112.92   |
| 22  | O     | 254 | LEU  | CA-C-N  | 7.82  | 130.75      | 120.28   |
| 22  | O     | 254 | LEU  | C-N-CA  | 7.82  | 130.75      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 20  | M     | 286 | ILE  | N-CA-C | -7.82 | 104.91      | 113.43   |
| 26  | S     | 156 | VAL  | CA-C-N | 7.82  | 130.60      | 120.44   |
| 26  | S     | 156 | VAL  | C-N-CA | 7.82  | 130.60      | 120.44   |
| 15  | H     | 383 | GLU  | O-C-N  | -7.81 | 113.84      | 122.12   |
| 26  | S     | 394 | ILE  | CA-C-N | 7.80  | 132.16      | 120.77   |
| 26  | S     | 394 | ILE  | C-N-CA | 7.80  | 132.16      | 120.77   |
| 18  | K     | 368 | LEU  | CA-C-N | 7.79  | 130.72      | 120.28   |
| 18  | K     | 368 | LEU  | C-N-CA | 7.79  | 130.72      | 120.28   |
| 33  | Z     | 107 | THR  | N-CA-C | -7.79 | 103.35      | 113.17   |
| 12  | E     | 173 | GLY  | CA-C-O | -7.78 | 113.83      | 122.24   |
| 24  | Q     | 270 | ILE  | CA-C-O | -7.78 | 112.86      | 120.95   |
| 21  | N     | 623 | PHE  | CA-C-N | 7.77  | 130.69      | 120.28   |
| 21  | N     | 623 | PHE  | C-N-CA | 7.77  | 130.69      | 120.28   |
| 33  | Z     | 77  | ASN  | N-CA-C | -7.77 | 94.24       | 110.80   |
| 15  | H     | 242 | PRO  | CA-C-N | 7.77  | 129.55      | 119.84   |
| 15  | H     | 242 | PRO  | C-N-CA | 7.77  | 129.55      | 119.84   |
| 18  | K     | 407 | LEU  | CA-C-N | 7.77  | 130.69      | 120.28   |
| 18  | K     | 407 | LEU  | C-N-CA | 7.77  | 130.69      | 120.28   |
| 24  | Q     | 121 | SER  | CA-C-N | 7.76  | 131.44      | 120.42   |
| 24  | Q     | 121 | SER  | C-N-CA | 7.76  | 131.44      | 120.42   |
| 12  | E     | 243 | LEU  | N-CA-C | -7.76 | 102.76      | 111.14   |
| 26  | S     | 127 | THR  | N-CA-C | 7.76  | 119.37      | 111.07   |
| 7   | 7     | 153 | ARG  | CA-C-N | 7.75  | 130.67      | 120.28   |
| 7   | 7     | 153 | ARG  | C-N-CA | 7.75  | 130.67      | 120.28   |
| 21  | N     | 722 | THR  | N-CA-C | -7.75 | 102.70      | 114.16   |
| 33  | Z     | 470 | ALA  | CA-C-N | 7.74  | 130.51      | 120.44   |
| 33  | Z     | 470 | ALA  | C-N-CA | 7.74  | 130.51      | 120.44   |
| 33  | Z     | 587 | THR  | N-CA-C | -7.74 | 102.78      | 111.07   |
| 26  | S     | 293 | ILE  | CA-C-N | 7.74  | 131.07      | 120.46   |
| 26  | S     | 293 | ILE  | C-N-CA | 7.74  | 131.07      | 120.46   |
| 33  | Z     | 64  | TYR  | N-CA-C | -7.74 | 102.79      | 111.07   |
| 10  | C     | 186 | VAL  | N-CA-C | 7.74  | 118.48      | 110.36   |
| 14  | G     | 20  | ASN  | CA-C-N | 7.73  | 130.97      | 120.38   |
| 14  | G     | 20  | ASN  | C-N-CA | 7.73  | 130.97      | 120.38   |
| 18  | K     | 220 | THR  | CA-C-N | 7.73  | 130.49      | 120.44   |
| 18  | K     | 220 | THR  | C-N-CA | 7.73  | 130.49      | 120.44   |
| 21  | N     | 573 | HIS  | CA-C-N | 7.73  | 130.30      | 120.56   |
| 21  | N     | 573 | HIS  | C-N-CA | 7.73  | 130.30      | 120.56   |
| 25  | R     | 150 | ALA  | N-CA-C | 7.73  | 119.71      | 111.28   |
| 4   | 4     | 12  | VAL  | O-C-N  | -7.72 | 114.92      | 123.26   |
| 27  | T     | 263 | ALA  | N-CA-C | 7.72  | 119.69      | 111.28   |
| 26  | S     | 215 | MET  | CA-C-N | 7.71  | 130.62      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 26  | S     | 215 | MET  | C-N-CA | 7.71  | 130.62      | 120.28   |
| 26  | S     | 223 | LEU  | CA-C-O | 7.71  | 128.96      | 119.78   |
| 7   | 7     | 168 | ALA  | CA-C-N | 7.71  | 130.28      | 120.56   |
| 7   | 7     | 168 | ALA  | C-N-CA | 7.71  | 130.28      | 120.56   |
| 21  | N     | 901 | GLY  | CA-C-N | 7.71  | 130.89      | 120.63   |
| 21  | N     | 901 | GLY  | C-N-CA | 7.71  | 130.89      | 120.63   |
| 5   | 5     | 204 | GLU  | CA-C-O | -7.71 | 110.60      | 120.00   |
| 14  | G     | 27  | VAL  | N-CA-C | 7.70  | 119.40      | 110.62   |
| 17  | J     | 201 | ALA  | N-CA-C | 7.69  | 119.30      | 111.07   |
| 24  | Q     | 31  | LEU  | CA-C-N | 7.69  | 132.00      | 120.31   |
| 24  | Q     | 31  | LEU  | C-N-CA | 7.69  | 132.00      | 120.31   |
| 2   | 2     | 160 | GLN  | CA-C-N | 7.69  | 130.58      | 120.28   |
| 2   | 2     | 160 | GLN  | C-N-CA | 7.69  | 130.58      | 120.28   |
| 20  | M     | 420 | SER  | O-C-N  | 7.68  | 130.26      | 122.12   |
| 22  | O     | 67  | SER  | N-CA-C | -7.67 | 103.00      | 111.36   |
| 13  | F     | 207 | THR  | CA-C-N | 7.67  | 130.23      | 120.56   |
| 13  | F     | 207 | THR  | C-N-CA | 7.67  | 130.23      | 120.56   |
| 2   | 2     | 161 | ALA  | CA-C-O | 7.67  | 128.68      | 120.55   |
| 25  | R     | 416 | LYS  | CA-C-N | 7.66  | 130.55      | 120.28   |
| 25  | R     | 416 | LYS  | C-N-CA | 7.66  | 130.55      | 120.28   |
| 26  | S     | 231 | ALA  | CA-C-O | -7.65 | 112.31      | 120.42   |
| 1   | 1     | 35  | THR  | N-CA-C | -7.65 | 96.43       | 108.90   |
| 1   | 1     | 134 | ILE  | N-CA-C | -7.64 | 105.40      | 112.43   |
| 3   | 3     | 81  | LEU  | CA-C-N | 7.63  | 130.18      | 120.56   |
| 3   | 3     | 81  | LEU  | C-N-CA | 7.63  | 130.18      | 120.56   |
| 4   | 4     | 81  | SER  | CA-C-O | 7.63  | 128.51      | 120.42   |
| 33  | Z     | 799 | PHE  | CA-C-N | 7.63  | 130.50      | 120.28   |
| 33  | Z     | 799 | PHE  | C-N-CA | 7.63  | 130.50      | 120.28   |
| 30  | W     | 121 | SER  | CA-C-N | 7.62  | 130.49      | 120.28   |
| 30  | W     | 121 | SER  | C-N-CA | 7.62  | 130.49      | 120.28   |
| 26  | S     | 268 | LEU  | CA-C-N | 7.62  | 130.34      | 120.44   |
| 26  | S     | 268 | LEU  | C-N-CA | 7.62  | 130.34      | 120.44   |
| 17  | J     | 192 | GLY  | CA-C-N | 7.62  | 130.49      | 120.28   |
| 17  | J     | 192 | GLY  | C-N-CA | 7.62  | 130.49      | 120.28   |
| 21  | N     | 313 | LEU  | CA-C-O | -7.62 | 112.82      | 120.82   |
| 8   | A     | 235 | THR  | CA-C-O | 7.61  | 129.25      | 120.80   |
| 23  | P     | 118 | VAL  | CA-C-N | 7.61  | 131.22      | 120.42   |
| 23  | P     | 118 | VAL  | C-N-CA | 7.61  | 131.22      | 120.42   |
| 17  | J     | 299 | ILE  | N-CA-C | -7.61 | 105.14      | 113.43   |
| 21  | N     | 378 | ASN  | N-CA-C | -7.61 | 96.50       | 108.90   |
| 22  | O     | 354 | GLN  | CA-C-O | -7.60 | 112.41      | 120.70   |
| 8   | A     | 211 | ILE  | N-CA-C | -7.60 | 103.12      | 110.42   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13  | F     | 117 | GLN  | CA-C-N | 7.60  | 131.22      | 120.28   |
| 13  | F     | 117 | GLN  | C-N-CA | 7.60  | 131.22      | 120.28   |
| 28  | U     | 289 | ASP  | O-C-N  | -7.60 | 114.19      | 122.09   |
| 21  | N     | 481 | ALA  | CA-C-N | 7.59  | 130.76      | 120.44   |
| 21  | N     | 481 | ALA  | C-N-CA | 7.59  | 130.76      | 120.44   |
| 27  | T     | 28  | PRO  | CA-C-N | 7.59  | 127.63      | 119.28   |
| 27  | T     | 28  | PRO  | C-N-CA | 7.59  | 127.63      | 119.28   |
| 11  | D     | 188 | VAL  | CA-C-N | 7.58  | 130.30      | 120.44   |
| 11  | D     | 188 | VAL  | C-N-CA | 7.58  | 130.30      | 120.44   |
| 14  | G     | 200 | TYR  | N-CA-C | 7.58  | 119.18      | 111.07   |
| 6   | 6     | 66  | TYR  | O-C-N  | 7.58  | 130.27      | 122.09   |
| 8   | A     | 224 | GLU  | N-CA-C | -7.58 | 94.84       | 108.48   |
| 24  | Q     | 150 | GLN  | N-CA-C | -7.58 | 99.03       | 109.71   |
| 29  | V     | 49  | VAL  | O-C-N  | -7.58 | 114.89      | 123.00   |
| 27  | T     | 261 | GLU  | CA-C-O | 7.57  | 128.50      | 120.70   |
| 4   | 4     | 167 | LEU  | N-CA-C | 7.57  | 119.53      | 111.28   |
| 2   | 2     | 59  | ILE  | CA-C-O | 7.56  | 128.86      | 120.85   |
| 14  | G     | 69  | VAL  | N-CA-C | -7.56 | 97.23       | 108.12   |
| 25  | R     | 355 | SER  | N-CA-C | 7.56  | 119.16      | 111.07   |
| 21  | N     | 921 | ARG  | N-CA-C | -7.56 | 103.52      | 112.89   |
| 28  | U     | 64  | ASP  | N-CA-C | -7.56 | 104.09      | 113.38   |
| 19  | L     | 351 | LEU  | CA-C-N | 7.55  | 128.00      | 119.92   |
| 19  | L     | 351 | LEU  | C-N-CA | 7.55  | 128.00      | 119.92   |
| 21  | N     | 735 | MET  | CA-C-N | 7.55  | 130.40      | 120.28   |
| 21  | N     | 735 | MET  | C-N-CA | 7.55  | 130.40      | 120.28   |
| 25  | R     | 368 | LEU  | CA-C-N | 7.55  | 129.57      | 120.14   |
| 25  | R     | 368 | LEU  | C-N-CA | 7.55  | 129.57      | 120.14   |
| 22  | O     | 361 | ASP  | N-CA-C | -7.55 | 103.06      | 112.72   |
| 25  | R     | 367 | ASP  | N-CA-C | -7.54 | 103.87      | 113.23   |
| 27  | T     | 207 | ALA  | N-CA-C | 7.54  | 119.58      | 111.36   |
| 15  | H     | 340 | LEU  | O-C-N  | 7.54  | 130.17      | 122.03   |
| 15  | H     | 345 | PRO  | CA-C-O | -7.54 | 112.71      | 121.98   |
| 33  | Z     | 418 | ALA  | CA-C-N | 7.53  | 130.05      | 120.56   |
| 33  | Z     | 418 | ALA  | C-N-CA | 7.53  | 130.05      | 120.56   |
| 33  | Z     | 775 | MET  | N-CA-C | 7.53  | 120.36      | 111.71   |
| 21  | N     | 582 | ASP  | CA-C-N | 7.52  | 130.77      | 120.46   |
| 21  | N     | 582 | ASP  | C-N-CA | 7.52  | 130.77      | 120.46   |
| 7   | 7     | 131 | SER  | N-CA-C | -7.52 | 101.45      | 108.22   |
| 20  | M     | 116 | ALA  | N-CA-C | -7.52 | 97.42       | 109.76   |
| 22  | O     | 259 | THR  | CA-C-N | 7.52  | 130.19      | 120.56   |
| 22  | O     | 259 | THR  | C-N-CA | 7.52  | 130.19      | 120.56   |
| 9   | B     | 243 | ILE  | CA-C-N | 7.52  | 130.68      | 120.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | B     | 243 | ILE  | C-N-CA | 7.52  | 130.68      | 120.38   |
| 22  | O     | 23  | HIS  | O-C-N  | -7.52 | 116.59      | 121.85   |
| 14  | G     | 55  | SER  | N-CA-C | -7.52 | 97.64       | 109.07   |
| 18  | K     | 265 | ALA  | O-C-N  | -7.52 | 112.68      | 121.32   |
| 22  | O     | 126 | ILE  | N-CA-C | 7.51  | 117.63      | 110.42   |
| 8   | A     | 210 | MET  | CA-C-N | 7.51  | 130.03      | 120.56   |
| 8   | A     | 210 | MET  | C-N-CA | 7.51  | 130.03      | 120.56   |
| 19  | L     | 355 | ALA  | CA-C-N | 7.51  | 128.26      | 120.00   |
| 19  | L     | 355 | ALA  | C-N-CA | 7.51  | 128.26      | 120.00   |
| 30  | W     | 64  | THR  | CA-C-N | 7.51  | 131.41      | 120.82   |
| 30  | W     | 64  | THR  | C-N-CA | 7.51  | 131.41      | 120.82   |
| 14  | G     | 232 | GLY  | CA-C-N | 7.50  | 130.67      | 120.54   |
| 14  | G     | 232 | GLY  | C-N-CA | 7.50  | 130.67      | 120.54   |
| 25  | R     | 77  | SER  | N-CA-C | -7.50 | 102.36      | 112.94   |
| 21  | N     | 166 | ILE  | CA-C-N | 7.50  | 130.55      | 120.65   |
| 21  | N     | 166 | ILE  | C-N-CA | 7.50  | 130.55      | 120.65   |
| 33  | Z     | 293 | MET  | CA-C-N | 7.50  | 130.74      | 120.46   |
| 33  | Z     | 293 | MET  | C-N-CA | 7.50  | 130.74      | 120.46   |
| 10  | C     | 175 | LEU  | CA-C-N | 7.50  | 130.64      | 120.44   |
| 10  | C     | 175 | LEU  | C-N-CA | 7.50  | 130.64      | 120.44   |
| 21  | N     | 912 | GLU  | N-CA-C | 7.50  | 114.97      | 108.22   |
| 1   | 1     | 26  | ILE  | CA-C-N | 7.50  | 130.33      | 120.28   |
| 1   | 1     | 26  | ILE  | C-N-CA | 7.50  | 130.33      | 120.28   |
| 4   | 4     | 110 | LYS  | N-CA-C | -7.50 | 106.08      | 114.62   |
| 3   | 3     | 123 | GLU  | N-CA-C | 7.49  | 121.17      | 107.99   |
| 10  | C     | 209 | ASP  | CA-C-O | 7.49  | 127.69      | 119.15   |
| 30  | W     | 194 | GLU  | CA-C-N | 7.49  | 128.25      | 119.94   |
| 30  | W     | 194 | GLU  | C-N-CA | 7.49  | 128.25      | 119.94   |
| 9   | B     | 71  | ILE  | CA-C-N | 7.49  | 128.02      | 121.58   |
| 9   | B     | 71  | ILE  | C-N-CA | 7.49  | 128.02      | 121.58   |
| 11  | D     | 56  | ASP  | N-CA-C | -7.48 | 98.92       | 109.69   |
| 17  | J     | 202 | VAL  | CA-C-N | 7.48  | 131.05      | 120.28   |
| 17  | J     | 202 | VAL  | C-N-CA | 7.48  | 131.05      | 120.28   |
| 33  | Z     | 826 | ARG  | CA-C-N | 7.48  | 131.05      | 120.28   |
| 33  | Z     | 826 | ARG  | C-N-CA | 7.48  | 131.05      | 120.28   |
| 14  | G     | 50  | GLU  | CA-C-N | -7.48 | 112.68      | 123.00   |
| 14  | G     | 50  | GLU  | C-N-CA | -7.48 | 112.68      | 123.00   |
| 26  | S     | 399 | TYR  | CA-C-N | 7.48  | 130.30      | 120.28   |
| 26  | S     | 399 | TYR  | C-N-CA | 7.48  | 130.30      | 120.28   |
| 25  | R     | 60  | ALA  | CA-C-O | -7.47 | 111.09      | 118.34   |
| 10  | C     | 141 | ASP  | N-CA-C | -7.47 | 97.71       | 109.07   |
| 9   | B     | 153 | SER  | O-C-N  | 7.47  | 130.04      | 122.12   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 22  | O     | 163 | ILE  | O-C-N  | -7.47 | 112.58      | 121.10   |
| 23  | P     | 145 | GLU  | CA-C-O | -7.47 | 112.64      | 120.55   |
| 20  | M     | 413 | GLU  | CA-C-N | 7.46  | 130.28      | 120.28   |
| 20  | M     | 413 | GLU  | C-N-CA | 7.46  | 130.28      | 120.28   |
| 10  | C     | 41  | SER  | N-CA-C | -7.46 | 104.06      | 113.02   |
| 15  | H     | 388 | ILE  | CA-C-N | 7.46  | 130.28      | 120.28   |
| 15  | H     | 388 | ILE  | C-N-CA | 7.46  | 130.28      | 120.28   |
| 21  | N     | 585 | ARG  | CA-C-N | 7.46  | 131.02      | 120.28   |
| 21  | N     | 585 | ARG  | C-N-CA | 7.46  | 131.02      | 120.28   |
| 6   | 6     | 158 | LYS  | N-CA-C | -7.46 | 103.58      | 114.39   |
| 33  | Z     | 830 | LEU  | CA-C-N | 7.45  | 130.27      | 120.28   |
| 33  | Z     | 830 | LEU  | C-N-CA | 7.45  | 130.27      | 120.28   |
| 9   | B     | 100 | ILE  | CA-C-O | 7.45  | 126.65      | 118.98   |
| 21  | N     | 586 | ALA  | N-CA-C | -7.45 | 103.14      | 111.71   |
| 28  | U     | 288 | PHE  | N-CA-C | -7.45 | 103.10      | 111.07   |
| 30  | W     | 188 | SER  | N-CA-C | -7.45 | 100.71      | 110.39   |
| 3   | 3     | 65  | TYR  | CA-C-N | 7.44  | 130.25      | 120.28   |
| 3   | 3     | 65  | TYR  | C-N-CA | 7.44  | 130.25      | 120.28   |
| 3   | 3     | 54  | LEU  | CA-C-N | 7.44  | 130.11      | 120.44   |
| 3   | 3     | 54  | LEU  | C-N-CA | 7.44  | 130.11      | 120.44   |
| 14  | G     | 172 | LYS  | CA-C-N | 7.44  | 130.11      | 120.44   |
| 14  | G     | 172 | LYS  | C-N-CA | 7.44  | 130.11      | 120.44   |
| 20  | M     | 359 | GLN  | CA-C-N | 7.44  | 130.65      | 120.46   |
| 20  | M     | 359 | GLN  | C-N-CA | 7.44  | 130.65      | 120.46   |
| 14  | G     | 91  | GLY  | CA-C-N | 7.44  | 130.55      | 120.44   |
| 14  | G     | 91  | GLY  | C-N-CA | 7.44  | 130.55      | 120.44   |
| 15  | H     | 375 | VAL  | CA-C-N | 7.44  | 132.05      | 121.42   |
| 15  | H     | 375 | VAL  | C-N-CA | 7.44  | 132.05      | 121.42   |
| 12  | E     | 26  | TYR  | CA-C-N | 7.43  | 130.24      | 120.28   |
| 12  | E     | 26  | TYR  | C-N-CA | 7.43  | 130.24      | 120.28   |
| 21  | N     | 257 | ILE  | O-C-N  | -7.43 | 114.63      | 121.91   |
| 33  | Z     | 917 | ASN  | N-CA-C | -7.42 | 104.26      | 113.38   |
| 12  | E     | 22  | PHE  | CA-C-N | 7.41  | 130.21      | 120.28   |
| 12  | E     | 22  | PHE  | C-N-CA | 7.41  | 130.21      | 120.28   |
| 23  | P     | 174 | SER  | O-C-N  | 7.41  | 129.98      | 122.12   |
| 1   | 1     | 61  | TYR  | CA-C-O | -7.41 | 113.04      | 120.82   |
| 33  | Z     | 599 | ILE  | O-C-N  | -7.41 | 113.43      | 121.80   |
| 24  | Q     | 135 | HIS  | N-CA-C | -7.41 | 103.28      | 111.36   |
| 26  | S     | 365 | THR  | CA-C-O | -7.41 | 112.98      | 120.90   |
| 32  | Y     | 77  | LEU  | O-C-N  | 7.41  | 129.70      | 122.07   |
| 31  | X     | 28  | PRO  | O-C-N  | 7.40  | 132.63      | 122.64   |
| 23  | P     | 267 | PHE  | CA-C-O | -7.40 | 113.05      | 120.82   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | I     | 392 | ILE  | CA-C-N | 7.40  | 130.19      | 120.28   |
| 16  | I     | 392 | ILE  | C-N-CA | 7.40  | 130.19      | 120.28   |
| 10  | C     | 169 | THR  | CA-C-N | 7.39  | 130.05      | 120.44   |
| 10  | C     | 169 | THR  | C-N-CA | 7.39  | 130.05      | 120.44   |
| 20  | M     | 222 | GLY  | CA-C-N | 7.39  | 128.00      | 120.38   |
| 20  | M     | 222 | GLY  | C-N-CA | 7.39  | 128.00      | 120.38   |
| 20  | M     | 400 | MET  | N-CA-C | 7.38  | 119.33      | 111.28   |
| 7   | 7     | 202 | LYS  | CA-C-N | 7.38  | 132.59      | 122.19   |
| 7   | 7     | 202 | LYS  | C-N-CA | 7.38  | 132.59      | 122.19   |
| 33  | Z     | 487 | SER  | CA-C-N | 7.37  | 130.75      | 120.29   |
| 33  | Z     | 487 | SER  | C-N-CA | 7.37  | 130.75      | 120.29   |
| 17  | J     | 395 | GLU  | CA-C-N | 7.36  | 134.95      | 121.70   |
| 17  | J     | 395 | GLU  | C-N-CA | 7.36  | 134.95      | 121.70   |
| 22  | O     | 10  | ILE  | CA-C-N | 7.36  | 130.14      | 120.28   |
| 22  | O     | 10  | ILE  | C-N-CA | 7.36  | 130.14      | 120.28   |
| 11  | D     | 114 | ALA  | CA-C-N | 7.36  | 128.15      | 119.98   |
| 11  | D     | 114 | ALA  | C-N-CA | 7.36  | 128.15      | 119.98   |
| 33  | Z     | 488 | ALA  | CA-C-O | -7.36 | 112.62      | 120.42   |
| 21  | N     | 70  | TYR  | CA-C-O | -7.36 | 113.03      | 120.90   |
| 25  | R     | 272 | ASP  | N-CA-C | -7.36 | 102.39      | 112.03   |
| 11  | D     | 54  | LEU  | N-CA-C | -7.35 | 101.38      | 113.50   |
| 13  | F     | 90  | GLN  | CA-C-N | 7.35  | 130.12      | 120.28   |
| 13  | F     | 90  | GLN  | C-N-CA | 7.35  | 130.12      | 120.28   |
| 28  | U     | 73  | ILE  | N-CA-C | -7.34 | 103.37      | 110.42   |
| 29  | V     | 236 | SER  | CA-C-N | 7.34  | 129.99      | 120.44   |
| 29  | V     | 236 | SER  | C-N-CA | 7.34  | 129.99      | 120.44   |
| 5   | 5     | 153 | ALA  | CA-C-O | -7.34 | 113.11      | 120.82   |
| 17  | J     | 24  | GLU  | CA-C-N | 7.34  | 130.12      | 120.28   |
| 17  | J     | 24  | GLU  | C-N-CA | 7.34  | 130.12      | 120.28   |
| 6   | 6     | 68  | PHE  | N-CA-C | 7.34  | 118.97      | 110.97   |
| 21  | N     | 389 | TYR  | N-CA-C | -7.34 | 102.30      | 113.89   |
| 26  | S     | 168 | LEU  | O-C-N  | 7.33  | 129.89      | 122.12   |
| 18  | K     | 264 | ASN  | N-CA-C | -7.33 | 102.28      | 112.25   |
| 21  | N     | 545 | SER  | CA-C-N | 7.33  | 130.10      | 120.28   |
| 21  | N     | 545 | SER  | C-N-CA | 7.33  | 130.10      | 120.28   |
| 21  | N     | 361 | ASN  | N-CA-C | 7.33  | 119.27      | 111.28   |
| 21  | N     | 410 | LEU  | N-CA-C | 7.33  | 119.90      | 111.11   |
| 24  | Q     | 267 | LEU  | CA-C-O | 7.32  | 128.31      | 120.55   |
| 14  | G     | 17  | ASP  | N-CA-C | -7.32 | 103.95      | 113.17   |
| 16  | I     | 250 | SER  | N-CA-C | 7.31  | 119.25      | 111.28   |
| 22  | O     | 369 | ARG  | CA-C-N | 7.31  | 130.41      | 120.54   |
| 22  | O     | 369 | ARG  | C-N-CA | 7.31  | 130.41      | 120.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | N     | 249 | ASN  | O-C-N   | 7.30  | 132.31      | 122.59   |
| 27  | T     | 35  | ILE  | CA-C-N  | 7.30  | 130.07      | 120.28   |
| 27  | T     | 35  | ILE  | C-N-CA  | 7.30  | 130.07      | 120.28   |
| 25  | R     | 48  | GLU  | N-CA-C  | 7.30  | 119.24      | 111.28   |
| 29  | V     | 144 | ILE  | N-CA-C  | -7.29 | 102.07      | 112.35   |
| 9   | B     | 154 | GLY  | CA-C-N  | 7.29  | 131.06      | 120.71   |
| 9   | B     | 154 | GLY  | C-N-CA  | 7.29  | 131.06      | 120.71   |
| 19  | L     | 90  | LYS  | CA-C-N  | 7.29  | 130.05      | 120.28   |
| 19  | L     | 90  | LYS  | C-N-CA  | 7.29  | 130.05      | 120.28   |
| 29  | V     | 37  | MET  | CA-C-N  | 7.29  | 130.64      | 120.29   |
| 29  | V     | 37  | MET  | C-N-CA  | 7.29  | 130.64      | 120.29   |
| 33  | Z     | 401 | VAL  | CA-C-N  | 7.29  | 129.91      | 120.44   |
| 33  | Z     | 401 | VAL  | C-N-CA  | 7.29  | 129.91      | 120.44   |
| 12  | E     | 160 | PRO  | CA-C-N  | 7.28  | 130.63      | 120.29   |
| 12  | E     | 160 | PRO  | C-N-CA  | 7.28  | 130.63      | 120.29   |
| 29  | V     | 239 | ALA  | CA-C-O  | -7.28 | 112.83      | 120.55   |
| 21  | N     | 32  | VAL  | CA-C-N  | 7.28  | 130.04      | 120.28   |
| 21  | N     | 32  | VAL  | C-N-CA  | 7.28  | 130.04      | 120.28   |
| 33  | Z     | 568 | LEU  | CA-C-N  | 7.28  | 130.04      | 120.28   |
| 33  | Z     | 568 | LEU  | C-N-CA  | 7.28  | 130.04      | 120.28   |
| 19  | L     | 264 | ARG  | CA-C-N  | 7.28  | 130.03      | 120.28   |
| 19  | L     | 264 | ARG  | C-N-CA  | 7.28  | 130.03      | 120.28   |
| 23  | P     | 299 | LEU  | CA-C-N  | 7.28  | 130.75      | 120.42   |
| 23  | P     | 299 | LEU  | C-N-CA  | 7.28  | 130.75      | 120.42   |
| 17  | J     | 368 | TYR  | CA-C-O  | -7.27 | 112.71      | 120.42   |
| 13  | F     | 150 | SER  | N-CA-C  | -7.27 | 102.34      | 112.45   |
| 19  | L     | 339 | ARG  | CA-C-O  | -7.27 | 112.53      | 119.80   |
| 24  | Q     | 233 | LYS  | CA-C-N  | 7.27  | 130.61      | 120.29   |
| 24  | Q     | 233 | LYS  | C-N-CA  | 7.27  | 130.61      | 120.29   |
| 33  | Z     | 207 | ILE  | CA-C-O  | -7.26 | 113.39      | 120.95   |
| 15  | H     | 452 | SER  | CA-C-N  | 7.26  | 129.21      | 120.14   |
| 15  | H     | 452 | SER  | C-N-CA  | 7.26  | 129.21      | 120.14   |
| 23  | P     | 109 | SER  | CB-CA-C | -7.26 | 108.19      | 116.54   |
| 20  | M     | 356 | SER  | N-CA-C  | 7.25  | 119.27      | 111.36   |
| 5   | 5     | 152 | ASP  | O-C-N   | 7.25  | 131.19      | 122.27   |
| 15  | H     | 207 | THR  | CA-C-O  | -7.25 | 112.96      | 121.44   |
| 21  | N     | 211 | PHE  | N-CA-C  | -7.25 | 102.56      | 111.40   |
| 2   | 2     | 163 | ILE  | O-C-N   | 7.24  | 129.01      | 121.91   |
| 5   | 5     | 186 | ILE  | N-CA-C  | -7.24 | 97.97       | 108.11   |
| 8   | A     | 132 | ALA  | N-CA-C  | -7.24 | 102.73      | 112.94   |
| 29  | V     | 102 | GLN  | N-CA-C  | -7.24 | 99.20       | 110.42   |
| 33  | Z     | 259 | PRO  | CA-C-N  | 7.23  | 130.29      | 120.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33  | Z     | 259 | PRO  | C-N-CA  | 7.23  | 130.29      | 120.38   |
| 6   | 6     | 79  | SER  | CA-C-N  | 7.23  | 129.97      | 120.28   |
| 6   | 6     | 79  | SER  | C-N-CA  | 7.23  | 129.97      | 120.28   |
| 3   | 3     | 75  | PRO  | CA-C-N  | 7.23  | 129.97      | 120.28   |
| 3   | 3     | 75  | PRO  | C-N-CA  | 7.23  | 129.97      | 120.28   |
| 30  | W     | 22  | PRO  | CA-C-N  | 7.23  | 134.71      | 121.70   |
| 30  | W     | 22  | PRO  | C-N-CA  | 7.23  | 134.71      | 121.70   |
| 16  | I     | 104 | LEU  | N-CA-C  | -7.22 | 97.18       | 109.24   |
| 12  | E     | 250 | GLU  | N-CA-C  | -7.22 | 104.34      | 113.72   |
| 21  | N     | 285 | ALA  | CA-C-N  | 7.22  | 129.95      | 120.28   |
| 21  | N     | 285 | ALA  | C-N-CA  | 7.22  | 129.95      | 120.28   |
| 33  | Z     | 623 | ARG  | CA-C-N  | 7.21  | 129.82      | 120.44   |
| 33  | Z     | 623 | ARG  | C-N-CA  | 7.21  | 129.82      | 120.44   |
| 8   | A     | 241 | ILE  | CA-C-N  | 7.21  | 129.94      | 120.28   |
| 8   | A     | 241 | ILE  | C-N-CA  | 7.21  | 129.94      | 120.28   |
| 6   | 6     | 98  | VAL  | O-C-N   | 7.21  | 131.17      | 123.02   |
| 21  | N     | 651 | PHE  | N-CA-C  | 7.21  | 121.33      | 112.54   |
| 24  | Q     | 97  | LEU  | N-CA-C  | 7.21  | 119.76      | 111.11   |
| 4   | 4     | 100 | ASN  | N-CA-C  | -7.21 | 97.66       | 109.40   |
| 28  | U     | 72  | TYR  | CA-C-N  | 7.21  | 129.64      | 120.56   |
| 28  | U     | 72  | TYR  | C-N-CA  | 7.21  | 129.64      | 120.56   |
| 28  | U     | 279 | SER  | CA-C-N  | 7.21  | 129.94      | 120.28   |
| 28  | U     | 279 | SER  | C-N-CA  | 7.21  | 129.94      | 120.28   |
| 19  | L     | 250 | GLY  | O-C-N   | -7.20 | 113.34      | 122.70   |
| 8   | A     | 205 | PHE  | CA-C-N  | 7.20  | 130.26      | 120.54   |
| 8   | A     | 205 | PHE  | C-N-CA  | 7.20  | 130.26      | 120.54   |
| 33  | Z     | 108 | ASP  | CA-C-O  | -7.20 | 112.55      | 120.69   |
| 18  | K     | 194 | GLN  | CA-C-N  | 7.20  | 130.51      | 120.29   |
| 18  | K     | 194 | GLN  | C-N-CA  | 7.20  | 130.51      | 120.29   |
| 26  | S     | 262 | THR  | N-CA-C  | -7.19 | 102.94      | 114.09   |
| 17  | J     | 59  | LYS  | CA-C-N  | 7.19  | 129.79      | 120.44   |
| 17  | J     | 59  | LYS  | C-N-CA  | 7.19  | 129.79      | 120.44   |
| 7   | 7     | 106 | ILE  | O-C-N   | 7.19  | 130.79      | 123.10   |
| 15  | H     | 389 | PHE  | CA-C-N  | 7.19  | 129.91      | 120.28   |
| 15  | H     | 389 | PHE  | C-N-CA  | 7.19  | 129.91      | 120.28   |
| 33  | Z     | 833 | GLN  | CA-C-N  | 7.19  | 129.91      | 120.28   |
| 33  | Z     | 833 | GLN  | C-N-CA  | 7.19  | 129.91      | 120.28   |
| 25  | R     | 372 | ILE  | CB-CA-C | -7.19 | 106.73      | 114.35   |
| 23  | P     | 309 | MET  | N-CA-C  | -7.18 | 104.13      | 114.12   |
| 33  | Z     | 256 | LEU  | O-C-N   | -7.18 | 113.06      | 121.32   |
| 33  | Z     | 353 | VAL  | CB-CA-C | -7.18 | 106.74      | 114.35   |
| 11  | D     | 216 | LYS  | CA-C-O  | -7.17 | 114.70      | 121.08   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | 2     | 179 | GLU  | CA-C-N  | 7.17  | 129.73      | 120.56   |
| 2   | 2     | 179 | GLU  | C-N-CA  | 7.17  | 129.73      | 120.56   |
| 7   | 7     | 104 | ASN  | N-CA-C  | -7.17 | 98.52       | 109.41   |
| 13  | F     | 144 | LEU  | N-CA-C  | -7.17 | 96.01       | 108.69   |
| 23  | P     | 202 | LYS  | CA-C-N  | 7.17  | 130.28      | 120.46   |
| 23  | P     | 202 | LYS  | C-N-CA  | 7.17  | 130.28      | 120.46   |
| 26  | S     | 390 | THR  | CA-C-N  | 7.17  | 127.93      | 119.98   |
| 26  | S     | 390 | THR  | C-N-CA  | 7.17  | 127.93      | 119.98   |
| 7   | 7     | 156 | ASP  | CA-C-N  | 7.16  | 126.06      | 120.33   |
| 7   | 7     | 156 | ASP  | C-N-CA  | 7.16  | 126.06      | 120.33   |
| 26  | S     | 382 | ARG  | CA-C-O  | 7.16  | 128.01      | 120.42   |
| 18  | K     | 53  | LYS  | CA-C-N  | 7.16  | 130.59      | 120.28   |
| 18  | K     | 53  | LYS  | C-N-CA  | 7.16  | 130.59      | 120.28   |
| 24  | Q     | 250 | THR  | CB-CA-C | -7.15 | 108.33      | 116.63   |
| 25  | R     | 309 | LEU  | O-C-N   | 7.15  | 130.31      | 122.15   |
| 13  | F     | 89  | ARG  | O-C-N   | -7.15 | 114.54      | 122.12   |
| 2   | 2     | 130 | GLY  | CA-C-N  | 7.15  | 130.19      | 120.54   |
| 2   | 2     | 130 | GLY  | C-N-CA  | 7.15  | 130.19      | 120.54   |
| 33  | Z     | 875 | LYS  | CA-C-N  | 7.15  | 130.25      | 120.46   |
| 33  | Z     | 875 | LYS  | C-N-CA  | 7.15  | 130.25      | 120.46   |
| 21  | N     | 878 | GLN  | CA-C-N  | 7.15  | 130.81      | 120.38   |
| 21  | N     | 878 | GLN  | C-N-CA  | 7.15  | 130.81      | 120.38   |
| 27  | T     | 102 | LYS  | CA-C-N  | 7.14  | 130.44      | 120.29   |
| 27  | T     | 102 | LYS  | C-N-CA  | 7.14  | 130.44      | 120.29   |
| 3   | 3     | 1   | GLY  | O-C-N   | 7.14  | 129.65      | 122.65   |
| 11  | D     | 83  | ARG  | CA-C-N  | 7.14  | 129.70      | 120.56   |
| 11  | D     | 83  | ARG  | C-N-CA  | 7.14  | 129.70      | 120.56   |
| 14  | G     | 215 | ILE  | N-CA-C  | -7.14 | 97.05       | 108.90   |
| 11  | D     | 240 | LYS  | CA-C-O  | -7.14 | 110.69      | 119.18   |
| 11  | D     | 108 | TYR  | CA-C-N  | 7.14  | 129.84      | 120.28   |
| 11  | D     | 108 | TYR  | C-N-CA  | 7.14  | 129.84      | 120.28   |
| 12  | E     | 109 | VAL  | CA-C-N  | 7.13  | 129.71      | 120.44   |
| 12  | E     | 109 | VAL  | C-N-CA  | 7.13  | 129.71      | 120.44   |
| 20  | M     | 354 | GLU  | CA-C-N  | 7.13  | 129.83      | 120.28   |
| 20  | M     | 354 | GLU  | C-N-CA  | 7.13  | 129.83      | 120.28   |
| 31  | X     | 76  | VAL  | CA-C-O  | -7.13 | 114.53      | 119.38   |
| 17  | J     | 366 | GLY  | CA-C-N  | 7.12  | 131.14      | 120.31   |
| 17  | J     | 366 | GLY  | C-N-CA  | 7.12  | 131.14      | 120.31   |
| 13  | F     | 223 | THR  | CA-C-N  | 7.12  | 132.29      | 123.10   |
| 13  | F     | 223 | THR  | C-N-CA  | 7.12  | 132.29      | 123.10   |
| 20  | M     | 283 | LEU  | CA-C-O  | 7.12  | 126.92      | 119.51   |
| 11  | D     | 241 | GLN  | N-CA-C  | -7.12 | 99.78       | 109.54   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 28  | U     | 69  | ASP  | CA-C-N | 7.12  | 130.12      | 120.44   |
| 28  | U     | 69  | ASP  | C-N-CA | 7.12  | 130.12      | 120.44   |
| 10  | C     | 177 | GLN  | N-CA-C | 7.12  | 119.90      | 111.71   |
| 31  | X     | 114 | LEU  | CA-C-N | 7.12  | 135.13      | 121.54   |
| 31  | X     | 114 | LEU  | C-N-CA | 7.12  | 135.13      | 121.54   |
| 9   | B     | 19  | GLY  | CA-C-N | 7.11  | 129.81      | 120.28   |
| 9   | B     | 19  | GLY  | C-N-CA | 7.11  | 129.81      | 120.28   |
| 4   | 4     | 1   | ASP  | N-CA-C | -7.11 | 96.74       | 108.76   |
| 22  | O     | 208 | ALA  | CA-C-N | 7.11  | 130.39      | 120.29   |
| 22  | O     | 208 | ALA  | C-N-CA | 7.11  | 130.39      | 120.29   |
| 28  | U     | 284 | SER  | CA-C-N | 7.11  | 130.19      | 120.46   |
| 28  | U     | 284 | SER  | C-N-CA | 7.11  | 130.19      | 120.46   |
| 21  | N     | 182 | ASN  | CA-C-N | 7.10  | 130.50      | 120.42   |
| 21  | N     | 182 | ASN  | C-N-CA | 7.10  | 130.50      | 120.42   |
| 33  | Z     | 838 | TYR  | CA-C-N | 7.10  | 134.16      | 121.66   |
| 33  | Z     | 838 | TYR  | C-N-CA | 7.10  | 134.16      | 121.66   |
| 23  | P     | 192 | ASP  | CA-C-N | 7.10  | 130.37      | 120.29   |
| 23  | P     | 192 | ASP  | C-N-CA | 7.10  | 130.37      | 120.29   |
| 4   | 4     | 143 | LEU  | N-CA-C | 7.10  | 118.67      | 111.07   |
| 14  | G     | 197 | LYS  | O-C-N  | -7.10 | 114.76      | 122.07   |
| 21  | N     | 70  | TYR  | O-C-N  | 7.10  | 129.47      | 122.09   |
| 27  | T     | 200 | LEU  | O-C-N  | -7.10 | 116.88      | 121.85   |
| 19  | L     | 179 | THR  | N-CA-C | -7.09 | 99.74       | 109.95   |
| 11  | D     | 134 | LEU  | N-CA-C | -7.09 | 96.78       | 108.76   |
| 17  | J     | 114 | CYS  | N-CA-C | -7.09 | 97.65       | 109.07   |
| 21  | N     | 555 | ILE  | CA-C-O | -7.09 | 112.59      | 120.25   |
| 27  | T     | 21  | ALA  | CA-C-N | 7.09  | 129.78      | 120.28   |
| 27  | T     | 21  | ALA  | C-N-CA | 7.09  | 129.78      | 120.28   |
| 33  | Z     | 268 | ALA  | CA-C-N | 7.09  | 129.65      | 120.44   |
| 33  | Z     | 268 | ALA  | C-N-CA | 7.09  | 129.65      | 120.44   |
| 33  | Z     | 772 | ILE  | CA-C-O | 7.09  | 128.32      | 120.95   |
| 21  | N     | 883 | SER  | N-CA-C | -7.08 | 98.96       | 108.74   |
| 6   | 6     | 93  | PHE  | N-CA-C | -7.08 | 104.67      | 113.38   |
| 24  | Q     | 76  | GLU  | CA-C-N | 7.08  | 130.34      | 120.29   |
| 24  | Q     | 76  | GLU  | C-N-CA | 7.08  | 130.34      | 120.29   |
| 5   | 5     | 26  | VAL  | CA-C-N | 7.08  | 130.34      | 120.29   |
| 5   | 5     | 26  | VAL  | C-N-CA | 7.08  | 130.34      | 120.29   |
| 15  | H     | 162 | ARG  | N-CA-C | 7.08  | 121.06      | 109.24   |
| 24  | Q     | 118 | CYS  | O-C-N  | -7.08 | 114.62      | 122.12   |
| 28  | U     | 107 | ASN  | CA-C-N | 7.08  | 129.77      | 120.28   |
| 28  | U     | 107 | ASN  | C-N-CA | 7.08  | 129.77      | 120.28   |
| 19  | L     | 389 | ALA  | CA-C-N | 7.07  | 130.34      | 120.29   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 19  | L     | 389 | ALA  | C-N-CA    | 7.07  | 130.34      | 120.29   |
| 22  | O     | 61  | LEU  | CA-C-N    | 7.07  | 130.33      | 120.29   |
| 22  | O     | 61  | LEU  | C-N-CA    | 7.07  | 130.33      | 120.29   |
| 24  | Q     | 355 | GLU  | CA-C-N    | 7.07  | 135.05      | 121.54   |
| 24  | Q     | 355 | GLU  | C-N-CA    | 7.07  | 135.05      | 121.54   |
| 21  | N     | 522 | ALA  | N-CA-C    | -7.07 | 103.51      | 111.14   |
| 28  | U     | 136 | ALA  | O-C-N     | -7.07 | 114.95      | 123.29   |
| 2   | 2     | 19  | ARG  | CA-C-O    | 7.07  | 128.13      | 120.43   |
| 27  | T     | 93  | ASN  | CA-C-N    | 7.07  | 135.03      | 121.54   |
| 27  | T     | 93  | ASN  | C-N-CA    | 7.07  | 135.03      | 121.54   |
| 19  | L     | 88  | TYR  | CA-C-N    | 7.06  | 129.75      | 120.28   |
| 19  | L     | 88  | TYR  | C-N-CA    | 7.06  | 129.75      | 120.28   |
| 3   | 3     | 168 | ARG  | N-CA-C    | -7.06 | 104.67      | 112.72   |
| 15  | H     | 215 | LYS  | CA-C-O    | 7.06  | 128.46      | 120.90   |
| 23  | P     | 100 | VAL  | CA-C-N    | 7.06  | 129.74      | 120.28   |
| 23  | P     | 100 | VAL  | C-N-CA    | 7.06  | 129.74      | 120.28   |
| 17  | J     | 266 | SER  | N-CA-C    | -7.06 | 104.29      | 113.12   |
| 3   | 3     | 12  | VAL  | N-CA-C    | -7.06 | 98.42       | 108.65   |
| 3   | 3     | 52  | THR  | N-CA-C    | 7.06  | 118.76      | 111.14   |
| 24  | Q     | 352 | GLU  | O-C-N     | -7.05 | 113.21      | 121.32   |
| 7   | 7     | 130 | SER  | CA-C-O    | 7.05  | 128.31      | 120.70   |
| 24  | Q     | 331 | THR  | CA-C-N    | 7.05  | 129.73      | 120.28   |
| 24  | Q     | 331 | THR  | C-N-CA    | 7.05  | 129.73      | 120.28   |
| 27  | T     | 114 | LEU  | N-CA-C    | 7.05  | 118.61      | 111.07   |
| 33  | Z     | 240 | ASN  | O-C-N     | -7.04 | 113.22      | 122.59   |
| 10  | C     | 215 | THR  | N-CA-C    | -7.04 | 98.61       | 109.24   |
| 19  | L     | 412 | PRO  | CA-C-N    | 7.04  | 130.29      | 120.29   |
| 19  | L     | 412 | PRO  | C-N-CA    | 7.04  | 130.29      | 120.29   |
| 21  | N     | 626 | GLY  | CA-C-N    | 7.04  | 129.50      | 120.70   |
| 21  | N     | 626 | GLY  | C-N-CA    | 7.04  | 129.50      | 120.70   |
| 33  | Z     | 906 | ALA  | CA-C-N    | 7.04  | 128.95      | 120.14   |
| 33  | Z     | 906 | ALA  | C-N-CA    | 7.04  | 128.95      | 120.14   |
| 16  | I     | 143 | PRO  | N-CA-C    | 7.04  | 121.87      | 111.03   |
| 24  | Q     | 210 | CYS  | CA-C-N    | 7.04  | 127.03      | 119.78   |
| 24  | Q     | 210 | CYS  | C-N-CA    | 7.04  | 127.03      | 119.78   |
| 26  | S     | 153 | GLU  | CA-C-N    | 7.04  | 129.71      | 120.28   |
| 26  | S     | 153 | GLU  | C-N-CA    | 7.04  | 129.71      | 120.28   |
| 24  | Q     | 25  | GLN  | CA-C-O    | -7.04 | 112.96      | 120.42   |
| 30  | W     | 43  | SER  | N-CA-C    | 7.04  | 118.95      | 111.28   |
| 15  | H     | 187 | LEU  | CA-C-N    | 7.04  | 127.63      | 120.38   |
| 15  | H     | 187 | LEU  | C-N-CA    | 7.04  | 127.63      | 120.38   |
| 20  | M     | 256 | ILE  | CA-CB-CG2 | -7.04 | 98.54       | 110.50   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | 7     | 85  | PHE  | N-CA-C | -7.03 | 103.31      | 110.97   |
| 14  | G     | 234 | LEU  | CA-C-O | -7.03 | 113.10      | 120.55   |
| 21  | N     | 134 | THR  | N-CA-C | 7.03  | 118.59      | 111.07   |
| 33  | Z     | 131 | LYS  | N-CA-C | -7.03 | 95.83       | 110.80   |
| 18  | K     | 94  | LEU  | CA-C-O | -7.02 | 112.91      | 121.06   |
| 6   | 6     | 195 | ILE  | N-CA-C | -7.02 | 98.28       | 108.11   |
| 15  | H     | 234 | ARG  | CA-C-N | 7.02  | 129.69      | 120.28   |
| 15  | H     | 234 | ARG  | C-N-CA | 7.02  | 129.69      | 120.28   |
| 20  | M     | 186 | LEU  | CA-C-N | 7.02  | 130.02      | 120.54   |
| 20  | M     | 186 | LEU  | C-N-CA | 7.02  | 130.02      | 120.54   |
| 14  | G     | 155 | SER  | N-CA-C | -7.02 | 98.25       | 109.76   |
| 21  | N     | 64  | ILE  | CA-C-N | 7.02  | 129.57      | 120.44   |
| 21  | N     | 64  | ILE  | C-N-CA | 7.02  | 129.57      | 120.44   |
| 7   | 7     | 86  | GLU  | CA-C-N | 7.02  | 129.91      | 120.65   |
| 7   | 7     | 86  | GLU  | C-N-CA | 7.02  | 129.91      | 120.65   |
| 26  | S     | 272 | TYR  | O-C-N  | 7.02  | 129.30      | 122.07   |
| 24  | Q     | 90  | LYS  | CA-C-N | 7.01  | 130.25      | 120.29   |
| 24  | Q     | 90  | LYS  | C-N-CA | 7.01  | 130.25      | 120.29   |
| 12  | E     | 56  | SER  | CA-C-O | -7.01 | 113.89      | 120.34   |
| 11  | D     | 235 | GLN  | CA-C-N | 7.01  | 130.37      | 120.42   |
| 11  | D     | 235 | GLN  | C-N-CA | 7.01  | 130.37      | 120.42   |
| 18  | K     | 289 | ASP  | N-CA-C | -7.01 | 101.70      | 112.99   |
| 22  | O     | 310 | PHE  | N-CA-C | -7.01 | 103.64      | 111.28   |
| 29  | V     | 164 | LEU  | N-CA-C | -7.01 | 105.08      | 112.93   |
| 21  | N     | 97  | PHE  | N-CA-C | 7.01  | 119.57      | 111.02   |
| 18  | K     | 390 | ALA  | CA-C-N | 7.00  | 127.70      | 120.00   |
| 18  | K     | 390 | ALA  | C-N-CA | 7.00  | 127.70      | 120.00   |
| 22  | O     | 287 | LEU  | CA-C-N | 6.99  | 129.53      | 120.44   |
| 22  | O     | 287 | LEU  | C-N-CA | 6.99  | 129.53      | 120.44   |
| 10  | C     | 240 | VAL  | N-CA-C | -6.99 | 104.04      | 110.82   |
| 20  | M     | 397 | GLU  | CA-C-N | 6.99  | 129.65      | 120.28   |
| 20  | M     | 397 | GLU  | C-N-CA | 6.99  | 129.65      | 120.28   |
| 7   | 7     | -6  | GLN  | CA-C-O | -6.99 | 113.05      | 119.62   |
| 7   | 7     | 123 | ASN  | CA-C-N | 6.99  | 131.78      | 120.60   |
| 7   | 7     | 123 | ASN  | C-N-CA | 6.99  | 131.78      | 120.60   |
| 20  | M     | 59  | LEU  | CA-C-N | 6.98  | 130.21      | 120.29   |
| 20  | M     | 59  | LEU  | C-N-CA | 6.98  | 130.21      | 120.29   |
| 23  | P     | 217 | LYS  | CA-C-O | 6.98  | 127.95      | 120.55   |
| 9   | B     | 136 | ILE  | N-CA-C | -6.98 | 98.40       | 108.17   |
| 23  | P     | 234 | TYR  | CA-C-N | 6.98  | 129.63      | 120.28   |
| 23  | P     | 234 | TYR  | C-N-CA | 6.98  | 129.63      | 120.28   |
| 1   | 1     | 60  | GLN  | CA-C-N | 6.98  | 129.51      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1     | 60  | GLN  | C-N-CA | 6.98  | 129.51      | 120.44   |
| 23  | P     | 235 | LEU  | CA-C-O | 6.98  | 127.95      | 120.55   |
| 9   | B     | 69  | PRO  | N-CA-C | 6.98  | 124.14      | 113.75   |
| 21  | N     | 165 | ILE  | CA-C-N | 6.97  | 129.35      | 120.56   |
| 21  | N     | 165 | ILE  | C-N-CA | 6.97  | 129.35      | 120.56   |
| 30  | W     | 19  | GLY  | O-C-N  | 6.97  | 131.77      | 122.70   |
| 30  | W     | 88  | ALA  | CA-C-O | 6.97  | 128.14      | 120.82   |
| 17  | J     | 316 | PHE  | CA-C-N | 6.97  | 127.56      | 120.38   |
| 17  | J     | 316 | PHE  | C-N-CA | 6.97  | 127.56      | 120.38   |
| 22  | O     | 60  | ARG  | N-CA-C | 6.97  | 119.91      | 111.82   |
| 6   | 6     | 14  | LEU  | CA-C-O | 6.97  | 129.03      | 120.25   |
| 19  | L     | 268 | ALA  | CA-C-N | 6.96  | 130.31      | 120.28   |
| 19  | L     | 268 | ALA  | C-N-CA | 6.96  | 130.31      | 120.28   |
| 24  | Q     | 401 | GLU  | N-CA-C | 6.96  | 119.18      | 109.15   |
| 17  | J     | 237 | ALA  | CA-C-N | 6.96  | 130.18      | 120.29   |
| 17  | J     | 237 | ALA  | C-N-CA | 6.96  | 130.18      | 120.29   |
| 15  | H     | 215 | LYS  | O-C-N  | -6.96 | 114.85      | 122.09   |
| 33  | Z     | 160 | GLU  | O-C-N  | 6.96  | 129.50      | 122.12   |
| 24  | Q     | 175 | VAL  | CA-C-N | 6.96  | 129.61      | 120.28   |
| 24  | Q     | 175 | VAL  | C-N-CA | 6.96  | 129.61      | 120.28   |
| 11  | D     | 60  | THR  | CA-C-N | 6.96  | 127.34      | 119.83   |
| 11  | D     | 60  | THR  | C-N-CA | 6.96  | 127.34      | 119.83   |
| 13  | F     | 153 | VAL  | O-C-N  | 6.96  | 130.57      | 123.20   |
| 10  | C     | 142 | ASP  | CA-C-O | 6.95  | 128.15      | 119.95   |
| 19  | L     | 260 | ALA  | O-C-N  | 6.95  | 129.49      | 122.12   |
| 26  | S     | 467 | PHE  | CA-C-N | 6.95  | 129.59      | 120.28   |
| 26  | S     | 467 | PHE  | C-N-CA | 6.95  | 129.59      | 120.28   |
| 27  | T     | 205 | ILE  | CA-C-N | 6.95  | 129.47      | 120.44   |
| 27  | T     | 205 | ILE  | C-N-CA | 6.95  | 129.47      | 120.44   |
| 28  | U     | 214 | VAL  | N-CA-C | 6.95  | 117.65      | 110.36   |
| 19  | L     | 182 | GLY  | N-CA-C | -6.94 | 103.75      | 115.62   |
| 21  | N     | 387 | ALA  | CA-C-N | 6.94  | 127.83      | 120.12   |
| 21  | N     | 387 | ALA  | C-N-CA | 6.94  | 127.83      | 120.12   |
| 24  | Q     | 211 | PRO  | CA-C-O | -6.94 | 113.51      | 121.56   |
| 24  | Q     | 234 | THR  | N-CA-C | -6.94 | 103.79      | 111.36   |
| 33  | Z     | 904 | LEU  | CA-C-N | 6.94  | 129.89      | 120.38   |
| 33  | Z     | 904 | LEU  | C-N-CA | 6.94  | 129.89      | 120.38   |
| 21  | N     | 526 | TYR  | N-CA-C | -6.94 | 96.02       | 110.80   |
| 1   | 1     | 59  | VAL  | CA-C-N | 6.94  | 129.46      | 120.44   |
| 1   | 1     | 59  | VAL  | C-N-CA | 6.94  | 129.46      | 120.44   |
| 20  | M     | 293 | SER  | N-CA-C | -6.94 | 104.39      | 112.92   |
| 21  | N     | 386 | MET  | CA-C-N | 6.94  | 129.74      | 120.58   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 386 | MET  | C-N-CA | 6.94  | 129.74      | 120.58   |
| 19  | L     | 238 | THR  | CA-C-N | 6.94  | 132.22      | 120.29   |
| 19  | L     | 238 | THR  | C-N-CA | 6.94  | 132.22      | 120.29   |
| 4   | 4     | 93  | SER  | CA-C-N | 6.93  | 129.45      | 120.44   |
| 4   | 4     | 93  | SER  | C-N-CA | 6.93  | 129.45      | 120.44   |
| 21  | N     | 230 | VAL  | CA-C-O | -6.93 | 113.74      | 120.95   |
| 25  | R     | 51  | LEU  | N-CA-C | 6.93  | 118.49      | 111.07   |
| 33  | Z     | 167 | ASP  | CA-C-N | 6.93  | 129.45      | 120.44   |
| 33  | Z     | 167 | ASP  | C-N-CA | 6.93  | 129.45      | 120.44   |
| 21  | N     | 390 | LEU  | CA-C-N | 6.93  | 128.50      | 119.84   |
| 21  | N     | 390 | LEU  | C-N-CA | 6.93  | 128.50      | 119.84   |
| 33  | Z     | 889 | VAL  | CA-C-O | -6.93 | 114.85      | 121.64   |
| 12  | E     | 232 | ASP  | CA-C-N | 6.93  | 129.56      | 120.28   |
| 12  | E     | 232 | ASP  | C-N-CA | 6.93  | 129.56      | 120.28   |
| 11  | D     | 42  | VAL  | N-CA-C | -6.93 | 98.78       | 108.27   |
| 22  | O     | 313 | ILE  | CA-C-N | 6.93  | 129.56      | 120.28   |
| 22  | O     | 313 | ILE  | C-N-CA | 6.93  | 129.56      | 120.28   |
| 15  | H     | 236 | ALA  | CA-C-N | 6.92  | 130.12      | 120.29   |
| 15  | H     | 236 | ALA  | C-N-CA | 6.92  | 130.12      | 120.29   |
| 18  | K     | 252 | ARG  | CA-C-N | 6.92  | 129.56      | 120.28   |
| 18  | K     | 252 | ARG  | C-N-CA | 6.92  | 129.56      | 120.28   |
| 13  | F     | 216 | VAL  | CA-C-O | -6.92 | 114.06      | 121.19   |
| 14  | G     | 99  | LYS  | O-C-N  | -6.92 | 114.94      | 122.07   |
| 17  | J     | 58  | ILE  | O-C-N  | 6.92  | 128.69      | 121.91   |
| 33  | Z     | 605 | SER  | CA-C-N | 6.92  | 129.85      | 120.44   |
| 33  | Z     | 605 | SER  | C-N-CA | 6.92  | 129.85      | 120.44   |
| 14  | G     | 190 | GLU  | O-C-N  | 6.92  | 129.45      | 122.12   |
| 22  | O     | 278 | PRO  | CA-C-N | 6.92  | 130.24      | 120.42   |
| 22  | O     | 278 | PRO  | C-N-CA | 6.92  | 130.24      | 120.42   |
| 22  | O     | 380 | LEU  | CA-C-N | 6.92  | 127.62      | 119.94   |
| 22  | O     | 380 | LEU  | C-N-CA | 6.92  | 127.62      | 119.94   |
| 20  | M     | 432 | PHE  | N-CA-C | -6.91 | 102.09      | 113.50   |
| 21  | N     | 92  | ASP  | N-CA-C | -6.91 | 104.88      | 113.38   |
| 12  | E     | 91  | HIS  | CA-C-O | -6.91 | 113.09      | 120.42   |
| 15  | H     | 276 | GLY  | CA-C-N | 6.91  | 129.54      | 120.28   |
| 15  | H     | 276 | GLY  | C-N-CA | 6.91  | 129.54      | 120.28   |
| 19  | L     | 150 | ILE  | N-CA-C | 6.91  | 119.69      | 111.05   |
| 19  | L     | 314 | GLY  | O-C-N  | 6.91  | 129.89      | 122.77   |
| 11  | D     | 228 | GLU  | CA-C-N | 6.91  | 129.40      | 120.56   |
| 11  | D     | 228 | GLU  | C-N-CA | 6.91  | 129.40      | 120.56   |
| 29  | V     | 85  | ASP  | CA-C-N | 6.91  | 129.26      | 120.56   |
| 29  | V     | 85  | ASP  | C-N-CA | 6.91  | 129.26      | 120.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 17  | J     | 176 | SER  | CA-C-N | 6.90  | 129.41      | 120.44   |
| 17  | J     | 176 | SER  | C-N-CA | 6.90  | 129.41      | 120.44   |
| 8   | A     | 22  | GLU  | CA-C-O | 6.90  | 127.90      | 120.24   |
| 24  | Q     | 122 | ILE  | N-CA-C | -6.90 | 103.75      | 110.72   |
| 19  | L     | 143 | GLY  | N-CA-C | -6.90 | 105.80      | 115.32   |
| 11  | D     | 161 | ALA  | O-C-N  | -6.90 | 115.34      | 123.41   |
| 24  | Q     | 341 | THR  | CA-C-N | 6.90  | 130.79      | 120.31   |
| 24  | Q     | 341 | THR  | C-N-CA | 6.90  | 130.79      | 120.31   |
| 33  | Z     | 51  | LEU  | N-CA-C | -6.89 | 97.11       | 108.76   |
| 22  | O     | 347 | LEU  | CA-C-O | 6.89  | 128.14      | 120.70   |
| 19  | L     | 248 | ALA  | N-CA-C | 6.89  | 118.79      | 111.28   |
| 21  | N     | 106 | ILE  | CA-C-O | -6.89 | 113.87      | 121.17   |
| 24  | Q     | 45  | SER  | N-CA-C | -6.89 | 99.27       | 109.81   |
| 33  | Z     | 586 | GLU  | CA-C-N | 6.89  | 129.40      | 120.44   |
| 33  | Z     | 586 | GLU  | C-N-CA | 6.89  | 129.40      | 120.44   |
| 6   | 6     | 83  | ASN  | CA-C-N | 6.89  | 130.20      | 120.42   |
| 6   | 6     | 83  | ASN  | C-N-CA | 6.89  | 130.20      | 120.42   |
| 33  | Z     | 387 | ASN  | CA-C-N | 6.89  | 127.62      | 119.98   |
| 33  | Z     | 387 | ASN  | C-N-CA | 6.89  | 127.62      | 119.98   |
| 21  | N     | 579 | SER  | N-CA-C | -6.88 | 104.62      | 113.16   |
| 22  | O     | 322 | ASP  | CA-C-N | 6.88  | 129.50      | 120.28   |
| 22  | O     | 322 | ASP  | C-N-CA | 6.88  | 129.50      | 120.28   |
| 22  | O     | 35  | GLU  | N-CA-C | -6.88 | 103.57      | 113.21   |
| 26  | S     | 298 | ARG  | CA-C-O | -6.88 | 113.60      | 121.72   |
| 26  | S     | 465 | ILE  | N-CA-C | 6.88  | 117.64      | 110.62   |
| 17  | J     | 275 | LEU  | CA-C-N | 6.87  | 129.49      | 120.28   |
| 17  | J     | 275 | LEU  | C-N-CA | 6.87  | 129.49      | 120.28   |
| 25  | R     | 396 | LYS  | CA-C-N | 6.87  | 129.49      | 120.28   |
| 25  | R     | 396 | LYS  | C-N-CA | 6.87  | 129.49      | 120.28   |
| 29  | V     | 34  | LEU  | CA-C-N | 6.87  | 129.79      | 120.38   |
| 29  | V     | 34  | LEU  | C-N-CA | 6.87  | 129.79      | 120.38   |
| 28  | U     | 96  | GLY  | O-C-N  | -6.87 | 114.90      | 121.77   |
| 17  | J     | 395 | GLU  | O-C-N  | -6.87 | 114.91      | 123.01   |
| 6   | 6     | 85  | GLN  | O-C-N  | 6.86  | 129.14      | 122.07   |
| 22  | O     | 327 | LEU  | N-CA-C | 6.86  | 118.76      | 111.28   |
| 20  | M     | 412 | HIS  | CA-C-N | 6.86  | 130.03      | 120.29   |
| 20  | M     | 412 | HIS  | C-N-CA | 6.86  | 130.03      | 120.29   |
| 21  | N     | 895 | LYS  | N-CA-C | 6.86  | 118.73      | 108.31   |
| 29  | V     | 257 | GLU  | CA-C-N | 6.86  | 129.47      | 120.28   |
| 29  | V     | 257 | GLU  | C-N-CA | 6.86  | 129.47      | 120.28   |
| 11  | D     | 209 | ASN  | N-CA-C | -6.86 | 104.23      | 112.59   |
| 20  | M     | 240 | ASN  | CA-C-N | 6.85  | 135.85      | 122.07   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | M     | 240 | ASN  | C-N-CA  | 6.85  | 135.85      | 122.07   |
| 1   | 1     | 76  | GLU  | CA-C-O  | 6.85  | 127.85      | 119.97   |
| 6   | 6     | 201 | ASP  | N-CA-C  | -6.85 | 104.66      | 113.16   |
| 11  | D     | 157 | SER  | O-C-N   | -6.85 | 116.68      | 123.46   |
| 22  | O     | 248 | TYR  | CA-C-N  | 6.85  | 129.46      | 120.28   |
| 22  | O     | 248 | TYR  | C-N-CA  | 6.85  | 129.46      | 120.28   |
| 1   | 1     | 183 | VAL  | N-CA-C  | -6.84 | 97.76       | 107.75   |
| 19  | L     | 187 | THR  | N-CA-C  | 6.84  | 125.37      | 110.80   |
| 23  | P     | 373 | GLU  | CA-C-N  | 6.84  | 129.45      | 120.28   |
| 23  | P     | 373 | GLU  | C-N-CA  | 6.84  | 129.45      | 120.28   |
| 27  | T     | 55  | LEU  | N-CA-C  | 6.84  | 118.73      | 111.28   |
| 4   | 4     | 23  | GLY  | CA-C-N  | 6.84  | 129.83      | 120.46   |
| 4   | 4     | 23  | GLY  | C-N-CA  | 6.84  | 129.83      | 120.46   |
| 17  | J     | 205 | HIS  | N-CA-C  | 6.84  | 118.73      | 111.28   |
| 33  | Z     | 593 | HIS  | N-CA-C  | -6.83 | 102.07      | 108.22   |
| 3   | 3     | 182 | LYS  | N-CA-C  | -6.83 | 99.36       | 109.81   |
| 13  | F     | 63  | ILE  | N-CA-C  | -6.83 | 98.61       | 108.17   |
| 23  | P     | 240 | TYR  | CA-C-N  | 6.83  | 130.11      | 120.28   |
| 23  | P     | 240 | TYR  | C-N-CA  | 6.83  | 130.11      | 120.28   |
| 16  | I     | 378 | GLU  | O-C-N   | 6.83  | 129.36      | 122.12   |
| 26  | S     | 315 | LYS  | CA-C-N  | 6.83  | 129.98      | 120.29   |
| 26  | S     | 315 | LYS  | C-N-CA  | 6.83  | 129.98      | 120.29   |
| 8   | A     | 135 | ARG  | CA-C-O  | -6.82 | 113.81      | 120.97   |
| 20  | M     | 311 | GLN  | N-CA-C  | 6.82  | 118.72      | 111.28   |
| 21  | N     | 111 | GLN  | CA-C-N  | 6.82  | 129.42      | 120.28   |
| 21  | N     | 111 | GLN  | C-N-CA  | 6.82  | 129.42      | 120.28   |
| 11  | D     | 179 | TYR  | N-CA-C  | -6.82 | 98.35       | 108.79   |
| 19  | L     | 248 | ALA  | N-CA-CB | -6.82 | 100.10      | 110.12   |
| 3   | 3     | 116 | ASP  | CA-C-N  | 6.82  | 129.41      | 120.28   |
| 3   | 3     | 116 | ASP  | C-N-CA  | 6.82  | 129.41      | 120.28   |
| 9   | B     | 94  | HIS  | N-CA-C  | -6.82 | 102.23      | 112.04   |
| 6   | 6     | 94  | PHE  | CA-C-N  | 6.81  | 128.36      | 119.84   |
| 6   | 6     | 94  | PHE  | C-N-CA  | 6.81  | 128.36      | 119.84   |
| 24  | Q     | 22  | GLU  | CA-C-N  | 6.81  | 129.41      | 120.28   |
| 24  | Q     | 22  | GLU  | C-N-CA  | 6.81  | 129.41      | 120.28   |
| 24  | Q     | 369 | ASP  | CA-C-O  | -6.81 | 114.11      | 121.94   |
| 33  | Z     | 595 | MET  | CA-C-N  | 6.80  | 129.95      | 120.29   |
| 33  | Z     | 595 | MET  | C-N-CA  | 6.80  | 129.95      | 120.29   |
| 21  | N     | 588 | VAL  | N-CA-C  | 6.80  | 117.59      | 110.72   |
| 21  | N     | 589 | ILE  | CA-C-N  | 6.80  | 130.07      | 120.28   |
| 21  | N     | 589 | ILE  | C-N-CA  | 6.80  | 130.07      | 120.28   |
| 33  | Z     | 323 | TYR  | CA-C-N  | 6.80  | 130.36      | 120.71   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 323 | TYR  | C-N-CA | 6.80  | 130.36      | 120.71   |
| 33  | Z     | 487 | SER  | CA-C-O | 6.80  | 127.70      | 120.70   |
| 14  | G     | 148 | TYR  | N-CA-C | -6.80 | 98.98       | 109.24   |
| 27  | T     | 130 | ASP  | CA-C-O | -6.80 | 113.63      | 120.90   |
| 4   | 4     | 4   | LEU  | CA-C-N | 6.79  | 129.67      | 121.38   |
| 4   | 4     | 4   | LEU  | C-N-CA | 6.79  | 129.67      | 121.38   |
| 22  | O     | 60  | ARG  | CA-C-N | 6.79  | 129.93      | 120.29   |
| 22  | O     | 60  | ARG  | C-N-CA | 6.79  | 129.93      | 120.29   |
| 13  | F     | 133 | LEU  | N-CA-C | -6.79 | 97.34       | 108.41   |
| 23  | P     | 311 | TRP  | CA-C-O | -6.79 | 112.27      | 118.79   |
| 23  | P     | 193 | TYR  | CA-C-N | 6.78  | 129.26      | 120.44   |
| 23  | P     | 193 | TYR  | C-N-CA | 6.78  | 129.26      | 120.44   |
| 22  | O     | 198 | THR  | CA-C-N | 6.78  | 129.25      | 120.44   |
| 22  | O     | 198 | THR  | C-N-CA | 6.78  | 129.25      | 120.44   |
| 25  | R     | 247 | GLU  | CA-C-N | 6.78  | 129.69      | 120.54   |
| 25  | R     | 247 | GLU  | C-N-CA | 6.78  | 129.69      | 120.54   |
| 12  | E     | 223 | THR  | N-CA-C | -6.78 | 98.79       | 109.50   |
| 10  | C     | 55  | THR  | CA-C-O | 6.77  | 127.24      | 119.18   |
| 10  | C     | 109 | GLU  | N-CA-C | 6.77  | 118.66      | 111.28   |
| 19  | L     | 172 | SER  | CA-C-O | 6.77  | 127.89      | 120.71   |
| 24  | Q     | 377 | LEU  | N-CA-C | -6.77 | 103.90      | 111.28   |
| 1   | 1     | 154 | PHE  | CA-C-N | 6.77  | 130.03      | 120.42   |
| 1   | 1     | 154 | PHE  | C-N-CA | 6.77  | 130.03      | 120.42   |
| 20  | M     | 181 | SER  | N-CA-C | -6.77 | 104.77      | 113.16   |
| 16  | I     | 369 | MET  | N-CA-C | 6.77  | 118.73      | 110.41   |
| 30  | W     | 34  | GLU  | CA-C-N | 6.77  | 129.90      | 120.29   |
| 30  | W     | 34  | GLU  | C-N-CA | 6.77  | 129.90      | 120.29   |
| 8   | A     | 214 | LEU  | N-CA-C | -6.77 | 105.03      | 113.28   |
| 20  | M     | 158 | THR  | N-CA-C | -6.77 | 98.70       | 109.59   |
| 23  | P     | 277 | GLN  | CA-C-N | 6.76  | 129.34      | 120.28   |
| 23  | P     | 277 | GLN  | C-N-CA | 6.76  | 129.34      | 120.28   |
| 12  | E     | 93  | ARG  | N-CA-C | -6.76 | 103.99      | 111.36   |
| 33  | Z     | 572 | ILE  | N-CA-C | 6.76  | 117.51      | 110.62   |
| 23  | P     | 250 | ILE  | CA-C-N | 6.75  | 129.62      | 120.44   |
| 23  | P     | 250 | ILE  | C-N-CA | 6.75  | 129.62      | 120.44   |
| 29  | V     | 267 | LYS  | CA-C-N | 6.75  | 129.22      | 120.44   |
| 29  | V     | 267 | LYS  | C-N-CA | 6.75  | 129.22      | 120.44   |
| 9   | B     | 207 | ASP  | CA-C-O | 6.75  | 127.35      | 119.32   |
| 17  | J     | 285 | SER  | N-CA-C | -6.75 | 97.58       | 109.06   |
| 27  | T     | 112 | ASN  | O-C-N  | 6.75  | 129.02      | 122.07   |
| 3   | 3     | 74  | GLU  | CA-C-N | 6.75  | 126.26      | 119.24   |
| 3   | 3     | 74  | GLU  | C-N-CA | 6.75  | 126.26      | 119.24   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 27  | T     | 29  | PRO  | CA-C-N | 6.75  | 130.00      | 120.42   |
| 27  | T     | 29  | PRO  | C-N-CA | 6.75  | 130.00      | 120.42   |
| 11  | D     | 152 | PRO  | CA-C-N | 6.75  | 129.99      | 120.28   |
| 11  | D     | 152 | PRO  | C-N-CA | 6.75  | 129.99      | 120.28   |
| 26  | S     | 362 | SER  | CA-C-N | 6.75  | 129.32      | 120.28   |
| 26  | S     | 362 | SER  | C-N-CA | 6.75  | 129.32      | 120.28   |
| 9   | B     | 100 | ILE  | N-CA-C | -6.74 | 106.92      | 113.53   |
| 7   | 7     | 87  | TYR  | N-CA-C | -6.74 | 103.62      | 110.97   |
| 21  | N     | 366 | THR  | CA-C-O | -6.74 | 113.74      | 120.82   |
| 33  | Z     | 605 | SER  | N-CA-C | 6.74  | 118.28      | 111.07   |
| 16  | I     | 433 | GLU  | N-CA-C | -6.74 | 104.97      | 113.72   |
| 17  | J     | 26  | LYS  | O-C-N  | 6.73  | 129.26      | 122.12   |
| 8   | A     | 237 | SER  | CA-C-N | 6.73  | 129.19      | 120.44   |
| 8   | A     | 237 | SER  | C-N-CA | 6.73  | 129.19      | 120.44   |
| 21  | N     | 393 | SER  | N-CA-C | -6.73 | 99.40       | 109.83   |
| 33  | Z     | 263 | ALA  | O-C-N  | 6.73  | 129.25      | 122.12   |
| 19  | L     | 214 | PRO  | N-CA-C | -6.73 | 102.49      | 110.70   |
| 13  | F     | 14  | SER  | CA-C-N | 6.72  | 126.68      | 119.28   |
| 13  | F     | 14  | SER  | C-N-CA | 6.72  | 126.68      | 119.28   |
| 29  | V     | 262 | THR  | O-C-N  | 6.72  | 129.00      | 122.07   |
| 2   | 2     | 43  | CYS  | N-CA-C | -6.72 | 97.25       | 108.75   |
| 21  | N     | 36  | TRP  | N-CA-C | 6.72  | 119.44      | 111.71   |
| 21  | N     | 236 | GLY  | O-C-N  | 6.72  | 128.64      | 122.19   |
| 25  | R     | 386 | GLY  | CA-C-N | -6.72 | 113.03      | 122.71   |
| 25  | R     | 386 | GLY  | C-N-CA | -6.72 | 113.03      | 122.71   |
| 2   | 2     | 219 | ASN  | CA-C-N | 6.72  | 130.25      | 120.91   |
| 2   | 2     | 219 | ASN  | C-N-CA | 6.72  | 130.25      | 120.91   |
| 16  | I     | 134 | SER  | CA-C-N | 6.72  | 134.37      | 121.54   |
| 16  | I     | 134 | SER  | C-N-CA | 6.72  | 134.37      | 121.54   |
| 8   | A     | 158 | ASP  | CA-C-O | -6.71 | 114.32      | 120.50   |
| 23  | P     | 269 | VAL  | O-C-N  | -6.71 | 115.36      | 121.87   |
| 18  | K     | 333 | ARG  | CA-C-N | 6.71  | 134.13      | 122.32   |
| 18  | K     | 333 | ARG  | C-N-CA | 6.71  | 134.13      | 122.32   |
| 28  | U     | 116 | ASN  | N-CA-C | -6.71 | 98.81       | 108.60   |
| 33  | Z     | 83  | THR  | N-CA-C | -6.71 | 99.11       | 109.24   |
| 33  | Z     | 770 | GLU  | CA-C-N | 6.71  | 129.16      | 120.44   |
| 33  | Z     | 770 | GLU  | C-N-CA | 6.71  | 129.16      | 120.44   |
| 29  | V     | 239 | ALA  | O-C-N  | 6.71  | 129.23      | 122.12   |
| 12  | E     | 11  | GLY  | O-C-N  | -6.70 | 116.54      | 123.31   |
| 27  | T     | 150 | ARG  | O-C-N  | -6.70 | 115.17      | 122.07   |
| 13  | F     | 198 | SER  | N-CA-C | 6.70  | 121.05      | 113.01   |
| 33  | Z     | 93  | ARG  | CA-C-N | 6.70  | 126.84      | 119.87   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 93  | ARG  | C-N-CA | 6.70  | 126.84      | 119.87   |
| 19  | L     | 181 | ASP  | N-CA-C | -6.70 | 105.14      | 113.38   |
| 20  | M     | 350 | PRO  | CA-C-N | 6.70  | 132.02      | 121.17   |
| 20  | M     | 350 | PRO  | C-N-CA | 6.70  | 132.02      | 121.17   |
| 15  | H     | 448 | ASP  | CA-C-N | 6.70  | 129.55      | 120.44   |
| 15  | H     | 448 | ASP  | C-N-CA | 6.70  | 129.55      | 120.44   |
| 21  | N     | 49  | LEU  | O-C-N  | 6.70  | 129.79      | 122.15   |
| 10  | C     | 61  | THR  | N-CA-C | -6.70 | 98.06       | 109.24   |
| 15  | H     | 302 | LYS  | CA-C-N | 6.69  | 134.32      | 121.54   |
| 15  | H     | 302 | LYS  | C-N-CA | 6.69  | 134.32      | 121.54   |
| 21  | N     | 555 | ILE  | CA-C-N | 6.69  | 129.25      | 120.28   |
| 21  | N     | 555 | ILE  | C-N-CA | 6.69  | 129.25      | 120.28   |
| 23  | P     | 280 | LEU  | CA-C-O | -6.69 | 113.45      | 120.55   |
| 26  | S     | 128 | ILE  | CA-C-N | 6.69  | 129.14      | 120.44   |
| 26  | S     | 128 | ILE  | C-N-CA | 6.69  | 129.14      | 120.44   |
| 9   | B     | 94  | HIS  | CA-C-O | 6.69  | 128.67      | 120.31   |
| 15  | H     | 289 | ARG  | CA-C-N | 6.69  | 129.79      | 120.29   |
| 15  | H     | 289 | ARG  | C-N-CA | 6.69  | 129.79      | 120.29   |
| 26  | S     | 382 | ARG  | N-CA-C | 6.69  | 118.65      | 111.36   |
| 33  | Z     | 400 | ILE  | N-CA-C | 6.69  | 117.44      | 110.62   |
| 1   | 1     | 57  | ASP  | O-C-N  | 6.68  | 129.21      | 122.12   |
| 2   | 2     | 146 | LEU  | N-CA-C | -6.68 | 100.63      | 110.52   |
| 9   | B     | 48  | GLU  | O-C-N  | 6.68  | 130.82      | 123.27   |
| 17  | J     | 245 | ILE  | CA-C-N | 6.68  | 131.66      | 122.77   |
| 17  | J     | 245 | ILE  | C-N-CA | 6.68  | 131.66      | 122.77   |
| 23  | P     | 313 | ILE  | N-CA-C | -6.68 | 104.25      | 110.53   |
| 26  | S     | 151 | GLU  | N-CA-C | -6.68 | 96.57       | 110.80   |
| 19  | L     | 237 | ALA  | N-CA-C | 6.67  | 118.56      | 111.28   |
| 2   | 2     | 75  | ARG  | CA-C-N | 6.67  | 131.24      | 120.30   |
| 2   | 2     | 75  | ARG  | C-N-CA | 6.67  | 131.24      | 120.30   |
| 15  | H     | 197 | MET  | O-C-N  | 6.67  | 131.08      | 123.27   |
| 19  | L     | 384 | ASP  | CA-C-O | -6.67 | 113.32      | 121.06   |
| 4   | 4     | 7   | ARG  | O-C-N  | -6.67 | 115.11      | 123.05   |
| 21  | N     | 410 | LEU  | CA-C-N | 6.67  | 128.97      | 120.56   |
| 21  | N     | 410 | LEU  | C-N-CA | 6.67  | 128.97      | 120.56   |
| 33  | Z     | 81  | SER  | N-CA-C | -6.67 | 100.92      | 110.59   |
| 2   | 2     | 42  | TRP  | N-CA-C | -6.67 | 99.31       | 109.85   |
| 21  | N     | 506 | GLN  | N-CA-C | -6.67 | 103.49      | 111.69   |
| 15  | H     | 257 | THR  | CA-C-N | 6.67  | 129.21      | 120.28   |
| 15  | H     | 257 | THR  | C-N-CA | 6.67  | 129.21      | 120.28   |
| 17  | J     | 226 | GLY  | O-C-N  | 6.66  | 128.65      | 122.19   |
| 29  | V     | 65  | VAL  | CA-C-N | 6.66  | 130.21      | 122.35   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 29  | V     | 65  | VAL  | C-N-CA | 6.66  | 130.21      | 122.35   |
| 21  | N     | 348 | PHE  | CA-C-N | 6.66  | 129.88      | 120.42   |
| 21  | N     | 348 | PHE  | C-N-CA | 6.66  | 129.88      | 120.42   |
| 9   | B     | 152 | PRO  | CA-C-N | 6.66  | 129.21      | 120.28   |
| 9   | B     | 152 | PRO  | C-N-CA | 6.66  | 129.21      | 120.28   |
| 26  | S     | 259 | TYR  | CA-C-N | 6.66  | 127.06      | 119.93   |
| 26  | S     | 259 | TYR  | C-N-CA | 6.66  | 127.06      | 119.93   |
| 26  | S     | 384 | ARG  | N-CA-C | 6.66  | 119.39      | 111.33   |
| 5   | 5     | 99  | THR  | O-C-N  | 6.66  | 130.84      | 123.25   |
| 18  | K     | 219 | LYS  | N-CA-C | 6.66  | 118.19      | 111.07   |
| 23  | P     | 194 | SER  | N-CA-C | 6.66  | 118.19      | 111.07   |
| 22  | O     | 183 | ASN  | N-CA-C | -6.66 | 104.73      | 112.92   |
| 14  | G     | 60  | PRO  | CA-C-O | -6.66 | 113.49      | 121.48   |
| 19  | L     | 235 | VAL  | CA-C-N | 6.65  | 129.20      | 120.28   |
| 19  | L     | 235 | VAL  | C-N-CA | 6.65  | 129.20      | 120.28   |
| 19  | L     | 323 | ILE  | CA-C-N | 6.65  | 132.23      | 122.99   |
| 19  | L     | 323 | ILE  | C-N-CA | 6.65  | 132.23      | 122.99   |
| 21  | N     | 414 | GLY  | N-CA-C | -6.64 | 105.69      | 115.72   |
| 26  | S     | 436 | ILE  | N-CA-C | -6.64 | 98.03       | 108.86   |
| 27  | T     | 32  | ILE  | O-C-N  | 6.64  | 128.31      | 121.87   |
| 3   | 3     | 136 | GLN  | N-CA-C | -6.64 | 103.96      | 111.07   |
| 8   | A     | 194 | ILE  | N-CA-C | -6.64 | 98.90       | 108.53   |
| 9   | B     | 169 | VAL  | N-CA-C | -6.64 | 104.28      | 110.53   |
| 20  | M     | 214 | ALA  | N-CA-C | -6.64 | 98.77       | 109.40   |
| 25  | R     | 286 | LEU  | CA-C-N | 6.64  | 131.85      | 122.08   |
| 25  | R     | 286 | LEU  | C-N-CA | 6.64  | 131.85      | 122.08   |
| 27  | T     | 30  | ILE  | N-CA-C | -6.64 | 104.02      | 110.72   |
| 15  | H     | 165 | PRO  | N-CA-C | 6.64  | 122.54      | 113.98   |
| 7   | 7     | 35  | ILE  | N-CA-C | -6.63 | 94.56       | 108.88   |
| 10  | C     | 170 | SER  | CA-C-N | 6.63  | 129.71      | 120.29   |
| 10  | C     | 170 | SER  | C-N-CA | 6.63  | 129.71      | 120.29   |
| 12  | E     | 238 | GLU  | CA-C-N | 6.63  | 130.39      | 120.31   |
| 12  | E     | 238 | GLU  | C-N-CA | 6.63  | 130.39      | 120.31   |
| 18  | K     | 213 | GLY  | N-CA-C | -6.63 | 98.81       | 112.34   |
| 21  | N     | 283 | ASP  | CA-C-N | 6.63  | 127.20      | 120.04   |
| 21  | N     | 283 | ASP  | C-N-CA | 6.63  | 127.20      | 120.04   |
| 12  | E     | 77  | ALA  | N-CA-C | -6.63 | 99.11       | 109.72   |
| 33  | Z     | 893 | PHE  | CA-C-N | 6.63  | 130.75      | 120.75   |
| 33  | Z     | 893 | PHE  | C-N-CA | 6.63  | 130.75      | 120.75   |
| 1   | 1     | 65  | LEU  | CA-C-N | 6.62  | 129.05      | 120.44   |
| 1   | 1     | 65  | LEU  | C-N-CA | 6.62  | 129.05      | 120.44   |
| 20  | M     | 262 | LEU  | CA-C-N | 6.62  | 129.53      | 120.46   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 20  | M     | 262 | LEU  | C-N-CA | 6.62  | 129.53      | 120.46   |
| 20  | M     | 270 | ALA  | CA-C-N | 6.62  | 129.69      | 120.29   |
| 20  | M     | 270 | ALA  | C-N-CA | 6.62  | 129.69      | 120.29   |
| 21  | N     | 226 | ASN  | CA-C-N | 6.62  | 130.75      | 120.82   |
| 21  | N     | 226 | ASN  | C-N-CA | 6.62  | 130.75      | 120.82   |
| 28  | U     | 136 | ALA  | CA-C-O | 6.62  | 127.60      | 120.38   |
| 3   | 3     | 144 | LEU  | N-CA-C | 6.61  | 118.57      | 111.36   |
| 27  | T     | 127 | GLN  | CA-C-N | 6.61  | 129.14      | 120.28   |
| 27  | T     | 127 | GLN  | C-N-CA | 6.61  | 129.14      | 120.28   |
| 7   | 7     | 206 | VAL  | O-C-N  | 6.61  | 129.82      | 122.61   |
| 20  | M     | 201 | MET  | CA-C-N | 6.61  | 129.43      | 120.44   |
| 20  | M     | 201 | MET  | C-N-CA | 6.61  | 129.43      | 120.44   |
| 21  | N     | 285 | ALA  | N-CA-C | -6.61 | 104.00      | 111.14   |
| 24  | Q     | 304 | GLU  | CA-C-N | 6.61  | 129.80      | 120.28   |
| 24  | Q     | 304 | GLU  | C-N-CA | 6.61  | 129.80      | 120.28   |
| 26  | S     | 133 | GLU  | O-C-N  | 6.61  | 128.88      | 122.07   |
| 9   | B     | 107 | THR  | CA-C-N | 6.61  | 129.13      | 120.28   |
| 9   | B     | 107 | THR  | C-N-CA | 6.61  | 129.13      | 120.28   |
| 23  | P     | 300 | VAL  | CA-C-O | -6.61 | 113.85      | 120.85   |
| 21  | N     | 20  | VAL  | N-CA-C | -6.60 | 104.05      | 110.72   |
| 10  | C     | 107 | PRO  | CA-C-N | 6.60  | 128.88      | 120.56   |
| 10  | C     | 107 | PRO  | C-N-CA | 6.60  | 128.88      | 120.56   |
| 24  | Q     | 411 | SER  | CA-C-N | 6.60  | 129.46      | 120.54   |
| 24  | Q     | 411 | SER  | C-N-CA | 6.60  | 129.46      | 120.54   |
| 33  | Z     | 207 | ILE  | O-C-N  | 6.60  | 128.28      | 121.87   |
| 13  | F     | 92  | CYS  | N-CA-C | -6.60 | 104.01      | 111.14   |
| 24  | Q     | 82  | THR  | O-C-N  | 6.60  | 128.87      | 122.07   |
| 15  | H     | 241 | ASP  | CA-C-O | -6.60 | 112.56      | 120.41   |
| 24  | Q     | 66  | VAL  | CA-C-O | -6.60 | 113.86      | 120.85   |
| 29  | V     | 49  | VAL  | N-CA-C | -6.60 | 98.11       | 108.86   |
| 21  | N     | 362 | TRP  | N-CA-C | -6.59 | 104.17      | 111.36   |
| 23  | P     | 137 | ALA  | CA-C-N | 6.59  | 129.12      | 120.28   |
| 23  | P     | 137 | ALA  | C-N-CA | 6.59  | 129.12      | 120.28   |
| 12  | E     | 136 | ARG  | O-C-N  | -6.59 | 117.23      | 121.85   |
| 7   | 7     | 19  | LEU  | O-C-N  | -6.59 | 115.70      | 123.41   |
| 21  | N     | 64  | ILE  | CA-C-O | -6.59 | 114.19      | 121.17   |
| 14  | G     | 179 | VAL  | CA-C-N | 6.59  | 131.84      | 120.58   |
| 14  | G     | 179 | VAL  | C-N-CA | 6.59  | 131.84      | 120.58   |
| 27  | T     | 52  | LEU  | CA-C-N | 6.58  | 131.96      | 122.35   |
| 27  | T     | 52  | LEU  | C-N-CA | 6.58  | 131.96      | 122.35   |
| 14  | G     | 34  | THR  | CA-C-N | 6.58  | 134.11      | 121.54   |
| 14  | G     | 34  | THR  | C-N-CA | 6.58  | 134.11      | 121.54   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 106 | ILE  | O-C-N  | 6.58  | 128.36      | 121.91   |
| 29  | V     | 293 | VAL  | CA-C-N | 6.58  | 129.10      | 120.28   |
| 29  | V     | 293 | VAL  | C-N-CA | 6.58  | 129.10      | 120.28   |
| 23  | P     | 69  | ARG  | N-CA-C | 6.58  | 118.45      | 111.28   |
| 26  | S     | 419 | VAL  | CA-C-N | 6.58  | 129.63      | 120.29   |
| 26  | S     | 419 | VAL  | C-N-CA | 6.58  | 129.63      | 120.29   |
| 33  | Z     | 245 | VAL  | N-CA-C | 6.58  | 117.36      | 110.72   |
| 21  | N     | 544 | GLU  | CA-C-N | 6.57  | 128.98      | 120.44   |
| 21  | N     | 544 | GLU  | C-N-CA | 6.57  | 128.98      | 120.44   |
| 4   | 4     | 134 | TYR  | N-CA-C | -6.57 | 105.39      | 113.41   |
| 30  | W     | 20  | ASP  | CA-C-N | 6.57  | 131.53      | 122.07   |
| 30  | W     | 20  | ASP  | C-N-CA | 6.57  | 131.53      | 122.07   |
| 17  | J     | 366 | GLY  | CA-C-O | -6.57 | 113.98      | 120.75   |
| 30  | W     | 30  | ILE  | N-CA-C | 6.57  | 117.32      | 110.62   |
| 29  | V     | 266 | LEU  | O-C-N  | 6.57  | 128.83      | 122.07   |
| 12  | E     | 148 | ASP  | N-CA-C | -6.56 | 99.33       | 109.24   |
| 33  | Z     | 543 | THR  | N-CA-C | 6.56  | 118.09      | 111.07   |
| 17  | J     | 164 | ILE  | CA-C-O | -6.56 | 114.43      | 120.73   |
| 28  | U     | 99  | LEU  | N-CA-C | 6.56  | 119.27      | 110.35   |
| 9   | B     | 39  | ALA  | N-CA-C | -6.56 | 105.31      | 113.38   |
| 5   | 5     | 152 | ASP  | CA-C-O | -6.56 | 112.43      | 119.97   |
| 23  | P     | 385 | ASN  | N-CA-C | 6.56  | 118.43      | 111.28   |
| 33  | Z     | 579 | GLU  | N-CA-C | 6.56  | 118.43      | 111.28   |
| 1   | 1     | 126 | ILE  | N-CA-C | -6.55 | 98.19       | 108.86   |
| 27  | T     | 25  | LYS  | CA-C-O | 6.55  | 127.49      | 120.55   |
| 1   | 1     | 164 | LYS  | CA-C-O | -6.55 | 113.61      | 120.55   |
| 24  | Q     | 50  | ARG  | CA-C-O | -6.54 | 113.61      | 120.55   |
| 18  | K     | 425 | ASP  | N-CA-C | -6.54 | 103.71      | 112.94   |
| 16  | I     | 97  | GLU  | CA-C-N | 6.54  | 129.04      | 120.28   |
| 16  | I     | 97  | GLU  | C-N-CA | 6.54  | 129.04      | 120.28   |
| 21  | N     | 532 | ALA  | N-CA-C | -6.54 | 105.33      | 113.38   |
| 19  | L     | 416 | MET  | CA-C-O | 6.54  | 127.48      | 120.55   |
| 23  | P     | 126 | THR  | N-CA-C | -6.54 | 106.51      | 114.75   |
| 9   | B     | 118 | MET  | CA-C-N | 6.54  | 129.57      | 120.29   |
| 9   | B     | 118 | MET  | C-N-CA | 6.54  | 129.57      | 120.29   |
| 2   | 2     | 55  | VAL  | CA-C-N | 6.53  | 130.24      | 120.31   |
| 2   | 2     | 55  | VAL  | C-N-CA | 6.53  | 130.24      | 120.31   |
| 25  | R     | 87  | SER  | CA-C-O | 6.53  | 129.06      | 121.87   |
| 10  | C     | 189 | ALA  | CA-C-N | 6.53  | 128.79      | 120.56   |
| 10  | C     | 189 | ALA  | C-N-CA | 6.53  | 128.79      | 120.56   |
| 21  | N     | 639 | ASP  | O-C-N  | 6.53  | 129.04      | 122.12   |
| 21  | N     | 399 | PHE  | CA-C-N | 6.53  | 129.41      | 120.46   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 399 | PHE  | C-N-CA | 6.53  | 129.41      | 120.46   |
| 26  | S     | 469 | ASN  | O-C-N  | 6.53  | 129.59      | 122.15   |
| 6   | 6     | 20  | ASN  | CA-C-O | 6.53  | 127.56      | 120.32   |
| 23  | P     | 332 | GLU  | N-CA-C | -6.53 | 105.21      | 113.43   |
| 10  | C     | 230 | PHE  | CA-C-N | 6.52  | 130.60      | 120.68   |
| 10  | C     | 230 | PHE  | C-N-CA | 6.52  | 130.60      | 120.68   |
| 25  | R     | 279 | LEU  | CA-C-N | 6.52  | 131.33      | 120.64   |
| 25  | R     | 279 | LEU  | C-N-CA | 6.52  | 131.33      | 120.64   |
| 15  | H     | 436 | LYS  | N-CA-C | 6.52  | 118.39      | 111.28   |
| 11  | D     | 183 | GLU  | O-C-N  | -6.52 | 113.83      | 121.32   |
| 21  | N     | 630 | ALA  | CA-C-N | 6.52  | 127.17      | 120.00   |
| 21  | N     | 630 | ALA  | C-N-CA | 6.52  | 127.17      | 120.00   |
| 13  | F     | 192 | ALA  | CA-C-N | 6.51  | 127.21      | 119.98   |
| 13  | F     | 192 | ALA  | C-N-CA | 6.51  | 127.21      | 119.98   |
| 15  | H     | 374 | LYS  | O-C-N  | -6.51 | 114.52      | 123.12   |
| 23  | P     | 251 | LYS  | N-CA-C | 6.51  | 118.17      | 111.14   |
| 17  | J     | 150 | VAL  | CA-C-O | -6.51 | 113.38      | 120.67   |
| 23  | P     | 257 | TRP  | N-CA-C | 6.51  | 118.46      | 111.36   |
| 25  | R     | 146 | ASP  | CA-C-O | -6.51 | 113.87      | 121.16   |
| 32  | Y     | 81  | LEU  | O-C-N  | 6.51  | 128.77      | 122.07   |
| 10  | C     | 51  | LYS  | N-CA-C | -6.50 | 99.61       | 109.95   |
| 21  | N     | 703 | GLN  | CA-C-N | 6.50  | 127.31      | 120.03   |
| 21  | N     | 703 | GLN  | C-N-CA | 6.50  | 127.31      | 120.03   |
| 23  | P     | 94  | GLN  | CA-C-N | 6.50  | 129.53      | 120.29   |
| 23  | P     | 94  | GLN  | C-N-CA | 6.50  | 129.53      | 120.29   |
| 19  | L     | 246 | SER  | CA-C-N | 6.50  | 127.97      | 119.84   |
| 19  | L     | 246 | SER  | C-N-CA | 6.50  | 127.97      | 119.84   |
| 26  | S     | 306 | SER  | N-CA-C | -6.50 | 104.66      | 112.59   |
| 16  | I     | 88  | LYS  | CA-C-O | -6.50 | 113.66      | 120.55   |
| 18  | K     | 421 | VAL  | N-CA-C | -6.50 | 98.38       | 107.80   |
| 20  | M     | 338 | LEU  | CA-C-N | 6.50  | 133.96      | 121.54   |
| 20  | M     | 338 | LEU  | C-N-CA | 6.50  | 133.96      | 121.54   |
| 21  | N     | 203 | ARG  | CA-C-N | 6.50  | 128.99      | 120.28   |
| 21  | N     | 203 | ARG  | C-N-CA | 6.50  | 128.99      | 120.28   |
| 19  | L     | 121 | ALA  | N-CA-C | -6.50 | 101.34      | 110.50   |
| 18  | K     | 145 | ALA  | N-CA-C | -6.49 | 98.80       | 108.99   |
| 21  | N     | 382 | GLY  | CA-C-N | 6.49  | 128.98      | 120.28   |
| 21  | N     | 382 | GLY  | C-N-CA | 6.49  | 128.98      | 120.28   |
| 6   | 6     | 2   | THR  | N-CA-C | -6.49 | 97.65       | 108.75   |
| 29  | V     | 287 | THR  | CA-C-N | 6.49  | 128.98      | 120.28   |
| 29  | V     | 287 | THR  | C-N-CA | 6.49  | 128.98      | 120.28   |
| 23  | P     | 136 | ARG  | CA-C-N | 6.49  | 128.97      | 120.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | P     | 136 | ARG  | C-N-CA  | 6.49  | 128.97      | 120.28   |
| 29  | V     | 247 | ILE  | N-CA-C  | 6.48  | 122.83      | 109.34   |
| 21  | N     | 61  | ALA  | CA-C-N  | 6.48  | 129.29      | 120.54   |
| 21  | N     | 61  | ALA  | C-N-CA  | 6.48  | 129.29      | 120.54   |
| 21  | N     | 674 | GLN  | N-CA-C  | -6.48 | 104.64      | 112.54   |
| 25  | R     | 229 | LYS  | CA-C-O  | -6.48 | 113.68      | 120.55   |
| 33  | Z     | 258 | PRO  | CA-C-O  | -6.48 | 111.17      | 120.56   |
| 9   | B     | 72  | GLY  | O-C-N   | -6.48 | 117.53      | 123.42   |
| 14  | G     | 154 | GLY  | CA-C-O  | 6.47  | 124.86      | 118.77   |
| 14  | G     | 168 | ARG  | CA-C-N  | 6.47  | 129.24      | 120.44   |
| 14  | G     | 168 | ARG  | C-N-CA  | 6.47  | 129.24      | 120.44   |
| 16  | I     | 108 | THR  | CA-C-N  | 6.47  | 131.10      | 121.72   |
| 16  | I     | 108 | THR  | C-N-CA  | 6.47  | 131.10      | 121.72   |
| 33  | Z     | 463 | HIS  | CA-C-N  | 6.47  | 133.90      | 121.54   |
| 33  | Z     | 463 | HIS  | C-N-CA  | 6.47  | 133.90      | 121.54   |
| 7   | 7     | 178 | TYR  | O-C-N   | 6.47  | 129.07      | 122.09   |
| 21  | N     | 83  | LEU  | O-C-N   | -6.47 | 115.41      | 122.07   |
| 23  | P     | 138 | ARG  | N-CA-C  | 6.47  | 118.33      | 111.28   |
| 25  | R     | 103 | CYS  | N-CA-C  | 6.47  | 119.15      | 111.71   |
| 25  | R     | 289 | ILE  | CA-C-O  | 6.47  | 124.50      | 119.46   |
| 13  | F     | 158 | GLY  | N-CA-C  | -6.46 | 99.50       | 111.14   |
| 15  | H     | 208 | TYR  | N-CA-C  | 6.46  | 118.64      | 110.24   |
| 15  | H     | 303 | ALA  | N-CA-C  | -6.46 | 97.03       | 110.80   |
| 19  | L     | 425 | VAL  | N-CA-C  | 6.46  | 121.40      | 113.00   |
| 25  | R     | 223 | ASN  | N-CA-C  | -6.46 | 103.52      | 111.40   |
| 33  | Z     | 253 | VAL  | CB-CA-C | -6.46 | 107.56      | 113.70   |
| 1   | 1     | 184 | GLU  | N-CA-C  | -6.46 | 98.87       | 109.40   |
| 4   | 4     | 7   | ARG  | CA-C-O  | 6.46  | 127.26      | 120.54   |
| 29  | V     | 240 | ALA  | CA-C-N  | 6.46  | 128.84      | 120.44   |
| 29  | V     | 240 | ALA  | C-N-CA  | 6.46  | 128.84      | 120.44   |
| 33  | Z     | 264 | PHE  | CA-C-N  | 6.46  | 128.84      | 120.44   |
| 33  | Z     | 264 | PHE  | C-N-CA  | 6.46  | 128.84      | 120.44   |
| 26  | S     | 197 | SER  | CA-C-O  | -6.46 | 111.27      | 120.51   |
| 15  | H     | 286 | GLU  | CA-C-O  | 6.46  | 129.74      | 120.51   |
| 22  | O     | 225 | ASP  | CA-C-N  | 6.46  | 129.46      | 120.29   |
| 22  | O     | 225 | ASP  | C-N-CA  | 6.46  | 129.46      | 120.29   |
| 14  | G     | 80  | LEU  | CA-C-N  | 6.45  | 125.49      | 120.33   |
| 14  | G     | 80  | LEU  | C-N-CA  | 6.45  | 125.49      | 120.33   |
| 9   | B     | 234 | ARG  | CA-C-N  | 6.45  | 130.64      | 121.42   |
| 9   | B     | 234 | ARG  | C-N-CA  | 6.45  | 130.64      | 121.42   |
| 11  | D     | 221 | ILE  | N-CA-C  | -6.45 | 99.08       | 108.11   |
| 5   | 5     | 13  | ILE  | CA-C-O  | 6.45  | 127.43      | 120.53   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 29  | V     | 279 | HIS  | CA-C-N | 6.45  | 128.92      | 120.28   |
| 29  | V     | 279 | HIS  | C-N-CA | 6.45  | 128.92      | 120.28   |
| 33  | Z     | 534 | PHE  | CA-C-N | 6.45  | 129.21      | 120.63   |
| 33  | Z     | 534 | PHE  | C-N-CA | 6.45  | 129.21      | 120.63   |
| 22  | O     | 225 | ASP  | N-CA-C | -6.45 | 104.19      | 113.21   |
| 9   | B     | 104 | TYR  | CA-C-N | 6.44  | 127.02      | 120.38   |
| 9   | B     | 104 | TYR  | C-N-CA | 6.44  | 127.02      | 120.38   |
| 14  | G     | 46  | VAL  | N-CA-C | -6.44 | 98.86       | 108.46   |
| 23  | P     | 275 | ASN  | CA-C-N | 6.44  | 129.56      | 120.28   |
| 23  | P     | 275 | ASN  | C-N-CA | 6.44  | 129.56      | 120.28   |
| 6   | 6     | 73  | LYS  | CA-C-N | 6.44  | 130.01      | 120.87   |
| 6   | 6     | 73  | LYS  | C-N-CA | 6.44  | 130.01      | 120.87   |
| 25  | R     | 101 | GLU  | N-CA-C | -6.44 | 103.54      | 111.40   |
| 27  | T     | 201 | PRO  | CA-C-N | 6.44  | 128.91      | 120.28   |
| 27  | T     | 201 | PRO  | C-N-CA | 6.44  | 128.91      | 120.28   |
| 12  | E     | 91  | HIS  | CA-C-N | 6.44  | 129.43      | 120.29   |
| 12  | E     | 91  | HIS  | C-N-CA | 6.44  | 129.43      | 120.29   |
| 21  | N     | 680 | LYS  | CA-C-O | -6.44 | 114.06      | 120.82   |
| 1   | 1     | 8   | PHE  | CA-C-N | 6.43  | 129.43      | 120.29   |
| 1   | 1     | 8   | PHE  | C-N-CA | 6.43  | 129.43      | 120.29   |
| 19  | L     | 248 | ALA  | CA-C-O | 6.43  | 127.37      | 120.55   |
| 30  | W     | 126 | ILE  | CA-C-O | -6.43 | 114.26      | 120.95   |
| 13  | F     | 230 | VAL  | CA-C-N | 6.43  | 129.19      | 120.38   |
| 13  | F     | 230 | VAL  | C-N-CA | 6.43  | 129.19      | 120.38   |
| 24  | Q     | 84  | TYR  | CA-C-O | -6.43 | 114.08      | 120.70   |
| 28  | U     | 200 | LEU  | CA-C-N | 6.43  | 129.22      | 120.54   |
| 28  | U     | 200 | LEU  | C-N-CA | 6.43  | 129.22      | 120.54   |
| 6   | 6     | 87  | LEU  | CA-C-N | 6.43  | 128.79      | 120.44   |
| 6   | 6     | 87  | LEU  | C-N-CA | 6.43  | 128.79      | 120.44   |
| 6   | 6     | 177 | ASP  | CA-C-N | 6.43  | 128.89      | 120.28   |
| 6   | 6     | 177 | ASP  | C-N-CA | 6.43  | 128.89      | 120.28   |
| 7   | 7     | 162 | VAL  | CA-C-O | 6.43  | 127.63      | 120.95   |
| 21  | N     | 75  | TYR  | CA-C-N | 6.43  | 128.89      | 120.28   |
| 21  | N     | 75  | TYR  | C-N-CA | 6.43  | 128.89      | 120.28   |
| 23  | P     | 281 | ILE  | CA-C-N | 6.43  | 128.89      | 120.28   |
| 23  | P     | 281 | ILE  | C-N-CA | 6.43  | 128.89      | 120.28   |
| 26  | S     | 298 | ARG  | CA-C-N | 6.43  | 133.81      | 121.54   |
| 26  | S     | 298 | ARG  | C-N-CA | 6.43  | 133.81      | 121.54   |
| 7   | 7     | 216 | ASP  | CA-C-N | 6.42  | 129.35      | 120.49   |
| 7   | 7     | 216 | ASP  | C-N-CA | 6.42  | 129.35      | 120.49   |
| 21  | N     | 250 | ASP  | CA-C-O | 6.42  | 127.30      | 120.36   |
| 23  | P     | 361 | THR  | N-CA-C | -6.42 | 101.01      | 110.52   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 18  | K     | 207 | ARG  | CA-C-N | 6.42  | 126.56      | 121.61   |
| 18  | K     | 207 | ARG  | C-N-CA | 6.42  | 126.56      | 121.61   |
| 24  | Q     | 61  | LEU  | CA-C-N | 6.42  | 128.38      | 120.22   |
| 24  | Q     | 61  | LEU  | C-N-CA | 6.42  | 128.38      | 120.22   |
| 33  | Z     | 174 | GLU  | O-C-N  | 6.42  | 129.03      | 122.09   |
| 23  | P     | 382 | ASP  | CA-C-N | 6.42  | 128.88      | 120.28   |
| 23  | P     | 382 | ASP  | C-N-CA | 6.42  | 128.88      | 120.28   |
| 27  | T     | 24  | GLU  | CA-C-N | 6.42  | 128.88      | 120.28   |
| 27  | T     | 24  | GLU  | C-N-CA | 6.42  | 128.88      | 120.28   |
| 4   | 4     | 30  | SER  | CA-C-N | 6.42  | 129.95      | 120.90   |
| 4   | 4     | 30  | SER  | C-N-CA | 6.42  | 129.95      | 120.90   |
| 17  | J     | 268 | VAL  | CA-C-N | 6.42  | 130.07      | 120.31   |
| 17  | J     | 268 | VAL  | C-N-CA | 6.42  | 130.07      | 120.31   |
| 19  | L     | 104 | LEU  | O-C-N  | 6.42  | 130.25      | 123.06   |
| 21  | N     | 888 | ASP  | N-CA-C | -6.42 | 104.70      | 113.30   |
| 33  | Z     | 842 | GLN  | N-CA-C | 6.41  | 119.26      | 111.82   |
| 13  | F     | 126 | ARG  | O-C-N  | -6.41 | 116.83      | 121.83   |
| 16  | I     | 96  | LEU  | N-CA-C | 6.41  | 118.27      | 111.28   |
| 18  | K     | 51  | LEU  | CA-C-N | 6.41  | 128.87      | 120.28   |
| 18  | K     | 51  | LEU  | C-N-CA | 6.41  | 128.87      | 120.28   |
| 23  | P     | 93  | ILE  | O-C-N  | 6.41  | 128.19      | 121.91   |
| 27  | T     | 182 | LYS  | O-C-N  | 6.41  | 128.91      | 122.12   |
| 31  | X     | 105 | ASN  | N-CA-C | -6.41 | 103.06      | 113.19   |
| 3   | 3     | 40  | VAL  | CA-C-N | 6.40  | 131.84      | 123.00   |
| 3   | 3     | 40  | VAL  | C-N-CA | 6.40  | 131.84      | 123.00   |
| 21  | N     | 642 | ASP  | CA-C-N | 6.40  | 125.90      | 119.24   |
| 21  | N     | 642 | ASP  | C-N-CA | 6.40  | 125.90      | 119.24   |
| 24  | Q     | 284 | ALA  | CA-C-N | 6.40  | 132.85      | 122.67   |
| 24  | Q     | 284 | ALA  | C-N-CA | 6.40  | 132.85      | 122.67   |
| 1   | 1     | 161 | GLN  | CA-C-O | -6.40 | 114.11      | 120.70   |
| 8   | A     | 68  | THR  | N-CA-C | -6.40 | 104.72      | 113.30   |
| 22  | O     | 225 | ASP  | O-C-N  | 6.40  | 127.80      | 121.85   |
| 33  | Z     | 488 | ALA  | O-C-N  | 6.40  | 129.44      | 122.15   |
| 9   | B     | 114 | VAL  | CA-C-N | 6.40  | 128.85      | 120.28   |
| 9   | B     | 114 | VAL  | C-N-CA | 6.40  | 128.85      | 120.28   |
| 26  | S     | 196 | ARG  | N-CA-C | -6.39 | 104.02      | 113.61   |
| 13  | F     | 96  | SER  | N-CA-C | 6.39  | 118.33      | 111.36   |
| 13  | F     | 116 | ALA  | CA-C-O | 6.39  | 127.20      | 120.42   |
| 25  | R     | 285 | ALA  | N-CA-C | -6.39 | 105.47      | 113.20   |
| 30  | W     | 70  | GLY  | CA-C-N | 6.39  | 128.85      | 120.28   |
| 30  | W     | 70  | GLY  | C-N-CA | 6.39  | 128.85      | 120.28   |
| 4   | 4     | 156 | GLY  | CA-C-N | 6.39  | 128.84      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | 4     | 156 | GLY  | C-N-CA | 6.39  | 128.84      | 120.28   |
| 19  | L     | 205 | GLU  | CA-C-N | 6.39  | 128.74      | 120.56   |
| 19  | L     | 205 | GLU  | C-N-CA | 6.39  | 128.74      | 120.56   |
| 22  | O     | 69  | PHE  | N-CA-C | 6.38  | 117.90      | 111.07   |
| 28  | U     | 138 | VAL  | O-C-N  | -6.38 | 116.18      | 123.07   |
| 2   | 2     | 2   | THR  | N-CA-C | -6.38 | 97.15       | 108.13   |
| 33  | Z     | 271 | ILE  | CA-C-N | 6.38  | 128.83      | 120.28   |
| 33  | Z     | 271 | ILE  | C-N-CA | 6.38  | 128.83      | 120.28   |
| 8   | A     | 96  | ARG  | CA-C-N | 6.38  | 128.83      | 120.28   |
| 8   | A     | 96  | ARG  | C-N-CA | 6.38  | 128.83      | 120.28   |
| 21  | N     | 214 | LEU  | CA-C-N | 6.38  | 130.00      | 120.31   |
| 21  | N     | 214 | LEU  | C-N-CA | 6.38  | 130.00      | 120.31   |
| 33  | Z     | 143 | VAL  | CA-C-N | 6.38  | 130.38      | 120.75   |
| 33  | Z     | 143 | VAL  | C-N-CA | 6.38  | 130.38      | 120.75   |
| 17  | J     | 315 | GLU  | N-CA-C | -6.38 | 100.13      | 110.20   |
| 33  | Z     | 589 | SER  | O-C-N  | 6.38  | 130.11      | 122.27   |
| 17  | J     | 381 | ASP  | CA-C-N | 6.37  | 129.34      | 120.29   |
| 17  | J     | 381 | ASP  | C-N-CA | 6.37  | 129.34      | 120.29   |
| 18  | K     | 405 | SER  | N-CA-C | 6.37  | 118.23      | 111.28   |
| 21  | N     | 69  | TYR  | CA-C-N | 6.37  | 129.15      | 120.54   |
| 21  | N     | 69  | TYR  | C-N-CA | 6.37  | 129.15      | 120.54   |
| 15  | H     | 340 | LEU  | CA-C-N | 6.37  | 131.36      | 120.72   |
| 15  | H     | 340 | LEU  | C-N-CA | 6.37  | 131.36      | 120.72   |
| 19  | L     | 197 | ILE  | N-CA-C | -6.37 | 106.08      | 111.56   |
| 24  | Q     | 133 | LEU  | N-CA-C | -6.37 | 103.59      | 112.45   |
| 24  | Q     | 3   | LEU  | CA-C-N | 6.37  | 126.12      | 119.05   |
| 24  | Q     | 3   | LEU  | C-N-CA | 6.37  | 126.12      | 119.05   |
| 4   | 4     | 193 | ASP  | CA-C-O | -6.37 | 113.77      | 121.28   |
| 19  | L     | 199 | LEU  | CA-C-N | 6.37  | 125.94      | 119.19   |
| 19  | L     | 199 | LEU  | C-N-CA | 6.37  | 125.94      | 119.19   |
| 5   | 5     | 198 | TRP  | CA-C-N | 6.37  | 129.06      | 120.65   |
| 5   | 5     | 198 | TRP  | C-N-CA | 6.37  | 129.06      | 120.65   |
| 17  | J     | 51  | LEU  | CA-C-N | 6.37  | 128.72      | 120.44   |
| 17  | J     | 51  | LEU  | C-N-CA | 6.37  | 128.72      | 120.44   |
| 1   | 1     | 189 | TYR  | CA-C-O | -6.37 | 114.02      | 120.96   |
| 8   | A     | 146 | VAL  | CA-C-N | 6.37  | 130.36      | 120.75   |
| 8   | A     | 146 | VAL  | C-N-CA | 6.37  | 130.36      | 120.75   |
| 20  | M     | 420 | SER  | N-CA-C | 6.37  | 118.22      | 111.28   |
| 28  | U     | 230 | GLN  | CA-C-N | 6.37  | 128.71      | 120.44   |
| 28  | U     | 230 | GLN  | C-N-CA | 6.37  | 128.71      | 120.44   |
| 20  | M     | 64  | ASP  | CA-C-N | 6.36  | 128.81      | 120.28   |
| 20  | M     | 64  | ASP  | C-N-CA | 6.36  | 128.81      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 23  | P     | 123 | ARG  | N-CA-C | -6.36 | 103.64      | 112.30   |
| 12  | E     | 236 | THR  | O-C-N  | -6.36 | 114.90      | 122.15   |
| 25  | R     | 214 | TYR  | CA-C-N | 6.36  | 127.04      | 119.98   |
| 25  | R     | 214 | TYR  | C-N-CA | 6.36  | 127.04      | 119.98   |
| 21  | N     | 518 | ALA  | CA-C-N | 6.36  | 129.17      | 120.46   |
| 21  | N     | 518 | ALA  | C-N-CA | 6.36  | 129.17      | 120.46   |
| 22  | O     | 200 | GLU  | CA-C-O | -6.36 | 111.45      | 120.16   |
| 15  | H     | 366 | LEU  | N-CA-C | 6.36  | 117.87      | 111.07   |
| 20  | M     | 250 | GLN  | N-CA-C | 6.36  | 119.19      | 111.82   |
| 25  | R     | 232 | VAL  | CA-C-N | 6.36  | 130.59      | 121.50   |
| 25  | R     | 232 | VAL  | C-N-CA | 6.36  | 130.59      | 121.50   |
| 27  | T     | 123 | HIS  | CA-C-O | 6.35  | 127.28      | 120.55   |
| 3   | 3     | 128 | ILE  | N-CA-C | -6.35 | 99.05       | 108.45   |
| 11  | D     | 123 | SER  | O-C-N  | 6.35  | 130.35      | 122.86   |
| 21  | N     | 548 | ARG  | CA-C-N | 6.35  | 128.69      | 120.44   |
| 21  | N     | 548 | ARG  | C-N-CA | 6.35  | 128.69      | 120.44   |
| 23  | P     | 420 | ASP  | CA-C-O | -6.35 | 113.82      | 120.55   |
| 25  | R     | 416 | LYS  | O-C-N  | -6.35 | 115.39      | 122.12   |
| 28  | U     | 192 | ASN  | CA-C-N | 6.35  | 128.69      | 120.44   |
| 28  | U     | 192 | ASN  | C-N-CA | 6.35  | 128.69      | 120.44   |
| 19  | L     | 295 | THR  | N-CA-C | -6.34 | 102.92      | 110.41   |
| 21  | N     | 708 | ALA  | CA-C-N | 6.34  | 133.85      | 121.41   |
| 21  | N     | 708 | ALA  | C-N-CA | 6.34  | 133.85      | 121.41   |
| 33  | Z     | 612 | GLY  | N-CA-C | -6.34 | 101.66      | 112.51   |
| 7   | 7     | 17  | ASP  | CA-C-O | -6.34 | 114.76      | 121.99   |
| 10  | C     | 84  | ALA  | CA-C-N | 6.34  | 129.41      | 120.28   |
| 10  | C     | 84  | ALA  | C-N-CA | 6.34  | 129.41      | 120.28   |
| 17  | J     | 347 | ALA  | N-CA-C | 6.34  | 118.19      | 111.28   |
| 24  | Q     | 274 | LEU  | CA-C-N | 6.34  | 129.42      | 120.42   |
| 24  | Q     | 274 | LEU  | C-N-CA | 6.34  | 129.42      | 120.42   |
| 4   | 4     | 120 | TYR  | CA-C-N | 6.33  | 128.67      | 120.44   |
| 4   | 4     | 120 | TYR  | C-N-CA | 6.33  | 128.67      | 120.44   |
| 16  | I     | 176 | SER  | CA-C-O | -6.33 | 111.48      | 120.16   |
| 25  | R     | 273 | SER  | N-CA-C | -6.33 | 100.76      | 110.32   |
| 21  | N     | 634 | LEU  | CA-C-N | 6.33  | 129.93      | 120.31   |
| 21  | N     | 634 | LEU  | C-N-CA | 6.33  | 129.93      | 120.31   |
| 30  | W     | 179 | ARG  | N-CA-C | -6.33 | 97.31       | 110.80   |
| 33  | Z     | 754 | LYS  | N-CA-C | 6.33  | 118.18      | 111.28   |
| 21  | N     | 728 | LYS  | CA-C-N | 6.33  | 128.76      | 120.28   |
| 21  | N     | 728 | LYS  | C-N-CA | 6.33  | 128.76      | 120.28   |
| 33  | Z     | 480 | ASN  | CA-C-O | -6.33 | 113.41      | 120.25   |
| 33  | Z     | 578 | GLY  | CA-C-N | 6.33  | 128.76      | 120.28   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 33  | Z     | 578 | GLY  | C-N-CA    | 6.33  | 128.76      | 120.28   |
| 18  | K     | 70  | ASP  | N-CA-C    | -6.33 | 104.47      | 111.36   |
| 21  | N     | 899 | ASN  | CA-C-O    | -6.33 | 114.46      | 121.23   |
| 22  | O     | 76  | LEU  | CA-C-N    | 6.33  | 129.62      | 120.38   |
| 22  | O     | 76  | LEU  | C-N-CA    | 6.33  | 129.62      | 120.38   |
| 22  | O     | 177 | GLN  | CA-C-N    | 6.33  | 129.27      | 120.29   |
| 22  | O     | 177 | GLN  | C-N-CA    | 6.33  | 129.27      | 120.29   |
| 23  | P     | 382 | ASP  | O-C-N     | 6.33  | 129.36      | 122.15   |
| 24  | Q     | 122 | ILE  | CA-C-N    | 6.33  | 128.76      | 120.28   |
| 24  | Q     | 122 | ILE  | C-N-CA    | 6.33  | 128.76      | 120.28   |
| 16  | I     | 352 | ASN  | CA-C-O    | -6.32 | 114.88      | 120.19   |
| 24  | Q     | 236 | PHE  | N-CA-C    | 6.32  | 118.17      | 111.28   |
| 26  | S     | 365 | THR  | CA-C-N    | 6.32  | 128.66      | 120.44   |
| 26  | S     | 365 | THR  | C-N-CA    | 6.32  | 128.66      | 120.44   |
| 23  | P     | 428 | THR  | CA-C-N    | 6.32  | 128.75      | 120.60   |
| 23  | P     | 428 | THR  | C-N-CA    | 6.32  | 128.75      | 120.60   |
| 33  | Z     | 224 | LEU  | CA-C-O    | -6.32 | 113.85      | 120.55   |
| 3   | 3     | 159 | SER  | N-CA-C    | 6.32  | 117.83      | 111.07   |
| 29  | V     | 252 | SER  | N-CA-C    | 6.31  | 118.97      | 111.71   |
| 33  | Z     | 135 | LEU  | CA-C-O    | -6.31 | 114.20      | 120.70   |
| 3   | 3     | 194 | ARG  | N-CA-C    | 6.31  | 118.44      | 110.24   |
| 19  | L     | 312 | MET  | CA-C-N    | 6.31  | 131.26      | 120.72   |
| 19  | L     | 312 | MET  | C-N-CA    | 6.31  | 131.26      | 120.72   |
| 11  | D     | 33  | ALA  | CA-C-O    | -6.31 | 113.03      | 120.60   |
| 20  | M     | 396 | VAL  | N-CA-C    | -6.31 | 104.35      | 110.72   |
| 25  | R     | 66  | LEU  | O-C-N     | 6.31  | 128.90      | 122.09   |
| 26  | S     | 127 | THR  | CA-C-O    | 6.31  | 127.44      | 120.82   |
| 14  | G     | 210 | ASP  | O-C-N     | -6.30 | 115.31      | 122.68   |
| 25  | R     | 362 | ALA  | N-CA-C    | 6.30  | 119.13      | 111.82   |
| 15  | H     | 288 | ALA  | N-CA-C    | 6.30  | 118.95      | 111.71   |
| 22  | O     | 115 | ARG  | N-CA-C    | -6.30 | 106.23      | 114.04   |
| 2   | 2     | 59  | ILE  | CA-C-N    | 6.30  | 126.97      | 119.98   |
| 2   | 2     | 59  | ILE  | C-N-CA    | 6.30  | 126.97      | 119.98   |
| 21  | N     | 661 | SER  | O-C-N     | 6.30  | 130.02      | 122.27   |
| 15  | H     | 278 | GLU  | N-CA-CB   | 6.30  | 120.04      | 110.28   |
| 19  | L     | 167 | VAL  | N-CA-C    | -6.30 | 107.16      | 113.20   |
| 11  | D     | 49  | ARG  | N-CA-C    | -6.29 | 97.81       | 108.26   |
| 11  | D     | 102 | ASP  | O-C-N     | -6.29 | 116.93      | 121.84   |
| 20  | M     | 299 | ARG  | NE-CZ-NH1 | 6.29  | 127.79      | 121.50   |
| 33  | Z     | 476 | ASP  | CA-C-N    | 6.29  | 128.71      | 120.28   |
| 33  | Z     | 476 | ASP  | C-N-CA    | 6.29  | 128.71      | 120.28   |
| 10  | C     | 51  | LYS  | CA-C-O    | 6.29  | 128.26      | 121.16   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 11  | D     | 194 | LEU  | CA-C-N | 6.29  | 129.22      | 120.29   |
| 11  | D     | 194 | LEU  | C-N-CA | 6.29  | 129.22      | 120.29   |
| 14  | G     | 113 | ASP  | CA-C-N | 6.29  | 128.70      | 120.28   |
| 14  | G     | 113 | ASP  | C-N-CA | 6.29  | 128.70      | 120.28   |
| 21  | N     | 875 | LEU  | CA-C-N | 6.29  | 126.03      | 119.05   |
| 21  | N     | 875 | LEU  | C-N-CA | 6.29  | 126.03      | 119.05   |
| 29  | V     | 113 | GLY  | CA-C-O | 6.29  | 125.03      | 119.56   |
| 22  | O     | 322 | ASP  | N-CA-C | 6.28  | 118.13      | 111.28   |
| 3   | 3     | 193 | MET  | CA-C-N | 6.28  | 130.05      | 120.82   |
| 3   | 3     | 193 | MET  | C-N-CA | 6.28  | 130.05      | 120.82   |
| 16  | I     | 92  | GLU  | CA-C-N | 6.28  | 129.21      | 120.29   |
| 16  | I     | 92  | GLU  | C-N-CA | 6.28  | 129.21      | 120.29   |
| 21  | N     | 351 | ALA  | O-C-N  | 6.28  | 128.87      | 122.09   |
| 20  | M     | 418 | GLY  | CA-C-N | 6.28  | 129.06      | 120.46   |
| 20  | M     | 418 | GLY  | C-N-CA | 6.28  | 129.06      | 120.46   |
| 4   | 4     | 172 | PRO  | N-CA-C | -6.28 | 105.81      | 114.98   |
| 18  | K     | 178 | ASP  | CA-C-N | 6.28  | 128.98      | 120.44   |
| 18  | K     | 178 | ASP  | C-N-CA | 6.28  | 128.98      | 120.44   |
| 18  | K     | 236 | ARG  | CA-C-O | 6.28  | 127.08      | 120.36   |
| 19  | L     | 80  | ASN  | CA-C-N | 6.28  | 129.06      | 120.46   |
| 19  | L     | 80  | ASN  | C-N-CA | 6.28  | 129.06      | 120.46   |
| 21  | N     | 363 | ALA  | O-C-N  | -6.28 | 114.88      | 122.22   |
| 21  | N     | 522 | ALA  | CA-C-N | 6.28  | 128.69      | 120.28   |
| 21  | N     | 522 | ALA  | C-N-CA | 6.28  | 128.69      | 120.28   |
| 21  | N     | 722 | THR  | CA-C-O | 6.28  | 125.42      | 118.52   |
| 23  | P     | 158 | ASP  | N-CA-C | 6.28  | 117.78      | 111.07   |
| 30  | W     | 80  | GLN  | N-CA-C | -6.28 | 99.01       | 109.24   |
| 24  | Q     | 69  | GLY  | CA-C-O | 6.27  | 127.52      | 119.68   |
| 29  | V     | 209 | GLU  | CA-C-N | 6.27  | 128.59      | 120.44   |
| 29  | V     | 209 | GLU  | C-N-CA | 6.27  | 128.59      | 120.44   |
| 19  | L     | 393 | ASN  | CA-C-O | 6.27  | 127.19      | 120.55   |
| 21  | N     | 423 | LEU  | N-CA-C | 6.27  | 119.09      | 111.82   |
| 22  | O     | 239 | MET  | N-CA-C | -6.27 | 104.44      | 113.21   |
| 27  | T     | 220 | PHE  | CA-C-N | 6.27  | 128.68      | 120.28   |
| 27  | T     | 220 | PHE  | C-N-CA | 6.27  | 128.68      | 120.28   |
| 5   | 5     | 57  | THR  | CA-C-N | 6.26  | 128.68      | 120.28   |
| 5   | 5     | 57  | THR  | C-N-CA | 6.26  | 128.68      | 120.28   |
| 8   | A     | 16  | ILE  | N-CA-C | -6.26 | 99.27       | 108.23   |
| 17  | J     | 188 | TYR  | N-CA-C | -6.26 | 98.04       | 108.75   |
| 28  | U     | 117 | ASN  | CA-C-N | 6.26  | 126.63      | 119.93   |
| 28  | U     | 117 | ASN  | C-N-CA | 6.26  | 126.63      | 119.93   |
| 19  | L     | 74  | LEU  | CA-C-N | 6.26  | 129.18      | 120.29   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | L     | 74  | LEU  | C-N-CA  | 6.26  | 129.18      | 120.29   |
| 20  | M     | 165 | SER  | N-CA-C  | 6.26  | 119.69      | 110.30   |
| 31  | X     | 55  | LYS  | CA-C-N  | 6.26  | 126.59      | 119.83   |
| 31  | X     | 55  | LYS  | C-N-CA  | 6.26  | 126.59      | 119.83   |
| 2   | 2     | 208 | GLY  | N-CA-C  | -6.25 | 105.26      | 115.46   |
| 6   | 6     | -6  | PRO  | N-CA-C  | -6.25 | 105.38      | 113.57   |
| 14  | G     | 36  | SER  | N-CA-C  | -6.25 | 99.62       | 109.50   |
| 23  | P     | 435 | LYS  | CA-C-N  | 6.25  | 128.57      | 120.44   |
| 23  | P     | 435 | LYS  | C-N-CA  | 6.25  | 128.57      | 120.44   |
| 33  | Z     | 989 | TYR  | N-CA-C  | -6.25 | 101.12      | 110.06   |
| 4   | 4     | 148 | ARG  | CA-C-N  | 6.25  | 127.66      | 119.84   |
| 4   | 4     | 148 | ARG  | C-N-CA  | 6.25  | 127.66      | 119.84   |
| 16  | I     | 130 | VAL  | CB-CA-C | -6.25 | 101.04      | 111.29   |
| 7   | 7     | 133 | THR  | N-CA-C  | -6.25 | 98.44       | 109.06   |
| 25  | R     | 56  | GLU  | N-CA-C  | -6.25 | 103.78      | 111.40   |
| 33  | Z     | 847 | ILE  | CA-C-N  | 6.25  | 129.16      | 120.29   |
| 33  | Z     | 847 | ILE  | C-N-CA  | 6.25  | 129.16      | 120.29   |
| 16  | I     | 248 | VAL  | N-CA-C  | -6.25 | 98.20       | 107.51   |
| 16  | I     | 331 | ILE  | N-CA-C  | -6.25 | 105.62      | 112.80   |
| 18  | K     | 391 | GLY  | N-CA-C  | -6.25 | 104.77      | 112.77   |
| 4   | 4     | 98  | GLN  | N-CA-C  | -6.25 | 102.80      | 110.61   |
| 17  | J     | 238 | ARG  | CA-C-O  | -6.24 | 113.80      | 120.42   |
| 21  | N     | 666 | GLN  | CA-C-O  | -6.24 | 114.40      | 122.14   |
| 6   | 6     | 140 | PHE  | CA-C-N  | 6.24  | 129.15      | 120.29   |
| 6   | 6     | 140 | PHE  | C-N-CA  | 6.24  | 129.15      | 120.29   |
| 14  | G     | 208 | GLU  | CA-C-N  | 6.24  | 132.32      | 122.21   |
| 14  | G     | 208 | GLU  | C-N-CA  | 6.24  | 132.32      | 122.21   |
| 17  | J     | 45  | GLU  | CA-C-N  | 6.24  | 129.15      | 120.29   |
| 17  | J     | 45  | GLU  | C-N-CA  | 6.24  | 129.15      | 120.29   |
| 9   | B     | 175 | LEU  | CA-C-N  | 6.24  | 128.64      | 120.28   |
| 9   | B     | 175 | LEU  | C-N-CA  | 6.24  | 128.64      | 120.28   |
| 16  | I     | 83  | LYS  | CA-C-O  | -6.24 | 112.80      | 118.79   |
| 18  | K     | 405 | SER  | CA-C-N  | 6.24  | 128.64      | 120.28   |
| 18  | K     | 405 | SER  | C-N-CA  | 6.24  | 128.64      | 120.28   |
| 5   | 5     | 160 | SER  | CA-C-N  | 6.23  | 129.00      | 120.46   |
| 5   | 5     | 160 | SER  | C-N-CA  | 6.23  | 129.00      | 120.46   |
| 21  | N     | 362 | TRP  | CA-C-N  | 6.23  | 129.26      | 120.28   |
| 21  | N     | 362 | TRP  | C-N-CA  | 6.23  | 129.26      | 120.28   |
| 20  | M     | 162 | GLU  | CA-C-N  | 6.23  | 130.73      | 120.94   |
| 20  | M     | 162 | GLU  | C-N-CA  | 6.23  | 130.73      | 120.94   |
| 21  | N     | 621 | THR  | CA-C-N  | 6.23  | 128.54      | 120.44   |
| 21  | N     | 621 | THR  | C-N-CA  | 6.23  | 128.54      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 22  | O     | 298 | GLU  | N-CA-C | -6.23 | 104.57      | 111.36   |
| 2   | 2     | 102 | GLY  | N-CA-C | -6.23 | 101.16      | 110.38   |
| 20  | M     | 373 | ASP  | N-CA-C | -6.22 | 104.44      | 114.09   |
| 3   | 3     | 59  | ARG  | CA-C-N | 6.22  | 128.53      | 120.44   |
| 3   | 3     | 59  | ARG  | C-N-CA | 6.22  | 128.53      | 120.44   |
| 32  | Y     | 79  | ALA  | CA-C-N | 6.22  | 128.62      | 120.28   |
| 32  | Y     | 79  | ALA  | C-N-CA | 6.22  | 128.62      | 120.28   |
| 2   | 2     | 14  | ILE  | O-C-N  | -6.22 | 116.31      | 122.97   |
| 15  | H     | 291 | VAL  | O-C-N  | -6.22 | 115.42      | 121.83   |
| 21  | N     | 887 | ASP  | N-CA-C | -6.22 | 103.38      | 111.71   |
| 9   | B     | 176 | GLU  | CA-C-O | 6.22  | 127.14      | 120.55   |
| 21  | N     | 282 | TYR  | N-CA-C | -6.22 | 100.16      | 108.74   |
| 21  | N     | 897 | LYS  | N-CA-C | -6.22 | 104.17      | 112.94   |
| 25  | R     | 115 | GLU  | CA-C-O | 6.22  | 127.01      | 120.42   |
| 30  | W     | 165 | GLN  | N-CA-C | -6.22 | 105.34      | 113.17   |
| 29  | V     | 31  | SER  | N-CA-C | 6.22  | 118.57      | 111.11   |
| 4   | 4     | 173 | MET  | CA-C-O | -6.21 | 114.31      | 121.15   |
| 14  | G     | 121 | ALA  | CA-C-O | -6.21 | 113.83      | 120.42   |
| 9   | B     | 211 | LEU  | CA-C-O | 6.21  | 127.80      | 120.66   |
| 23  | P     | 439 | MET  | CA-C-N | 6.21  | 128.60      | 120.28   |
| 23  | P     | 439 | MET  | C-N-CA | 6.21  | 128.60      | 120.28   |
| 33  | Z     | 884 | THR  | CA-C-O | -6.21 | 113.08      | 120.10   |
| 21  | N     | 7   | ALA  | N-CA-C | 6.21  | 121.97      | 113.16   |
| 24  | Q     | 267 | LEU  | O-C-N  | -6.21 | 115.54      | 122.12   |
| 11  | D     | 121 | THR  | CA-C-N | 6.21  | 131.07      | 120.71   |
| 11  | D     | 121 | THR  | C-N-CA | 6.21  | 131.07      | 120.71   |
| 20  | M     | 389 | ALA  | CA-C-N | 6.21  | 129.10      | 120.29   |
| 20  | M     | 389 | ALA  | C-N-CA | 6.21  | 129.10      | 120.29   |
| 22  | O     | 292 | CYS  | N-CA-C | -6.21 | 104.60      | 111.36   |
| 19  | L     | 379 | ALA  | CA-C-N | 6.20  | 128.96      | 120.46   |
| 19  | L     | 379 | ALA  | C-N-CA | 6.20  | 128.96      | 120.46   |
| 2   | 2     | 214 | LYS  | N-CA-C | -6.20 | 98.87       | 108.42   |
| 27  | T     | 38  | ASN  | N-CA-C | -6.20 | 105.29      | 112.92   |
| 10  | C     | 136 | ILE  | CA-C-O | -6.20 | 113.94      | 120.39   |
| 24  | Q     | 208 | ILE  | N-CA-C | -6.20 | 99.37       | 108.23   |
| 28  | U     | 291 | LEU  | CA-C-N | 6.20  | 128.37      | 120.56   |
| 28  | U     | 291 | LEU  | C-N-CA | 6.20  | 128.37      | 120.56   |
| 20  | M     | 229 | THR  | CA-C-N | 6.20  | 128.58      | 120.28   |
| 20  | M     | 229 | THR  | C-N-CA | 6.20  | 128.58      | 120.28   |
| 2   | 2     | 155 | ALA  | CA-C-N | 6.20  | 128.49      | 120.44   |
| 2   | 2     | 155 | ALA  | C-N-CA | 6.20  | 128.49      | 120.44   |
| 16  | I     | 180 | SER  | CA-C-N | 6.20  | 129.20      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | I     | 180 | SER  | C-N-CA | 6.20  | 129.20      | 120.28   |
| 23  | P     | 282 | HIS  | CA-C-O | -6.20 | 113.98      | 120.55   |
| 24  | Q     | 287 | THR  | CA-C-O | -6.20 | 112.59      | 119.34   |
| 30  | W     | 75  | GLY  | CA-C-N | 6.20  | 131.07      | 120.72   |
| 30  | W     | 75  | GLY  | C-N-CA | 6.20  | 131.07      | 120.72   |
| 2   | 2     | 92  | GLY  | N-CA-C | 6.19  | 123.26      | 115.21   |
| 23  | P     | 359 | ARG  | N-CA-C | -6.19 | 99.72       | 109.50   |
| 33  | Z     | 493 | LEU  | CA-C-O | 6.19  | 127.09      | 119.97   |
| 4   | 4     | 165 | GLN  | CA-C-N | 6.19  | 128.57      | 120.28   |
| 4   | 4     | 165 | GLN  | C-N-CA | 6.19  | 128.57      | 120.28   |
| 28  | U     | 173 | HIS  | N-CA-C | -6.19 | 104.61      | 111.36   |
| 13  | F     | 192 | ALA  | N-CA-C | 6.19  | 118.02      | 111.28   |
| 22  | O     | 136 | THR  | CA-C-N | 6.19  | 128.57      | 120.28   |
| 22  | O     | 136 | THR  | C-N-CA | 6.19  | 128.57      | 120.28   |
| 21  | N     | 351 | ALA  | CA-C-O | -6.19 | 114.33      | 120.70   |
| 1   | 1     | 76  | GLU  | O-C-N  | -6.18 | 114.67      | 122.27   |
| 16  | I     | 312 | GLN  | N-CA-C | 6.18  | 118.02      | 111.28   |
| 29  | V     | 187 | ALA  | CA-C-N | 6.18  | 128.84      | 120.44   |
| 29  | V     | 187 | ALA  | C-N-CA | 6.18  | 128.84      | 120.44   |
| 18  | K     | 369 | ASP  | CA-C-N | 6.18  | 128.47      | 120.44   |
| 18  | K     | 369 | ASP  | C-N-CA | 6.18  | 128.47      | 120.44   |
| 23  | P     | 112 | LEU  | CA-C-N | 6.18  | 128.56      | 120.28   |
| 23  | P     | 112 | LEU  | C-N-CA | 6.18  | 128.56      | 120.28   |
| 5   | 5     | 66  | HIS  | CA-C-N | 6.17  | 129.70      | 120.31   |
| 5   | 5     | 66  | HIS  | C-N-CA | 6.17  | 129.70      | 120.31   |
| 20  | M     | 349 | PHE  | CA-C-O | -6.17 | 114.77      | 119.59   |
| 9   | B     | 53  | SER  | O-C-N  | -6.17 | 117.02      | 121.83   |
| 18  | K     | 397 | LYS  | N-CA-C | 6.17  | 123.95      | 110.80   |
| 22  | O     | 179 | PHE  | CA-C-N | 6.17  | 128.46      | 120.44   |
| 22  | O     | 179 | PHE  | C-N-CA | 6.17  | 128.46      | 120.44   |
| 24  | Q     | 203 | THR  | CA-C-N | 6.17  | 128.55      | 120.28   |
| 24  | Q     | 203 | THR  | C-N-CA | 6.17  | 128.55      | 120.28   |
| 24  | Q     | 205 | ALA  | N-CA-C | 6.17  | 118.09      | 111.36   |
| 5   | 5     | 119 | GLY  | CA-C-N | 6.17  | 129.52      | 120.82   |
| 5   | 5     | 119 | GLY  | C-N-CA | 6.17  | 129.52      | 120.82   |
| 26  | S     | 382 | ARG  | O-C-N  | -6.17 | 115.12      | 122.15   |
| 32  | Y     | 76  | GLU  | CA-C-O | 6.17  | 127.30      | 120.82   |
| 16  | I     | 221 | LEU  | N-CA-C | -6.17 | 98.85       | 108.90   |
| 18  | K     | 362 | LEU  | CA-C-O | -6.17 | 114.23      | 121.44   |
| 17  | J     | 354 | SER  | CA-C-N | 6.17  | 126.78      | 120.00   |
| 17  | J     | 354 | SER  | C-N-CA | 6.17  | 126.78      | 120.00   |
| 1   | 1     | 160 | SER  | CA-C-N | 6.16  | 128.82      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1     | 160 | SER  | C-N-CA | 6.16  | 128.82      | 120.44   |
| 14  | G     | 199 | ILE  | N-CA-C | -6.16 | 104.50      | 110.72   |
| 15  | H     | 214 | CYS  | CA-C-N | 6.16  | 128.86      | 120.54   |
| 15  | H     | 214 | CYS  | C-N-CA | 6.16  | 128.86      | 120.54   |
| 24  | Q     | 100 | LEU  | N-CA-C | 6.16  | 118.00      | 111.28   |
| 28  | U     | 105 | LYS  | N-CA-C | -6.16 | 104.11      | 111.69   |
| 29  | V     | 152 | VAL  | CA-C-O | 6.16  | 127.17      | 120.57   |
| 33  | Z     | 73  | GLU  | O-C-N  | 6.16  | 128.42      | 122.07   |
| 21  | N     | 338 | PHE  | CA-C-N | 6.16  | 128.54      | 120.28   |
| 21  | N     | 338 | PHE  | C-N-CA | 6.16  | 128.54      | 120.28   |
| 25  | R     | 279 | LEU  | N-CA-C | 6.16  | 118.08      | 111.36   |
| 27  | T     | 16  | GLU  | CA-C-O | -6.16 | 113.89      | 120.42   |
| 23  | P     | 440 | HIS  | O-C-N  | 6.16  | 128.65      | 122.12   |
| 5   | 5     | 183 | ASP  | N-CA-C | -6.16 | 105.81      | 113.38   |
| 17  | J     | 387 | GLY  | CA-C-N | 6.16  | 128.82      | 120.44   |
| 17  | J     | 387 | GLY  | C-N-CA | 6.16  | 128.82      | 120.44   |
| 23  | P     | 275 | ASN  | O-C-N  | 6.16  | 129.17      | 122.15   |
| 27  | T     | 214 | GLU  | CA-C-N | 6.16  | 128.53      | 120.28   |
| 27  | T     | 214 | GLU  | C-N-CA | 6.16  | 128.53      | 120.28   |
| 12  | E     | 126 | GLY  | O-C-N  | 6.16  | 128.84      | 122.75   |
| 25  | R     | 249 | ILE  | CA-C-O | 6.16  | 127.38      | 120.85   |
| 26  | S     | 471 | LEU  | N-CA-C | 6.16  | 117.99      | 111.28   |
| 23  | P     | 93  | ILE  | CA-C-N | 6.15  | 128.53      | 120.28   |
| 23  | P     | 93  | ILE  | C-N-CA | 6.15  | 128.53      | 120.28   |
| 27  | T     | 193 | THR  | CA-C-N | 6.15  | 128.53      | 120.28   |
| 27  | T     | 193 | THR  | C-N-CA | 6.15  | 128.53      | 120.28   |
| 30  | W     | 151 | THR  | N-CA-C | -6.15 | 101.67      | 110.59   |
| 33  | Z     | 63  | LEU  | CA-C-O | 6.15  | 126.94      | 120.42   |
| 10  | C     | 57  | LEU  | N-CA-C | -6.15 | 101.38      | 110.48   |
| 1   | 1     | 176 | VAL  | CA-C-N | 6.15  | 130.77      | 122.90   |
| 1   | 1     | 176 | VAL  | C-N-CA | 6.15  | 130.77      | 122.90   |
| 23  | P     | 313 | ILE  | CA-C-N | 6.15  | 129.15      | 120.42   |
| 23  | P     | 313 | ILE  | C-N-CA | 6.15  | 129.15      | 120.42   |
| 13  | F     | 13  | PHE  | N-CA-C | -6.15 | 99.80       | 108.96   |
| 26  | S     | 198 | SER  | CA-C-N | 6.15  | 133.28      | 121.54   |
| 26  | S     | 198 | SER  | C-N-CA | 6.15  | 133.28      | 121.54   |
| 16  | I     | 81  | ILE  | CA-C-O | -6.14 | 114.34      | 120.85   |
| 26  | S     | 238 | LEU  | N-CA-C | 6.14  | 117.98      | 111.28   |
| 33  | Z     | 303 | ASP  | CA-C-O | -6.14 | 113.65      | 119.55   |
| 11  | D     | 112 | TYR  | CA-C-O | 6.14  | 127.06      | 120.24   |
| 18  | K     | 207 | ARG  | N-CA-C | -6.14 | 107.62      | 114.62   |
| 33  | Z     | 352 | LYS  | CA-C-N | 6.14  | 124.11      | 120.24   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 33  | Z     | 352 | LYS  | C-N-CA   | 6.14  | 124.11      | 120.24   |
| 27  | T     | 59  | LYS  | N-CA-C   | 6.14  | 117.97      | 111.28   |
| 18  | K     | 348 | GLU  | CA-C-N   | 6.14  | 128.42      | 120.44   |
| 18  | K     | 348 | GLU  | C-N-CA   | 6.14  | 128.42      | 120.44   |
| 23  | P     | 307 | GLU  | CA-C-N   | 6.14  | 130.84      | 122.19   |
| 23  | P     | 307 | GLU  | C-N-CA   | 6.14  | 130.84      | 122.19   |
| 6   | 6     | 92  | ARG  | CA-C-N   | 6.14  | 132.88      | 122.26   |
| 6   | 6     | 92  | ARG  | C-N-CA   | 6.14  | 132.88      | 122.26   |
| 8   | A     | 201 | LYS  | CA-C-O   | 6.14  | 127.03      | 119.97   |
| 14  | G     | 30  | VAL  | CA-C-N   | 6.14  | 130.42      | 120.60   |
| 14  | G     | 30  | VAL  | C-N-CA   | 6.14  | 130.42      | 120.60   |
| 24  | Q     | 313 | ASP  | CA-C-N   | 6.14  | 128.50      | 120.28   |
| 24  | Q     | 313 | ASP  | C-N-CA   | 6.14  | 128.50      | 120.28   |
| 25  | R     | 217 | HIS  | N-CA-C   | 6.14  | 117.97      | 111.28   |
| 15  | H     | 368 | PRO  | O-C-N    | 6.13  | 130.68      | 122.89   |
| 29  | V     | 44  | GLY  | O-C-N    | 6.13  | 129.61      | 122.68   |
| 10  | C     | 51  | LYS  | CA-C-N   | 6.13  | 133.01      | 121.97   |
| 10  | C     | 51  | LYS  | C-N-CA   | 6.13  | 133.01      | 121.97   |
| 15  | H     | 368 | PRO  | CA-C-O   | -6.13 | 114.43      | 121.36   |
| 22  | O     | 44  | SER  | CB-CA-C  | -6.13 | 109.52      | 116.63   |
| 27  | T     | 26  | LEU  | CA-C-N   | 6.13  | 128.47      | 120.26   |
| 27  | T     | 26  | LEU  | C-N-CA   | 6.13  | 128.47      | 120.26   |
| 33  | Z     | 208 | VAL  | CA-C-N   | 6.13  | 125.75      | 119.56   |
| 33  | Z     | 208 | VAL  | C-N-CA   | 6.13  | 125.75      | 119.56   |
| 13  | F     | 102 | LYS  | N-CA-C   | -6.13 | 105.09      | 113.30   |
| 33  | Z     | 260 | GLU  | CB-CG-CD | 6.13  | 123.02      | 112.60   |
| 13  | F     | 140 | SER  | N-CA-C   | -6.12 | 105.39      | 112.92   |
| 13  | F     | 47  | VAL  | O-C-N    | -6.12 | 116.59      | 123.20   |
| 17  | J     | 32  | LEU  | CA-C-N   | 6.12  | 129.61      | 120.31   |
| 17  | J     | 32  | LEU  | C-N-CA   | 6.12  | 129.61      | 120.31   |
| 10  | C     | 82  | ALA  | CA-C-O   | -6.12 | 114.40      | 120.82   |
| 11  | D     | 118 | GLN  | CA-C-N   | 6.12  | 128.48      | 120.28   |
| 11  | D     | 118 | GLN  | C-N-CA   | 6.12  | 128.48      | 120.28   |
| 1   | 1     | 175 | MET  | O-C-N    | 6.12  | 130.57      | 123.17   |
| 5   | 5     | 208 | ASN  | CA-C-N   | 6.11  | 129.08      | 120.28   |
| 5   | 5     | 208 | ASN  | C-N-CA   | 6.11  | 129.08      | 120.28   |
| 21  | N     | 701 | VAL  | CA-C-O   | -6.11 | 114.37      | 120.85   |
| 22  | O     | 256 | ASN  | N-CA-C   | -6.11 | 104.54      | 111.14   |
| 23  | P     | 324 | GLU  | CA-C-O   | 6.11  | 127.93      | 121.33   |
| 18  | K     | 60  | LEU  | CA-C-O   | -6.11 | 114.40      | 120.82   |
| 7   | 7     | -2  | THR  | CA-C-O   | -6.11 | 113.96      | 121.11   |
| 8   | A     | 117 | LEU  | O-C-N    | 6.11  | 128.59      | 122.12   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 15  | H     | 301 | LYS  | CA-C-N | 6.11  | 129.38      | 120.71   |
| 15  | H     | 301 | LYS  | C-N-CA | 6.11  | 129.38      | 120.71   |
| 9   | B     | 232 | GLY  | CA-C-N | 6.11  | 126.13      | 119.90   |
| 9   | B     | 232 | GLY  | C-N-CA | 6.11  | 126.13      | 119.90   |
| 20  | M     | 56  | ASN  | O-C-N  | 6.11  | 129.11      | 122.15   |
| 21  | N     | 654 | GLN  | O-C-N  | 6.11  | 128.36      | 122.07   |
| 33  | Z     | 298 | PHE  | CA-C-N | 6.11  | 128.46      | 120.28   |
| 33  | Z     | 298 | PHE  | C-N-CA | 6.11  | 128.46      | 120.28   |
| 33  | Z     | 504 | GLU  | CA-C-N | 6.11  | 129.09      | 120.42   |
| 33  | Z     | 504 | GLU  | C-N-CA | 6.11  | 129.09      | 120.42   |
| 5   | 5     | 181 | THR  | N-CA-C | -6.10 | 101.17      | 110.14   |
| 21  | N     | 873 | ARG  | CA-C-N | 6.10  | 132.95      | 121.97   |
| 21  | N     | 873 | ARG  | C-N-CA | 6.10  | 132.95      | 121.97   |
| 18  | K     | 143 | SER  | N-CA-C | -6.10 | 106.44      | 114.31   |
| 2   | 2     | 196 | ARG  | N-CA-C | 6.10  | 118.89      | 110.35   |
| 12  | E     | 160 | PRO  | N-CA-C | -6.10 | 106.03      | 114.27   |
| 16  | I     | 376 | ASN  | CA-C-N | 6.10  | 128.45      | 120.28   |
| 16  | I     | 376 | ASN  | C-N-CA | 6.10  | 128.45      | 120.28   |
| 19  | L     | 395 | ALA  | N-CA-C | 6.10  | 117.60      | 111.07   |
| 22  | O     | 163 | ILE  | CA-C-N | 6.10  | 127.46      | 119.84   |
| 22  | O     | 163 | ILE  | C-N-CA | 6.10  | 127.46      | 119.84   |
| 22  | O     | 281 | ALA  | N-CA-C | 6.10  | 117.93      | 111.28   |
| 25  | R     | 44  | LYS  | CA-C-N | 6.10  | 128.45      | 120.28   |
| 25  | R     | 44  | LYS  | C-N-CA | 6.10  | 128.45      | 120.28   |
| 30  | W     | 29  | GLN  | CA-C-N | 6.10  | 128.81      | 120.46   |
| 30  | W     | 29  | GLN  | C-N-CA | 6.10  | 128.81      | 120.46   |
| 31  | X     | 113 | GLU  | N-CA-C | -6.10 | 105.15      | 112.59   |
| 2   | 2     | 23  | GLY  | CA-C-O | -6.10 | 112.80      | 121.52   |
| 7   | 7     | 2   | SER  | N-CA-C | 6.10  | 123.78      | 110.80   |
| 12  | E     | 244 | LYS  | N-CA-C | 6.10  | 117.92      | 111.28   |
| 15  | H     | 334 | LEU  | CA-C-N | 6.10  | 128.45      | 120.28   |
| 15  | H     | 334 | LEU  | C-N-CA | 6.10  | 128.45      | 120.28   |
| 19  | L     | 145 | ARG  | CA-C-O | 6.10  | 127.93      | 120.92   |
| 19  | L     | 183 | ILE  | CA-C-N | 6.10  | 125.77      | 119.92   |
| 19  | L     | 183 | ILE  | C-N-CA | 6.10  | 125.77      | 119.92   |
| 27  | T     | 213 | ASN  | O-C-N  | -6.10 | 116.18      | 123.31   |
| 10  | C     | 29  | ILE  | CA-C-O | -6.09 | 114.61      | 120.95   |
| 11  | D     | 135 | ILE  | N-CA-C | -6.09 | 99.58       | 108.11   |
| 26  | S     | 443 | ILE  | N-CA-C | -6.09 | 99.64       | 108.17   |
| 27  | T     | 22  | ALA  | CA-C-N | 6.09  | 128.44      | 120.28   |
| 27  | T     | 22  | ALA  | C-N-CA | 6.09  | 128.44      | 120.28   |
| 27  | T     | 224 | ARG  | CA-C-N | 6.09  | 130.81      | 122.34   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 27  | T     | 224 | ARG  | C-N-CA | 6.09  | 130.81      | 122.34   |
| 17  | J     | 345 | LYS  | CA-C-O | 6.09  | 126.88      | 120.42   |
| 11  | D     | 227 | GLU  | CA-C-N | 6.09  | 128.44      | 120.28   |
| 11  | D     | 227 | GLU  | C-N-CA | 6.09  | 128.44      | 120.28   |
| 18  | K     | 103 | ILE  | CA-C-O | -6.09 | 113.71      | 120.96   |
| 31  | X     | 15  | CYS  | N-CA-C | -6.09 | 100.92      | 109.69   |
| 31  | X     | 107 | GLY  | N-CA-C | -6.09 | 106.03      | 116.01   |
| 13  | F     | 207 | THR  | N-CA-C | -6.09 | 100.05      | 109.24   |
| 13  | F     | 219 | ASP  | CA-C-O | 6.08  | 125.84      | 119.51   |
| 7   | 7     | 199 | THR  | N-CA-C | -6.08 | 98.49       | 108.41   |
| 16  | I     | 294 | SER  | N-CA-C | -6.08 | 105.44      | 112.92   |
| 20  | M     | 49  | GLN  | O-C-N  | 6.08  | 128.57      | 122.12   |
| 25  | R     | 416 | LYS  | N-CA-C | 6.08  | 117.91      | 111.28   |
| 33  | Z     | 567 | ALA  | O-C-N  | 6.08  | 128.36      | 122.03   |
| 17  | J     | 383 | GLU  | CA-C-N | 6.08  | 128.93      | 120.29   |
| 17  | J     | 383 | GLU  | C-N-CA | 6.08  | 128.93      | 120.29   |
| 18  | K     | 180 | GLN  | N-CA-C | 6.08  | 118.70      | 111.71   |
| 20  | M     | 403 | LEU  | CA-C-N | 6.08  | 128.43      | 120.28   |
| 20  | M     | 403 | LEU  | C-N-CA | 6.08  | 128.43      | 120.28   |
| 21  | N     | 67  | LYS  | CA-C-O | 6.08  | 127.20      | 120.63   |
| 21  | N     | 168 | SER  | CA-C-N | 6.08  | 128.34      | 120.44   |
| 21  | N     | 168 | SER  | C-N-CA | 6.08  | 128.34      | 120.44   |
| 29  | V     | 83  | VAL  | CA-C-N | 6.08  | 131.14      | 121.66   |
| 29  | V     | 83  | VAL  | C-N-CA | 6.08  | 131.14      | 121.66   |
| 10  | C     | 107 | PRO  | CA-C-O | -6.08 | 114.26      | 121.67   |
| 29  | V     | 150 | LYS  | N-CA-C | -6.08 | 99.73       | 108.60   |
| 21  | N     | 479 | GLU  | CA-C-N | 6.08  | 128.34      | 120.44   |
| 21  | N     | 479 | GLU  | C-N-CA | 6.08  | 128.34      | 120.44   |
| 30  | W     | 136 | ASN  | N-CA-C | 6.08  | 123.74      | 110.80   |
| 1   | 1     | 33  | LYS  | N-CA-C | -6.07 | 105.52      | 113.17   |
| 4   | 4     | 82  | PHE  | CA-C-O | 6.07  | 127.19      | 120.82   |
| 13  | F     | 108 | ALA  | N-CA-C | 6.07  | 117.90      | 111.28   |
| 17  | J     | 240 | HIS  | CA-C-N | 6.07  | 129.51      | 120.83   |
| 17  | J     | 240 | HIS  | C-N-CA | 6.07  | 129.51      | 120.83   |
| 20  | M     | 267 | PHE  | CA-C-N | 6.07  | 128.33      | 120.44   |
| 20  | M     | 267 | PHE  | C-N-CA | 6.07  | 128.33      | 120.44   |
| 23  | P     | 254 | GLU  | CA-C-N | 6.07  | 128.91      | 120.29   |
| 23  | P     | 254 | GLU  | C-N-CA | 6.07  | 128.91      | 120.29   |
| 6   | 6     | 90  | GLY  | CA-C-O | 6.07  | 126.66      | 119.50   |
| 10  | C     | 185 | LYS  | CA-C-O | -6.07 | 114.19      | 120.99   |
| 20  | M     | 217 | GLY  | CA-C-O | -6.07 | 116.01      | 121.47   |
| 21  | N     | 253 | LEU  | N-CA-C | 6.07  | 117.56      | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 67  | SER  | CA-C-N | 6.07  | 128.41      | 120.28   |
| 33  | Z     | 67  | SER  | C-N-CA | 6.07  | 128.41      | 120.28   |
| 33  | Z     | 101 | SER  | CA-C-N | 6.07  | 130.25      | 120.30   |
| 33  | Z     | 101 | SER  | C-N-CA | 6.07  | 130.25      | 120.30   |
| 8   | A     | 38  | THR  | CA-C-N | 6.07  | 131.37      | 122.63   |
| 8   | A     | 38  | THR  | C-N-CA | 6.07  | 131.37      | 122.63   |
| 21  | N     | 326 | SER  | N-CA-C | 6.07  | 120.52      | 113.18   |
| 28  | U     | 223 | HIS  | CA-C-N | 6.07  | 128.41      | 120.28   |
| 28  | U     | 223 | HIS  | C-N-CA | 6.07  | 128.41      | 120.28   |
| 4   | 4     | 157 | LEU  | N-CA-C | -6.06 | 104.67      | 111.28   |
| 11  | D     | 36  | VAL  | N-CA-C | -6.06 | 99.48       | 108.45   |
| 18  | K     | 60  | LEU  | O-C-N  | 6.06  | 128.31      | 122.07   |
| 11  | D     | 131 | VAL  | CA-C-O | -6.06 | 114.09      | 120.76   |
| 4   | 4     | 97  | TYR  | N-CA-C | -6.06 | 101.96      | 110.50   |
| 5   | 5     | 161 | ILE  | CA-C-N | 6.06  | 128.32      | 120.44   |
| 5   | 5     | 161 | ILE  | C-N-CA | 6.06  | 128.32      | 120.44   |
| 19  | L     | 422 | VAL  | CA-C-O | 6.06  | 127.25      | 120.95   |
| 29  | V     | 98  | THR  | CA-C-N | 6.06  | 130.72      | 120.91   |
| 29  | V     | 98  | THR  | C-N-CA | 6.06  | 130.72      | 120.91   |
| 22  | O     | 377 | VAL  | CA-C-N | 6.05  | 128.31      | 120.44   |
| 22  | O     | 377 | VAL  | C-N-CA | 6.05  | 128.31      | 120.44   |
| 1   | 1     | 55  | ILE  | CA-C-O | -6.05 | 114.76      | 121.17   |
| 1   | 1     | 145 | ASN  | CA-C-N | 6.05  | 132.69      | 121.62   |
| 1   | 1     | 145 | ASN  | C-N-CA | 6.05  | 132.69      | 121.62   |
| 27  | T     | 134 | LYS  | O-C-N  | 6.05  | 128.63      | 122.09   |
| 22  | O     | 385 | GLU  | CA-C-N | 6.05  | 128.63      | 120.65   |
| 22  | O     | 385 | GLU  | C-N-CA | 6.05  | 128.63      | 120.65   |
| 29  | V     | 30  | SER  | CA-C-N | 6.05  | 128.71      | 120.54   |
| 29  | V     | 30  | SER  | C-N-CA | 6.05  | 128.71      | 120.54   |
| 33  | Z     | 877 | THR  | O-C-N  | 6.05  | 129.05      | 122.15   |
| 2   | 2     | 63  | ILE  | CA-C-N | 6.05  | 128.99      | 120.28   |
| 2   | 2     | 63  | ILE  | C-N-CA | 6.05  | 128.99      | 120.28   |
| 14  | G     | 124 | LEU  | N-CA-C | -6.05 | 105.55      | 113.17   |
| 7   | 7     | 61  | ASP  | CA-C-N | 6.05  | 128.38      | 120.28   |
| 7   | 7     | 61  | ASP  | C-N-CA | 6.05  | 128.38      | 120.28   |
| 7   | 7     | 84  | ILE  | O-C-N  | 6.05  | 128.06      | 121.83   |
| 15  | H     | 202 | GLU  | N-CA-C | -6.05 | 100.89      | 109.96   |
| 21  | N     | 757 | THR  | N-CA-C | -6.05 | 97.92       | 110.80   |
| 13  | F     | 164 | ARG  | O-C-N  | -6.04 | 115.72      | 122.91   |
| 33  | Z     | 331 | GLY  | CA-C-N | 6.04  | 128.30      | 120.44   |
| 33  | Z     | 331 | GLY  | C-N-CA | 6.04  | 128.30      | 120.44   |
| 7   | 7     | 192 | ILE  | CA-C-O | 6.04  | 127.13      | 120.48   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 17  | J     | 287 | ASN  | N-CA-C | -6.04 | 104.72      | 114.09   |
| 18  | K     | 417 | THR  | N-CA-C | -6.04 | 105.45      | 114.64   |
| 20  | M     | 278 | ILE  | N-CA-C | -6.04 | 98.50       | 107.51   |
| 25  | R     | 109 | LYS  | N-CA-C | 6.04  | 117.87      | 111.28   |
| 33  | Z     | 473 | LEU  | CA-C-N | 6.04  | 128.87      | 120.29   |
| 33  | Z     | 473 | LEU  | C-N-CA | 6.04  | 128.87      | 120.29   |
| 15  | H     | 147 | ILE  | O-C-N  | -6.04 | 116.04      | 123.10   |
| 20  | M     | 69  | ILE  | CA-C-N | 6.04  | 128.37      | 120.28   |
| 20  | M     | 69  | ILE  | C-N-CA | 6.04  | 128.37      | 120.28   |
| 4   | 4     | 7   | ARG  | CA-C-N | 6.04  | 132.83      | 121.97   |
| 4   | 4     | 7   | ARG  | C-N-CA | 6.04  | 132.83      | 121.97   |
| 12  | E     | 151 | ASP  | N-CA-C | -6.03 | 104.77      | 113.21   |
| 29  | V     | 88  | GLN  | CA-C-N | 6.03  | 128.85      | 120.29   |
| 29  | V     | 88  | GLN  | C-N-CA | 6.03  | 128.85      | 120.29   |
| 33  | Z     | 90  | LYS  | CA-C-N | 6.03  | 128.36      | 120.28   |
| 33  | Z     | 90  | LYS  | C-N-CA | 6.03  | 128.36      | 120.28   |
| 16  | I     | 420 | LYS  | CA-C-N | 6.03  | 128.36      | 120.28   |
| 16  | I     | 420 | LYS  | C-N-CA | 6.03  | 128.36      | 120.28   |
| 16  | I     | 412 | THR  | CA-C-N | 6.03  | 128.64      | 120.38   |
| 16  | I     | 412 | THR  | C-N-CA | 6.03  | 128.64      | 120.38   |
| 33  | Z     | 209 | PRO  | N-CA-C | 6.03  | 121.39      | 113.86   |
| 9   | B     | 10  | THR  | N-CA-C | -6.02 | 98.46       | 108.34   |
| 19  | L     | 145 | ARG  | O-C-N  | -6.02 | 116.17      | 123.16   |
| 31  | X     | 21  | SER  | CA-C-N | 6.02  | 131.14      | 122.35   |
| 31  | X     | 21  | SER  | C-N-CA | 6.02  | 131.14      | 122.35   |
| 28  | U     | 95  | SER  | CA-C-O | 6.02  | 126.72      | 119.43   |
| 30  | W     | 123 | ASP  | CA-C-N | 6.02  | 128.84      | 120.29   |
| 30  | W     | 123 | ASP  | C-N-CA | 6.02  | 128.84      | 120.29   |
| 6   | 6     | 107 | GLU  | CA-C-N | 6.02  | 128.62      | 120.44   |
| 6   | 6     | 107 | GLU  | C-N-CA | 6.02  | 128.62      | 120.44   |
| 20  | M     | 67  | GLU  | N-CA-C | -6.02 | 104.80      | 111.36   |
| 14  | G     | 219 | SER  | N-CA-C | -6.02 | 98.46       | 108.75   |
| 9   | B     | 238 | LEU  | CA-C-N | 6.01  | 131.04      | 120.87   |
| 9   | B     | 238 | LEU  | C-N-CA | 6.01  | 131.04      | 120.87   |
| 13  | F     | 111 | LEU  | CA-C-N | 6.01  | 128.34      | 120.28   |
| 13  | F     | 111 | LEU  | C-N-CA | 6.01  | 128.34      | 120.28   |
| 22  | O     | 354 | GLN  | N-CA-C | 6.01  | 118.38      | 110.08   |
| 17  | J     | 196 | THR  | CA-C-N | 6.01  | 128.34      | 120.28   |
| 17  | J     | 196 | THR  | C-N-CA | 6.01  | 128.34      | 120.28   |
| 17  | J     | 345 | LYS  | CA-C-N | 6.01  | 128.96      | 120.42   |
| 17  | J     | 345 | LYS  | C-N-CA | 6.01  | 128.96      | 120.42   |
| 21  | N     | 21  | LYS  | O-C-N  | 6.01  | 129.00      | 122.15   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 870 | ALA  | CA-C-N | 6.01  | 130.90      | 122.36   |
| 33  | Z     | 870 | ALA  | C-N-CA | 6.01  | 130.90      | 122.36   |
| 12  | E     | 242 | GLU  | CA-C-N | 6.01  | 128.61      | 120.44   |
| 12  | E     | 242 | GLU  | C-N-CA | 6.01  | 128.61      | 120.44   |
| 28  | U     | 294 | ASN  | CA-C-O | 6.01  | 127.13      | 120.82   |
| 15  | H     | 192 | ASP  | CA-C-N | 6.01  | 125.56      | 119.19   |
| 15  | H     | 192 | ASP  | C-N-CA | 6.01  | 125.56      | 119.19   |
| 17  | J     | 81  | ASP  | O-C-N  | 6.01  | 129.85      | 122.34   |
| 23  | P     | 105 | LYS  | CA-C-N | 6.01  | 128.25      | 120.44   |
| 23  | P     | 105 | LYS  | C-N-CA | 6.01  | 128.25      | 120.44   |
| 29  | V     | 77  | GLY  | CA-C-N | 6.01  | 132.78      | 121.97   |
| 29  | V     | 77  | GLY  | C-N-CA | 6.01  | 132.78      | 121.97   |
| 4   | 4     | 172 | PRO  | CA-C-N | 6.00  | 129.37      | 120.90   |
| 4   | 4     | 172 | PRO  | C-N-CA | 6.00  | 129.37      | 120.90   |
| 33  | Z     | 839 | SER  | N-CA-C | -6.00 | 105.78      | 113.23   |
| 13  | F     | 11  | VAL  | CA-C-N | 6.00  | 131.65      | 122.11   |
| 13  | F     | 11  | VAL  | C-N-CA | 6.00  | 131.65      | 122.11   |
| 27  | T     | 69  | SER  | CA-C-N | 6.00  | 128.12      | 120.56   |
| 27  | T     | 69  | SER  | C-N-CA | 6.00  | 128.12      | 120.56   |
| 33  | Z     | 816 | GLY  | CA-C-N | 6.00  | 128.61      | 120.44   |
| 33  | Z     | 816 | GLY  | C-N-CA | 6.00  | 128.61      | 120.44   |
| 4   | 4     | 4   | LEU  | N-CA-C | -6.00 | 100.37      | 109.85   |
| 11  | D     | 174 | PHE  | CA-C-O | -6.00 | 114.52      | 120.82   |
| 7   | 7     | -2  | THR  | O-C-N  | 6.00  | 130.62      | 123.24   |
| 8   | A     | 133 | TYR  | N-CA-C | -6.00 | 104.79      | 114.09   |
| 11  | D     | 97  | ARG  | CA-C-N | 6.00  | 128.24      | 120.44   |
| 11  | D     | 97  | ARG  | C-N-CA | 6.00  | 128.24      | 120.44   |
| 31  | X     | 73  | THR  | N-CA-C | -6.00 | 97.34       | 108.02   |
| 3   | 3     | 165 | ALA  | CA-C-O | 6.00  | 126.78      | 120.42   |
| 33  | Z     | 880 | SER  | CA-C-N | 6.00  | 128.68      | 120.46   |
| 33  | Z     | 880 | SER  | C-N-CA | 6.00  | 128.68      | 120.46   |
| 23  | P     | 135 | GLU  | N-CA-C | 5.99  | 118.77      | 111.82   |
| 17  | J     | 369 | ALA  | CA-C-N | 5.99  | 128.31      | 120.28   |
| 17  | J     | 369 | ALA  | C-N-CA | 5.99  | 128.31      | 120.28   |
| 21  | N     | 677 | ASP  | CA-C-N | 5.99  | 128.11      | 120.56   |
| 21  | N     | 677 | ASP  | C-N-CA | 5.99  | 128.11      | 120.56   |
| 9   | B     | 172 | LYS  | CA-C-N | 5.99  | 128.31      | 120.28   |
| 9   | B     | 172 | LYS  | C-N-CA | 5.99  | 128.31      | 120.28   |
| 16  | I     | 377 | LEU  | O-C-N  | 5.99  | 128.47      | 122.12   |
| 23  | P     | 115 | ARG  | CA-C-N | 5.99  | 128.98      | 120.53   |
| 23  | P     | 115 | ARG  | C-N-CA | 5.99  | 128.98      | 120.53   |
| 33  | Z     | 909 | ARG  | O-C-N  | -5.99 | 116.03      | 121.66   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | 7     | 167 | GLU  | CA-C-N | 5.99  | 128.22      | 120.44   |
| 7   | 7     | 167 | GLU  | C-N-CA | 5.99  | 128.22      | 120.44   |
| 18  | K     | 189 | GLU  | CA-C-N | 5.99  | 127.57      | 120.09   |
| 18  | K     | 189 | GLU  | C-N-CA | 5.99  | 127.57      | 120.09   |
| 26  | S     | 477 | VAL  | N-CA-C | 5.99  | 117.45      | 110.62   |
| 9   | B     | 68  | THR  | CA-C-N | 5.99  | 126.14      | 119.32   |
| 9   | B     | 68  | THR  | C-N-CA | 5.99  | 126.14      | 119.32   |
| 13  | F     | 179 | PHE  | N-CA-C | 5.99  | 117.81      | 111.28   |
| 21  | N     | 862 | SER  | CA-C-O | -5.99 | 113.18      | 120.54   |
| 29  | V     | 53  | MET  | N-CA-C | -5.99 | 99.95       | 109.59   |
| 9   | B     | 23  | TYR  | CA-C-N | 5.99  | 128.90      | 120.28   |
| 9   | B     | 23  | TYR  | C-N-CA | 5.99  | 128.90      | 120.28   |
| 12  | E     | 203 | ILE  | CA-C-N | 5.98  | 128.30      | 120.28   |
| 12  | E     | 203 | ILE  | C-N-CA | 5.98  | 128.30      | 120.28   |
| 22  | O     | 138 | LEU  | CA-C-N | 5.98  | 128.30      | 120.28   |
| 22  | O     | 138 | LEU  | C-N-CA | 5.98  | 128.30      | 120.28   |
| 24  | Q     | 162 | LEU  | CA-C-N | 5.98  | 128.78      | 120.29   |
| 24  | Q     | 162 | LEU  | C-N-CA | 5.98  | 128.78      | 120.29   |
| 24  | Q     | 187 | LYS  | N-CA-C | 5.98  | 117.88      | 111.36   |
| 22  | O     | 365 | LYS  | CA-C-N | 5.98  | 128.22      | 120.44   |
| 22  | O     | 365 | LYS  | C-N-CA | 5.98  | 128.22      | 120.44   |
| 24  | Q     | 107 | VAL  | CA-C-N | 5.98  | 127.31      | 119.84   |
| 24  | Q     | 107 | VAL  | C-N-CA | 5.98  | 127.31      | 119.84   |
| 33  | Z     | 869 | ASP  | N-CA-C | -5.98 | 106.23      | 112.93   |
| 21  | N     | 742 | TRP  | CA-C-N | 5.98  | 127.19      | 119.78   |
| 21  | N     | 742 | TRP  | C-N-CA | 5.98  | 127.19      | 119.78   |
| 21  | N     | 293 | LEU  | N-CA-C | 5.98  | 121.02      | 113.25   |
| 14  | G     | 241 | PHE  | CA-C-O | 5.97  | 126.85      | 120.10   |
| 22  | O     | 346 | GLU  | CA-C-N | 5.97  | 131.90      | 122.94   |
| 22  | O     | 346 | GLU  | C-N-CA | 5.97  | 131.90      | 122.94   |
| 19  | L     | 414 | ASP  | N-CA-C | 5.97  | 117.79      | 111.28   |
| 3   | 3     | 161 | ALA  | CA-C-N | 5.97  | 128.56      | 120.44   |
| 3   | 3     | 161 | ALA  | C-N-CA | 5.97  | 128.56      | 120.44   |
| 15  | H     | 344 | ASP  | CA-C-N | 5.97  | 128.31      | 120.25   |
| 15  | H     | 344 | ASP  | C-N-CA | 5.97  | 128.31      | 120.25   |
| 20  | M     | 336 | ALA  | CA-C-O | 5.97  | 126.72      | 119.38   |
| 25  | R     | 151 | GLU  | N-CA-C | 5.97  | 117.58      | 111.14   |
| 25  | R     | 215 | GLY  | CA-C-O | -5.97 | 114.61      | 120.75   |
| 2   | 2     | 153 | LYS  | CA-C-N | 5.96  | 128.19      | 120.44   |
| 2   | 2     | 153 | LYS  | C-N-CA | 5.96  | 128.19      | 120.44   |
| 6   | 6     | 19  | ARG  | CA-C-N | 5.96  | 131.92      | 122.74   |
| 6   | 6     | 19  | ARG  | C-N-CA | 5.96  | 131.92      | 122.74   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | C     | 73  | ILE  | N-CA-C  | -5.96 | 99.57       | 108.46   |
| 20  | M     | 65  | ASN  | O-C-N   | -5.96 | 115.80      | 122.12   |
| 20  | M     | 127 | VAL  | CA-C-O  | 5.96  | 128.20      | 121.28   |
| 17  | J     | 28  | GLN  | CA-C-N  | 5.96  | 128.19      | 120.44   |
| 17  | J     | 28  | GLN  | C-N-CA  | 5.96  | 128.19      | 120.44   |
| 12  | E     | 197 | GLU  | N-CA-C  | 5.96  | 117.78      | 111.28   |
| 27  | T     | 4   | LEU  | N-CA-C  | -5.96 | 98.10       | 110.80   |
| 14  | G     | 112 | ALA  | CA-C-O  | -5.96 | 114.56      | 120.82   |
| 21  | N     | 899 | ASN  | CA-C-N  | 5.96  | 129.75      | 120.75   |
| 21  | N     | 899 | ASN  | C-N-CA  | 5.96  | 129.75      | 120.75   |
| 27  | T     | 270 | ILE  | CB-CA-C | -5.96 | 104.18      | 111.87   |
| 5   | 5     | 95  | LEU  | O-C-N   | -5.96 | 115.45      | 122.96   |
| 10  | C     | 193 | ALA  | CA-C-O  | -5.96 | 114.56      | 120.82   |
| 21  | N     | 497 | ALA  | O-C-N   | 5.96  | 128.21      | 122.07   |
| 3   | 3     | 188 | LYS  | CA-C-O  | -5.96 | 113.93      | 120.30   |
| 4   | 4     | 134 | TYR  | CA-C-N  | 5.96  | 132.92      | 121.54   |
| 4   | 4     | 134 | TYR  | C-N-CA  | 5.96  | 132.92      | 121.54   |
| 9   | B     | 58  | SER  | N-CA-C  | -5.96 | 104.68      | 113.61   |
| 12  | E     | 113 | THR  | CA-C-N  | 5.96  | 128.18      | 120.44   |
| 12  | E     | 113 | THR  | C-N-CA  | 5.96  | 128.18      | 120.44   |
| 8   | A     | 22  | GLU  | N-CA-C  | -5.95 | 104.37      | 111.69   |
| 20  | M     | 321 | VAL  | N-CA-C  | -5.95 | 99.91       | 108.48   |
| 21  | N     | 65  | ALA  | CA-C-N  | 5.95  | 128.58      | 120.54   |
| 21  | N     | 65  | ALA  | C-N-CA  | 5.95  | 128.58      | 120.54   |
| 21  | N     | 565 | ASN  | CA-C-N  | 5.95  | 128.18      | 120.44   |
| 21  | N     | 565 | ASN  | C-N-CA  | 5.95  | 128.18      | 120.44   |
| 2   | 2     | 203 | TYR  | N-CA-C  | -5.95 | 99.91       | 108.60   |
| 17  | J     | 204 | HIS  | CA-C-N  | 5.95  | 128.25      | 120.28   |
| 17  | J     | 204 | HIS  | C-N-CA  | 5.95  | 128.25      | 120.28   |
| 21  | N     | 486 | GLY  | CA-C-N  | 5.95  | 128.53      | 120.44   |
| 21  | N     | 486 | GLY  | C-N-CA  | 5.95  | 128.53      | 120.44   |
| 24  | Q     | 25  | GLN  | O-C-N   | 5.95  | 128.93      | 122.15   |
| 18  | K     | 55  | GLU  | CA-C-O  | -5.95 | 114.11      | 120.42   |
| 20  | M     | 229 | THR  | N-CA-C  | -5.95 | 104.88      | 111.36   |
| 21  | N     | 515 | ARG  | CA-C-N  | 5.95  | 126.42      | 119.94   |
| 21  | N     | 515 | ARG  | C-N-CA  | 5.95  | 126.42      | 119.94   |
| 33  | Z     | 407 | VAL  | CA-C-N  | 5.95  | 128.25      | 120.28   |
| 33  | Z     | 407 | VAL  | C-N-CA  | 5.95  | 128.25      | 120.28   |
| 3   | 3     | 49  | THR  | CA-C-N  | 5.95  | 130.75      | 120.58   |
| 3   | 3     | 49  | THR  | C-N-CA  | 5.95  | 130.75      | 120.58   |
| 11  | D     | 90  | ARG  | CA-C-O  | -5.95 | 114.25      | 120.55   |
| 17  | J     | 105 | LYS  | N-CA-C  | -5.95 | 105.21      | 112.88   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 745 | LEU  | CA-C-N | 5.95  | 132.90      | 121.54   |
| 21  | N     | 745 | LEU  | C-N-CA | 5.95  | 132.90      | 121.54   |
| 18  | K     | 384 | ALA  | CA-C-N | 5.94  | 128.17      | 120.44   |
| 18  | K     | 384 | ALA  | C-N-CA | 5.94  | 128.17      | 120.44   |
| 28  | U     | 225 | ILE  | O-C-N  | 5.94  | 127.73      | 121.91   |
| 2   | 2     | 191 | LEU  | CA-C-N | 5.94  | 130.28      | 123.21   |
| 2   | 2     | 191 | LEU  | C-N-CA | 5.94  | 130.28      | 123.21   |
| 33  | Z     | 504 | GLU  | N-CA-C | 5.94  | 117.75      | 111.28   |
| 33  | Z     | 527 | SER  | N-CA-C | 5.94  | 119.35      | 111.75   |
| 22  | O     | 58  | ARG  | CA-C-N | 5.94  | 128.72      | 120.29   |
| 22  | O     | 58  | ARG  | C-N-CA | 5.94  | 128.72      | 120.29   |
| 29  | V     | 68  | VAL  | CA-C-O | -5.94 | 115.38      | 120.96   |
| 10  | C     | 96  | GLN  | O-C-N  | -5.94 | 115.27      | 122.22   |
| 27  | T     | 235 | PHE  | O-C-N  | -5.94 | 115.94      | 123.24   |
| 11  | D     | 17  | ILE  | CA-C-N | 5.93  | 129.04      | 120.79   |
| 11  | D     | 17  | ILE  | C-N-CA | 5.93  | 129.04      | 120.79   |
| 16  | I     | 104 | LEU  | O-C-N  | -5.93 | 116.03      | 123.27   |
| 16  | I     | 348 | ILE  | CA-C-N | 5.93  | 132.79      | 122.82   |
| 16  | I     | 348 | ILE  | C-N-CA | 5.93  | 132.79      | 122.82   |
| 17  | J     | 95  | ILE  | N-CA-C | -5.93 | 99.87       | 108.36   |
| 20  | M     | 65  | ASN  | CA-C-N | 5.93  | 128.72      | 120.29   |
| 20  | M     | 65  | ASN  | C-N-CA | 5.93  | 128.72      | 120.29   |
| 23  | P     | 280 | LEU  | O-C-N  | 5.93  | 128.41      | 122.12   |
| 26  | S     | 144 | LEU  | O-C-N  | -5.93 | 114.70      | 122.59   |
| 33  | Z     | 119 | LEU  | CA-C-O | -5.93 | 114.26      | 120.55   |
| 19  | L     | 359 | GLU  | N-CA-C | 5.93  | 117.55      | 111.14   |
| 14  | G     | 167 | GLY  | CA-C-N | 5.93  | 128.50      | 120.38   |
| 14  | G     | 167 | GLY  | C-N-CA | 5.93  | 128.50      | 120.38   |
| 22  | O     | 167 | ILE  | N-CA-C | 5.93  | 116.67      | 110.62   |
| 26  | S     | 330 | LEU  | CA-C-N | 5.93  | 128.55      | 120.54   |
| 26  | S     | 330 | LEU  | C-N-CA | 5.93  | 128.55      | 120.54   |
| 5   | 5     | 92  | GLY  | N-CA-C | -5.93 | 106.59      | 114.95   |
| 24  | Q     | 71  | LYS  | CA-C-O | 5.93  | 127.03      | 120.63   |
| 2   | 2     | 150 | GLU  | CA-C-N | 5.93  | 128.71      | 120.29   |
| 2   | 2     | 150 | GLU  | C-N-CA | 5.93  | 128.71      | 120.29   |
| 18  | K     | 109 | ILE  | CA-C-O | 5.93  | 126.91      | 120.57   |
| 20  | M     | 138 | ASP  | N-CA-C | -5.93 | 105.70      | 113.17   |
| 30  | W     | 82  | GLU  | O-C-N  | -5.93 | 116.48      | 123.41   |
| 23  | P     | 186 | LEU  | CA-C-N | 5.92  | 128.70      | 120.29   |
| 23  | P     | 186 | LEU  | C-N-CA | 5.92  | 128.70      | 120.29   |
| 26  | S     | 150 | LYS  | CA-C-N | 5.92  | 132.86      | 121.54   |
| 26  | S     | 150 | LYS  | C-N-CA | 5.92  | 132.86      | 121.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | H     | 256 | LYS  | O-C-N   | 5.92  | 128.49      | 122.09   |
| 22  | O     | 66  | VAL  | O-C-N   | 5.92  | 127.61      | 121.87   |
| 33  | Z     | 975 | SER  | CA-C-N  | 5.92  | 131.16      | 122.63   |
| 33  | Z     | 975 | SER  | C-N-CA  | 5.92  | 131.16      | 122.63   |
| 15  | H     | 194 | SER  | CB-CA-C | -5.92 | 109.73      | 116.54   |
| 19  | L     | 214 | PRO  | CA-C-N  | 5.92  | 127.24      | 119.84   |
| 19  | L     | 214 | PRO  | C-N-CA  | 5.92  | 127.24      | 119.84   |
| 28  | U     | 159 | CYS  | O-C-N   | -5.92 | 116.38      | 123.31   |
| 1   | 1     | 41  | ILE  | CA-C-O  | -5.92 | 114.51      | 120.31   |
| 2   | 2     | 166 | ASP  | N-CA-C  | -5.92 | 98.76       | 108.41   |
| 10  | C     | 134 | SER  | CA-C-N  | 5.92  | 131.51      | 122.93   |
| 10  | C     | 134 | SER  | C-N-CA  | 5.92  | 131.51      | 122.93   |
| 11  | D     | 93  | ALA  | CA-C-O  | 5.92  | 126.82      | 120.55   |
| 22  | O     | 221 | ALA  | N-CA-C  | -5.92 | 104.74      | 111.07   |
| 24  | Q     | 72  | ASP  | CA-C-N  | 5.92  | 128.69      | 120.29   |
| 24  | Q     | 72  | ASP  | C-N-CA  | 5.92  | 128.69      | 120.29   |
| 12  | E     | 151 | ASP  | O-C-N   | 5.91  | 127.35      | 121.85   |
| 2   | 2     | 41  | ILE  | CB-CA-C | 5.91  | 118.67      | 110.99   |
| 8   | A     | 27  | GLN  | CA-C-N  | 5.91  | 128.81      | 120.42   |
| 8   | A     | 27  | GLN  | C-N-CA  | 5.91  | 128.81      | 120.42   |
| 10  | C     | 217 | ARG  | N-CA-C  | -5.91 | 100.77      | 109.81   |
| 14  | G     | 126 | ASN  | N-CA-C  | -5.91 | 105.16      | 112.90   |
| 24  | Q     | 125 | ALA  | CA-C-N  | 5.91  | 129.29      | 120.31   |
| 24  | Q     | 125 | ALA  | C-N-CA  | 5.91  | 129.29      | 120.31   |
| 7   | 7     | 218 | LYS  | N-CA-C  | -5.91 | 105.66      | 114.64   |
| 20  | M     | 173 | ASP  | O-C-N   | -5.91 | 114.01      | 122.99   |
| 19  | L     | 260 | ALA  | N-CA-C  | 5.90  | 117.72      | 111.28   |
| 22  | O     | 12  | SER  | CA-C-N  | 5.90  | 128.19      | 120.28   |
| 22  | O     | 12  | SER  | C-N-CA  | 5.90  | 128.19      | 120.28   |
| 17  | J     | 128 | ASN  | N-CA-C  | 5.90  | 118.82      | 110.50   |
| 20  | M     | 398 | ALA  | CA-C-N  | 5.90  | 126.49      | 120.00   |
| 20  | M     | 398 | ALA  | C-N-CA  | 5.90  | 126.49      | 120.00   |
| 21  | N     | 407 | GLY  | CA-C-N  | 5.90  | 128.67      | 120.29   |
| 21  | N     | 407 | GLY  | C-N-CA  | 5.90  | 128.67      | 120.29   |
| 1   | 1     | 106 | ASN  | N-CA-C  | -5.90 | 105.43      | 114.16   |
| 21  | N     | 347 | SER  | CA-C-O  | -5.90 | 114.26      | 120.63   |
| 12  | E     | 145 | ALA  | CA-C-O  | 5.90  | 128.01      | 121.11   |
| 18  | K     | 246 | TYR  | N-CA-C  | 5.90  | 115.63      | 107.73   |
| 21  | N     | 191 | THR  | CA-C-N  | 5.90  | 128.46      | 120.44   |
| 21  | N     | 191 | THR  | C-N-CA  | 5.90  | 128.46      | 120.44   |
| 22  | O     | 89  | SER  | CA-C-N  | 5.90  | 130.74      | 122.36   |
| 22  | O     | 89  | SER  | C-N-CA  | 5.90  | 130.74      | 122.36   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | 6     | 133 | ALA  | CA-C-N | 5.90  | 128.46      | 120.38   |
| 6   | 6     | 133 | ALA  | C-N-CA | 5.90  | 128.46      | 120.38   |
| 17  | J     | 81  | ASP  | N-CA-C | -5.90 | 105.74      | 113.17   |
| 26  | S     | 178 | LEU  | N-CA-C | -5.90 | 106.09      | 113.28   |
| 33  | Z     | 111 | LEU  | CA-C-O | -5.90 | 113.19      | 119.97   |
| 29  | V     | 95  | LEU  | CA-C-N | 5.89  | 128.46      | 120.38   |
| 29  | V     | 95  | LEU  | C-N-CA | 5.89  | 128.46      | 120.38   |
| 7   | 7     | 102 | LEU  | N-CA-C | -5.89 | 98.92       | 108.41   |
| 18  | K     | 92  | VAL  | O-C-N  | -5.89 | 114.38      | 121.10   |
| 3   | 3     | 97  | GLY  | CA-C-N | 5.89  | 125.80      | 119.85   |
| 3   | 3     | 97  | GLY  | C-N-CA | 5.89  | 125.80      | 119.85   |
| 13  | F     | 178 | THR  | CA-C-N | 5.89  | 128.17      | 120.28   |
| 13  | F     | 178 | THR  | C-N-CA | 5.89  | 128.17      | 120.28   |
| 18  | K     | 427 | TYR  | O-C-N  | 5.89  | 130.42      | 122.59   |
| 33  | Z     | 305 | VAL  | O-C-N  | 5.89  | 127.68      | 121.91   |
| 11  | D     | 146 | LYS  | CA-C-N | 5.89  | 131.10      | 122.39   |
| 11  | D     | 146 | LYS  | C-N-CA | 5.89  | 131.10      | 122.39   |
| 12  | E     | 101 | LEU  | CA-C-N | 5.89  | 129.26      | 120.31   |
| 12  | E     | 101 | LEU  | C-N-CA | 5.89  | 129.26      | 120.31   |
| 17  | J     | 198 | LEU  | CA-C-N | 5.89  | 128.17      | 120.28   |
| 17  | J     | 198 | LEU  | C-N-CA | 5.89  | 128.17      | 120.28   |
| 23  | P     | 73  | ASP  | N-CA-C | -5.89 | 104.94      | 111.36   |
| 9   | B     | 135 | LEU  | N-CA-C | -5.88 | 98.82       | 108.41   |
| 20  | M     | 71  | ASN  | CA-C-O | -5.88 | 114.31      | 120.55   |
| 21  | N     | 563 | GLY  | O-C-N  | 5.88  | 128.47      | 122.88   |
| 27  | T     | 137 | GLU  | CA-C-N | 5.88  | 128.16      | 120.28   |
| 27  | T     | 137 | GLU  | C-N-CA | 5.88  | 128.16      | 120.28   |
| 4   | 4     | 136 | GLY  | CA-C-N | 5.88  | 128.16      | 120.28   |
| 4   | 4     | 136 | GLY  | C-N-CA | 5.88  | 128.16      | 120.28   |
| 8   | A     | 36  | ASN  | N-CA-C | -5.88 | 106.34      | 112.93   |
| 21  | N     | 607 | GLN  | CA-C-N | 5.88  | 128.09      | 120.44   |
| 21  | N     | 607 | GLN  | C-N-CA | 5.88  | 128.09      | 120.44   |
| 25  | R     | 238 | PHE  | N-CA-C | -5.88 | 100.20      | 108.96   |
| 21  | N     | 82  | ALA  | CA-C-N | 5.88  | 128.08      | 120.44   |
| 21  | N     | 82  | ALA  | C-N-CA | 5.88  | 128.08      | 120.44   |
| 22  | O     | 191 | THR  | N-CA-C | 5.88  | 117.36      | 111.07   |
| 2   | 2     | 122 | GLY  | CA-C-O | -5.88 | 114.73      | 121.49   |
| 33  | Z     | 811 | SER  | O-C-N  | -5.88 | 116.02      | 122.07   |
| 12  | E     | 83  | ALA  | N-CA-C | 5.87  | 117.76      | 111.36   |
| 21  | N     | 17  | GLN  | N-CA-C | -5.87 | 98.29       | 110.80   |
| 30  | W     | 169 | SER  | N-CA-C | 5.87  | 123.31      | 110.80   |
| 8   | A     | 70  | SER  | CA-C-O | 5.87  | 127.57      | 120.99   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | K     | 144 | ASN  | CA-C-O  | -5.87 | 114.69      | 122.44   |
| 21  | N     | 779 | GLU  | N-CA-C  | -5.87 | 105.94      | 112.57   |
| 8   | A     | 174 | LYS  | CA-C-N  | 5.87  | 128.46      | 120.54   |
| 8   | A     | 174 | LYS  | C-N-CA  | 5.87  | 128.46      | 120.54   |
| 3   | 3     | 76  | GLU  | O-C-N   | -5.87 | 115.90      | 122.12   |
| 24  | Q     | 150 | GLN  | CA-C-N  | 5.87  | 128.62      | 120.29   |
| 24  | Q     | 150 | GLN  | C-N-CA  | 5.87  | 128.62      | 120.29   |
| 28  | U     | 281 | LEU  | O-C-N   | 5.87  | 128.11      | 122.07   |
| 6   | 6     | 149 | ASN  | N-CA-C  | -5.86 | 106.08      | 113.23   |
| 7   | 7     | 157 | ILE  | CA-C-O  | -5.86 | 114.76      | 118.69   |
| 11  | D     | 199 | LEU  | N-CA-C  | -5.86 | 105.62      | 112.89   |
| 14  | G     | 17  | ASP  | O-C-N   | -5.86 | 115.01      | 122.34   |
| 2   | 2     | 180 | ILE  | N-CA-C  | -5.86 | 105.02      | 110.53   |
| 9   | B     | 162 | THR  | N-CA-C  | -5.86 | 99.23       | 108.14   |
| 23  | P     | 179 | PHE  | N-CA-C  | -5.86 | 104.97      | 111.36   |
| 33  | Z     | 101 | SER  | CA-C-O  | -5.86 | 114.34      | 120.55   |
| 18  | K     | 302 | GLN  | CA-C-O  | -5.86 | 114.34      | 120.55   |
| 21  | N     | 61  | ALA  | O-C-N   | 5.86  | 128.35      | 122.08   |
| 22  | O     | 367 | LYS  | CA-C-N  | 5.86  | 128.06      | 120.44   |
| 22  | O     | 367 | LYS  | C-N-CA  | 5.86  | 128.06      | 120.44   |
| 24  | Q     | 169 | ASP  | N-CA-C  | 5.86  | 123.28      | 110.80   |
| 25  | R     | 186 | TYR  | N-CA-C  | -5.86 | 105.96      | 113.23   |
| 21  | N     | 32  | VAL  | N-CA-C  | 5.86  | 116.04      | 110.42   |
| 25  | R     | 291 | SER  | N-CA-C  | 5.86  | 117.34      | 111.07   |
| 25  | R     | 179 | PHE  | O-C-N   | -5.86 | 115.47      | 122.15   |
| 22  | O     | 291 | ILE  | CB-CA-C | -5.85 | 104.14      | 112.22   |
| 31  | X     | 26  | PRO  | CA-C-O  | -5.85 | 114.94      | 121.32   |
| 8   | A     | 229 | THR  | N-CA-C  | -5.85 | 100.42      | 109.14   |
| 13  | F     | 16  | THR  | CA-C-N  | 5.85  | 130.70      | 122.63   |
| 13  | F     | 16  | THR  | C-N-CA  | 5.85  | 130.70      | 122.63   |
| 20  | M     | 302 | GLN  | CA-C-N  | 5.85  | 128.60      | 120.29   |
| 20  | M     | 302 | GLN  | C-N-CA  | 5.85  | 128.60      | 120.29   |
| 21  | N     | 253 | LEU  | CA-C-N  | 5.85  | 128.71      | 120.28   |
| 21  | N     | 253 | LEU  | C-N-CA  | 5.85  | 128.71      | 120.28   |
| 5   | 5     | 112 | ILE  | N-CA-C  | -5.85 | 99.70       | 108.12   |
| 14  | G     | 247 | ASN  | N-CA-C  | -5.85 | 104.37      | 112.03   |
| 1   | 1     | 127 | ALA  | N-CA-C  | -5.85 | 100.49      | 108.38   |
| 21  | N     | 549 | TYR  | O-C-N   | 5.85  | 128.09      | 122.07   |
| 23  | P     | 118 | VAL  | N-CA-C  | 5.85  | 116.58      | 110.62   |
| 26  | S     | 440 | ASP  | N-CA-C  | -5.85 | 106.15      | 113.28   |
| 1   | 1     | 24  | ALA  | N-CA-C  | -5.84 | 105.51      | 114.16   |
| 21  | N     | 111 | GLN  | N-CA-C  | 5.84  | 117.32      | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 248 | TYR  | CA-C-N | 5.84  | 128.11      | 120.28   |
| 33  | Z     | 248 | TYR  | C-N-CA | 5.84  | 128.11      | 120.28   |
| 24  | Q     | 59  | LEU  | CA-C-N | 5.84  | 128.11      | 120.28   |
| 24  | Q     | 59  | LEU  | C-N-CA | 5.84  | 128.11      | 120.28   |
| 28  | U     | 126 | LYS  | CA-C-N | 5.84  | 130.46      | 122.34   |
| 28  | U     | 126 | LYS  | C-N-CA | 5.84  | 130.46      | 122.34   |
| 6   | 6     | 5   | GLY  | O-C-N  | -5.84 | 117.99      | 123.48   |
| 9   | B     | 172 | LYS  | CA-C-O | 5.84  | 126.74      | 120.55   |
| 32  | Y     | 87  | GLU  | N-CA-C | 5.84  | 119.51      | 112.38   |
| 10  | C     | 123 | THR  | N-CA-C | -5.84 | 106.49      | 113.97   |
| 29  | V     | 241 | THR  | O-C-N  | 5.84  | 128.08      | 122.07   |
| 25  | R     | 286 | LEU  | CA-C-O | 5.84  | 126.13      | 119.18   |
| 19  | L     | 425 | VAL  | CA-C-O | 5.84  | 127.17      | 119.53   |
| 26  | S     | 256 | LYS  | CA-C-N | 5.84  | 128.10      | 120.28   |
| 26  | S     | 256 | LYS  | C-N-CA | 5.84  | 128.10      | 120.28   |
| 23  | P     | 267 | PHE  | N-CA-C | -5.83 | 104.83      | 111.07   |
| 33  | Z     | 471 | LEU  | O-C-N  | 5.83  | 128.08      | 122.07   |
| 2   | 2     | 1   | THR  | CA-C-N | 5.83  | 131.07      | 121.86   |
| 2   | 2     | 1   | THR  | C-N-CA | 5.83  | 131.07      | 121.86   |
| 23  | P     | 428 | THR  | O-C-N  | 5.83  | 128.30      | 122.12   |
| 24  | Q     | 428 | GLU  | CA-C-N | 5.83  | 128.02      | 120.44   |
| 24  | Q     | 428 | GLU  | C-N-CA | 5.83  | 128.02      | 120.44   |
| 26  | S     | 192 | GLU  | CA-C-N | 5.83  | 128.56      | 120.63   |
| 26  | S     | 192 | GLU  | C-N-CA | 5.83  | 128.56      | 120.63   |
| 5   | 5     | 65  | LEU  | CA-C-N | 5.83  | 128.09      | 120.28   |
| 5   | 5     | 65  | LEU  | C-N-CA | 5.83  | 128.09      | 120.28   |
| 11  | D     | 189 | GLU  | CA-C-O | -5.83 | 114.70      | 120.82   |
| 20  | M     | 433 | TYR  | CA-C-O | -5.83 | 114.46      | 120.99   |
| 28  | U     | 233 | PHE  | CA-C-O | -5.83 | 114.66      | 120.90   |
| 9   | B     | 117 | ILE  | O-C-N  | 5.83  | 127.52      | 121.87   |
| 18  | K     | 191 | PRO  | CA-C-N | 5.83  | 128.37      | 120.44   |
| 18  | K     | 191 | PRO  | C-N-CA | 5.83  | 128.37      | 120.44   |
| 20  | M     | 265 | ASP  | CA-C-N | 5.83  | 128.37      | 120.44   |
| 20  | M     | 265 | ASP  | C-N-CA | 5.83  | 128.37      | 120.44   |
| 11  | D     | 23  | ALA  | CA-C-N | 5.83  | 129.17      | 120.31   |
| 11  | D     | 23  | ALA  | C-N-CA | 5.83  | 129.17      | 120.31   |
| 23  | P     | 229 | LEU  | O-C-N  | 5.83  | 129.04      | 122.22   |
| 23  | P     | 261 | LEU  | N-CA-C | 5.83  | 117.63      | 111.28   |
| 5   | 5     | 151 | GLU  | CA-C-N | 5.83  | 129.17      | 120.31   |
| 5   | 5     | 151 | GLU  | C-N-CA | 5.83  | 129.17      | 120.31   |
| 9   | B     | 138 | GLY  | CA-C-N | 5.83  | 131.90      | 122.29   |
| 9   | B     | 138 | GLY  | C-N-CA | 5.83  | 131.90      | 122.29   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13  | F     | 21  | GLN  | CA-C-N | 5.83  | 129.87      | 120.55   |
| 13  | F     | 21  | GLN  | C-N-CA | 5.83  | 129.87      | 120.55   |
| 20  | M     | 255 | TYR  | CA-C-N | 5.83  | 132.45      | 121.97   |
| 20  | M     | 255 | TYR  | C-N-CA | 5.83  | 132.45      | 121.97   |
| 25  | R     | 312 | TYR  | O-C-N  | -5.83 | 115.97      | 122.03   |
| 7   | 7     | 72  | LEU  | N-CA-C | -5.82 | 99.88       | 108.79   |
| 15  | H     | 260 | ALA  | N-CA-C | 5.82  | 117.30      | 111.07   |
| 25  | R     | 165 | GLY  | CA-C-N | 5.82  | 128.40      | 120.54   |
| 25  | R     | 165 | GLY  | C-N-CA | 5.82  | 128.40      | 120.54   |
| 25  | R     | 328 | PHE  | CA-C-O | 5.82  | 126.93      | 120.82   |
| 10  | C     | 219 | GLY  | N-CA-C | -5.82 | 105.44      | 112.48   |
| 10  | C     | 231 | LYS  | CA-C-O | -5.82 | 114.36      | 120.70   |
| 21  | N     | 872 | THR  | CA-C-N | 5.82  | 129.10      | 120.95   |
| 21  | N     | 872 | THR  | C-N-CA | 5.82  | 129.10      | 120.95   |
| 17  | J     | 174 | PHE  | CA-C-N | 5.82  | 128.00      | 120.44   |
| 17  | J     | 174 | PHE  | C-N-CA | 5.82  | 128.00      | 120.44   |
| 2   | 2     | 180 | ILE  | O-C-N  | 5.82  | 127.95      | 121.90   |
| 12  | E     | 220 | SER  | CA-C-O | -5.82 | 115.01      | 121.23   |
| 31  | X     | 120 | GLU  | N-CA-C | 5.82  | 117.30      | 111.07   |
| 32  | Y     | 72  | ASP  | CA-C-N | 5.82  | 128.00      | 120.44   |
| 32  | Y     | 72  | ASP  | C-N-CA | 5.82  | 128.00      | 120.44   |
| 19  | L     | 336 | ALA  | CA-C-O | 5.82  | 126.71      | 120.55   |
| 11  | D     | 18  | PHE  | CA-C-N | 5.81  | 128.65      | 120.28   |
| 11  | D     | 18  | PHE  | C-N-CA | 5.81  | 128.65      | 120.28   |
| 13  | F     | 163 | ALA  | O-C-N  | 5.81  | 130.16      | 122.95   |
| 26  | S     | 234 | ILE  | N-CA-C | 5.81  | 116.55      | 110.62   |
| 26  | S     | 173 | LEU  | N-CA-C | 5.81  | 117.71      | 110.91   |
| 21  | N     | 777 | ALA  | CA-C-N | 5.81  | 129.52      | 120.75   |
| 21  | N     | 777 | ALA  | C-N-CA | 5.81  | 129.52      | 120.75   |
| 25  | R     | 282 | THR  | N-CA-C | -5.81 | 107.18      | 114.56   |
| 20  | M     | 230 | LEU  | CA-C-N | 5.81  | 128.54      | 120.29   |
| 20  | M     | 230 | LEU  | C-N-CA | 5.81  | 128.54      | 120.29   |
| 20  | M     | 384 | ASP  | N-CA-C | -5.81 | 98.62       | 108.26   |
| 21  | N     | 659 | ALA  | CA-C-N | 5.81  | 128.38      | 120.54   |
| 21  | N     | 659 | ALA  | C-N-CA | 5.81  | 128.38      | 120.54   |
| 25  | R     | 339 | ALA  | CA-C-O | -5.81 | 114.72      | 120.70   |
| 19  | L     | 344 | ASP  | N-CA-C | -5.81 | 104.18      | 112.13   |
| 23  | P     | 334 | ASN  | O-C-N  | 5.81  | 128.27      | 122.12   |
| 25  | R     | 327 | ASP  | CA-C-N | 5.81  | 127.99      | 120.44   |
| 25  | R     | 327 | ASP  | C-N-CA | 5.81  | 127.99      | 120.44   |
| 6   | 6     | 111 | GLY  | N-CA-C | 5.80  | 118.60      | 111.93   |
| 17  | J     | 299 | ILE  | CA-C-O | 5.80  | 124.47      | 118.96   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 18  | K     | 69  | LYS  | CA-C-N | 5.80  | 128.53      | 120.29   |
| 18  | K     | 69  | LYS  | C-N-CA | 5.80  | 128.53      | 120.29   |
| 27  | T     | 182 | LYS  | CA-C-O | -5.80 | 114.40      | 120.55   |
| 28  | U     | 198 | LYS  | CA-C-N | 5.80  | 126.38      | 119.94   |
| 28  | U     | 198 | LYS  | C-N-CA | 5.80  | 126.38      | 119.94   |
| 29  | V     | 193 | ASN  | N-CA-C | -5.80 | 99.73       | 109.07   |
| 33  | Z     | 581 | VAL  | CA-C-N | 5.80  | 128.85      | 120.38   |
| 33  | Z     | 581 | VAL  | C-N-CA | 5.80  | 128.85      | 120.38   |
| 26  | S     | 231 | ALA  | O-C-N  | 5.80  | 128.76      | 122.15   |
| 14  | G     | 86  | HIS  | O-C-N  | 5.80  | 128.04      | 122.07   |
| 26  | S     | 132 | ALA  | CA-C-N | 5.80  | 127.97      | 120.44   |
| 26  | S     | 132 | ALA  | C-N-CA | 5.80  | 127.97      | 120.44   |
| 2   | 2     | 58  | LEU  | CA-C-N | 5.79  | 128.65      | 120.42   |
| 2   | 2     | 58  | LEU  | C-N-CA | 5.79  | 128.65      | 120.42   |
| 22  | O     | 242 | ILE  | CA-C-N | 5.79  | 128.40      | 120.35   |
| 22  | O     | 242 | ILE  | C-N-CA | 5.79  | 128.40      | 120.35   |
| 29  | V     | 28  | TYR  | N-CA-C | -5.79 | 99.29       | 108.73   |
| 32  | Y     | 81  | LEU  | N-CA-C | 5.79  | 117.27      | 111.07   |
| 7   | 7     | 3   | VAL  | N-CA-C | -5.79 | 99.71       | 108.17   |
| 17  | J     | 232 | GLU  | CA-C-N | 5.79  | 127.97      | 120.44   |
| 17  | J     | 232 | GLU  | C-N-CA | 5.79  | 127.97      | 120.44   |
| 21  | N     | 499 | HIS  | CA-C-N | 5.79  | 127.97      | 120.44   |
| 21  | N     | 499 | HIS  | C-N-CA | 5.79  | 127.97      | 120.44   |
| 8   | A     | 125 | SER  | CA-C-N | 5.79  | 128.04      | 120.28   |
| 8   | A     | 125 | SER  | C-N-CA | 5.79  | 128.04      | 120.28   |
| 16  | I     | 390 | ALA  | CA-C-N | 5.79  | 129.11      | 120.31   |
| 16  | I     | 390 | ALA  | C-N-CA | 5.79  | 129.11      | 120.31   |
| 23  | P     | 383 | LEU  | N-CA-C | 5.79  | 117.59      | 111.28   |
| 10  | C     | 207 | THR  | CA-C-N | 5.79  | 129.86      | 120.60   |
| 10  | C     | 207 | THR  | C-N-CA | 5.79  | 129.86      | 120.60   |
| 21  | N     | 888 | ASP  | CA-C-N | 5.79  | 132.59      | 121.54   |
| 21  | N     | 888 | ASP  | C-N-CA | 5.79  | 132.59      | 121.54   |
| 28  | U     | 194 | LEU  | CA-C-O | 5.79  | 126.89      | 120.82   |
| 18  | K     | 407 | LEU  | O-C-N  | -5.78 | 115.99      | 122.12   |
| 22  | O     | 248 | TYR  | N-CA-C | -5.78 | 104.75      | 113.89   |
| 25  | R     | 161 | ALA  | CA-C-O | 5.78  | 127.46      | 120.81   |
| 31  | X     | 75  | TRP  | N-CA-C | -5.78 | 99.30       | 108.73   |
| 21  | N     | 686 | ILE  | CA-C-N | 5.78  | 128.50      | 120.29   |
| 21  | N     | 686 | ILE  | C-N-CA | 5.78  | 128.50      | 120.29   |
| 28  | U     | 286 | ILE  | N-CA-C | 5.78  | 116.52      | 110.62   |
| 5   | 5     | 79  | ALA  | N-CA-C | 5.78  | 117.38      | 111.14   |
| 21  | N     | 161 | TYR  | N-CA-C | 5.78  | 119.40      | 111.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | B     | 76  | SER  | N-CA-C  | -5.78 | 98.87       | 108.75   |
| 27  | T     | 74  | ASN  | CA-C-N  | 5.78  | 128.50      | 120.29   |
| 27  | T     | 74  | ASN  | C-N-CA  | 5.78  | 128.50      | 120.29   |
| 11  | D     | 235 | GLN  | O-C-N   | -5.78 | 115.46      | 122.22   |
| 29  | V     | 71  | MET  | N-CA-C  | -5.78 | 103.48      | 110.13   |
| 33  | Z     | 107 | THR  | CA-C-N  | 5.78  | 129.44      | 120.60   |
| 33  | Z     | 107 | THR  | C-N-CA  | 5.78  | 129.44      | 120.60   |
| 3   | 3     | 150 | GLU  | CA-C-N  | 5.78  | 127.06      | 119.84   |
| 3   | 3     | 150 | GLU  | C-N-CA  | 5.78  | 127.06      | 119.84   |
| 8   | A     | 103 | GLU  | CA-C-N  | 5.78  | 127.95      | 120.44   |
| 8   | A     | 103 | GLU  | C-N-CA  | 5.78  | 127.95      | 120.44   |
| 21  | N     | 641 | LEU  | N-CA-C  | 5.78  | 119.43      | 112.38   |
| 13  | F     | 176 | LEU  | CA-C-N  | 5.77  | 128.29      | 120.38   |
| 13  | F     | 176 | LEU  | C-N-CA  | 5.77  | 128.29      | 120.38   |
| 12  | E     | 86  | ARG  | O-C-N   | -5.77 | 115.57      | 122.15   |
| 12  | E     | 112 | LEU  | N-CA-C  | 5.77  | 117.57      | 111.28   |
| 21  | N     | 658 | ILE  | N-CA-C  | 5.77  | 117.20      | 110.62   |
| 6   | 6     | 94  | PHE  | CA-C-O  | -5.77 | 114.53      | 121.22   |
| 15  | H     | 395 | SER  | CA-C-N  | 5.77  | 132.56      | 121.54   |
| 15  | H     | 395 | SER  | C-N-CA  | 5.77  | 132.56      | 121.54   |
| 18  | K     | 311 | ASN  | N-CA-C  | -5.77 | 104.43      | 113.02   |
| 22  | O     | 217 | LEU  | CA-C-N  | 5.77  | 128.01      | 120.28   |
| 22  | O     | 217 | LEU  | C-N-CA  | 5.77  | 128.01      | 120.28   |
| 24  | Q     | 124 | PHE  | CA-C-N  | 5.77  | 128.59      | 120.28   |
| 24  | Q     | 124 | PHE  | C-N-CA  | 5.77  | 128.59      | 120.28   |
| 2   | 2     | 61  | SER  | CA-C-O  | -5.77 | 114.77      | 120.82   |
| 6   | 6     | 5   | GLY  | CA-C-O  | 5.77  | 126.05      | 120.57   |
| 25  | R     | 301 | TYR  | N-CA-C  | -5.77 | 105.63      | 114.16   |
| 29  | V     | 255 | ILE  | N-CA-C  | -5.77 | 104.90      | 110.72   |
| 21  | N     | 586 | ALA  | O-C-N   | -5.76 | 115.48      | 122.22   |
| 19  | L     | 181 | ASP  | CA-C-O  | -5.76 | 112.58      | 119.15   |
| 24  | Q     | 270 | ILE  | CA-C-N  | 5.76  | 128.00      | 120.28   |
| 24  | Q     | 270 | ILE  | C-N-CA  | 5.76  | 128.00      | 120.28   |
| 9   | B     | 167 | GLY  | CA-C-N  | 5.76  | 128.27      | 120.44   |
| 9   | B     | 167 | GLY  | C-N-CA  | 5.76  | 128.27      | 120.44   |
| 2   | 2     | 56  | THR  | CA-C-N  | 5.75  | 128.46      | 120.29   |
| 2   | 2     | 56  | THR  | C-N-CA  | 5.75  | 128.46      | 120.29   |
| 3   | 3     | 62  | THR  | CA-C-N  | 5.75  | 127.92      | 120.44   |
| 3   | 3     | 62  | THR  | C-N-CA  | 5.75  | 127.92      | 120.44   |
| 22  | O     | 291 | ILE  | CA-C-O  | 5.75  | 126.95      | 120.85   |
| 22  | O     | 120 | LYS  | N-CA-C  | -5.75 | 98.91       | 108.75   |
| 22  | O     | 356 | ARG  | CB-CA-C | -5.75 | 103.71      | 112.11   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | R     | 372 | ILE  | O-C-N  | -5.75 | 115.98      | 120.07   |
| 27  | T     | 109 | TYR  | CA-C-O | -5.75 | 114.32      | 120.42   |
| 7   | 7     | 174 | ARG  | CA-C-N | 5.75  | 128.34      | 120.46   |
| 7   | 7     | 174 | ARG  | C-N-CA | 5.75  | 128.34      | 120.46   |
| 14  | G     | 13  | VAL  | CA-C-O | -5.75 | 115.68      | 121.49   |
| 26  | S     | 152 | LEU  | N-CA-C | 5.75  | 117.55      | 111.28   |
| 30  | W     | 110 | ILE  | N-CA-C | -5.75 | 100.06      | 108.11   |
| 3   | 3     | 124 | ALA  | N-CA-C | -5.75 | 99.96       | 108.99   |
| 12  | E     | 127 | ALA  | CA-C-N | 5.75  | 131.85      | 122.65   |
| 12  | E     | 127 | ALA  | C-N-CA | 5.75  | 131.85      | 122.65   |
| 15  | H     | 330 | GLN  | CA-C-N | 5.75  | 127.98      | 120.28   |
| 15  | H     | 330 | GLN  | C-N-CA | 5.75  | 127.98      | 120.28   |
| 25  | R     | 243 | LEU  | CA-C-N | 5.75  | 132.52      | 121.54   |
| 25  | R     | 243 | LEU  | C-N-CA | 5.75  | 132.52      | 121.54   |
| 26  | S     | 368 | LYS  | O-C-N  | 5.75  | 128.70      | 122.15   |
| 30  | W     | 180 | LEU  | CA-C-N | 5.75  | 128.45      | 120.29   |
| 30  | W     | 180 | LEU  | C-N-CA | 5.75  | 128.45      | 120.29   |
| 17  | J     | 146 | THR  | N-CA-C | -5.75 | 100.62      | 108.38   |
| 22  | O     | 313 | ILE  | CA-C-O | -5.75 | 114.76      | 120.85   |
| 8   | A     | 112 | MET  | O-C-N  | -5.75 | 116.31      | 121.31   |
| 12  | E     | 213 | ASP  | N-CA-C | -5.75 | 100.34      | 109.07   |
| 30  | W     | 96  | LEU  | CA-C-N | 5.75  | 127.98      | 120.28   |
| 30  | W     | 96  | LEU  | C-N-CA | 5.75  | 127.98      | 120.28   |
| 16  | I     | 175 | LYS  | O-C-N  | 5.74  | 129.82      | 122.93   |
| 18  | K     | 323 | THR  | N-CA-C | -5.74 | 104.03      | 113.50   |
| 21  | N     | 731 | VAL  | CA-C-N | 5.74  | 126.31      | 119.94   |
| 21  | N     | 731 | VAL  | C-N-CA | 5.74  | 126.31      | 119.94   |
| 26  | S     | 233 | LEU  | N-CA-C | -5.74 | 105.10      | 111.36   |
| 4   | 4     | 164 | VAL  | O-C-N  | 5.74  | 128.29      | 121.80   |
| 22  | O     | 129 | ILE  | CA-C-N | 5.74  | 127.97      | 120.28   |
| 22  | O     | 129 | ILE  | C-N-CA | 5.74  | 127.97      | 120.28   |
| 18  | K     | 182 | GLN  | N-CA-C | -5.74 | 105.11      | 111.36   |
| 7   | 7     | 43  | VAL  | CA-C-O | 5.74  | 126.67      | 120.53   |
| 10  | C     | 99  | LEU  | CA-C-O | -5.74 | 114.80      | 120.82   |
| 22  | O     | 75  | GLN  | CA-C-N | 5.74  | 127.96      | 120.28   |
| 22  | O     | 75  | GLN  | C-N-CA | 5.74  | 127.96      | 120.28   |
| 27  | T     | 140 | SER  | CA-C-N | 5.74  | 128.24      | 120.44   |
| 27  | T     | 140 | SER  | C-N-CA | 5.74  | 128.24      | 120.44   |
| 20  | M     | 373 | ASP  | O-C-N  | 5.73  | 128.34      | 122.09   |
| 12  | E     | 101 | LEU  | N-CA-C | 5.73  | 117.20      | 111.07   |
| 19  | L     | 306 | MET  | N-CA-C | 5.73  | 117.53      | 111.28   |
| 20  | M     | 371 | ASP  | O-C-N  | -5.73 | 115.31      | 122.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | N     | 468 | GLU  | N-CA-C  | -5.73 | 105.78      | 112.89   |
| 31  | X     | 102 | GLN  | N-CA-C  | 5.73  | 118.26      | 111.33   |
| 14  | G     | 81  | ILE  | CB-CA-C | -5.73 | 106.50      | 114.00   |
| 19  | L     | 188 | GLU  | CA-C-N  | 5.73  | 127.96      | 120.28   |
| 19  | L     | 188 | GLU  | C-N-CA  | 5.73  | 127.96      | 120.28   |
| 29  | V     | 192 | LEU  | N-CA-C  | -5.73 | 98.60       | 110.80   |
| 4   | 4     | 148 | ARG  | CA-C-O  | -5.73 | 114.51      | 119.72   |
| 19  | L     | 260 | ALA  | CA-C-N  | 5.73  | 127.96      | 120.28   |
| 19  | L     | 260 | ALA  | C-N-CA  | 5.73  | 127.96      | 120.28   |
| 19  | L     | 279 | PHE  | CA-C-O  | 5.73  | 126.62      | 120.32   |
| 24  | Q     | 85  | MET  | CA-C-N  | 5.73  | 128.53      | 120.28   |
| 24  | Q     | 85  | MET  | C-N-CA  | 5.73  | 128.53      | 120.28   |
| 26  | S     | 401 | LYS  | CA-C-O  | 5.73  | 127.25      | 120.66   |
| 30  | W     | 146 | GLU  | CA-C-N  | 5.73  | 132.28      | 121.97   |
| 30  | W     | 146 | GLU  | C-N-CA  | 5.73  | 132.28      | 121.97   |
| 21  | N     | 550 | GLY  | CA-C-N  | 5.73  | 126.34      | 119.98   |
| 21  | N     | 550 | GLY  | C-N-CA  | 5.73  | 126.34      | 119.98   |
| 23  | P     | 241 | LEU  | CA-C-N  | 5.73  | 128.42      | 120.29   |
| 23  | P     | 241 | LEU  | C-N-CA  | 5.73  | 128.42      | 120.29   |
| 33  | Z     | 852 | GLN  | CA-C-O  | 5.72  | 126.62      | 120.55   |
| 6   | 6     | 147 | PHE  | CA-C-N  | 5.72  | 131.06      | 122.99   |
| 6   | 6     | 147 | PHE  | C-N-CA  | 5.72  | 131.06      | 122.99   |
| 7   | 7     | 176 | LEU  | CA-C-O  | -5.72 | 114.48      | 120.55   |
| 33  | Z     | 245 | VAL  | CA-C-O  | -5.72 | 114.78      | 120.85   |
| 8   | A     | 51  | THR  | N-CA-C  | -5.72 | 98.56       | 108.69   |
| 22  | O     | 187 | SER  | CA-C-N  | 5.72  | 127.88      | 120.44   |
| 22  | O     | 187 | SER  | C-N-CA  | 5.72  | 127.88      | 120.44   |
| 11  | D     | 240 | LYS  | O-C-N   | 5.72  | 130.53      | 122.41   |
| 12  | E     | 207 | VAL  | N-CA-C  | -5.72 | 104.55      | 112.50   |
| 28  | U     | 194 | LEU  | N-CA-C  | 5.72  | 117.19      | 111.07   |
| 25  | R     | 303 | SER  | N-CA-C  | -5.72 | 106.85      | 113.88   |
| 29  | V     | 103 | MET  | O-C-N   | -5.72 | 115.99      | 122.68   |
| 7   | 7     | 177 | TYR  | N-CA-C  | -5.72 | 105.03      | 112.23   |
| 24  | Q     | 289 | GLU  | CB-CA-C | -5.72 | 109.97      | 116.54   |
| 30  | W     | 52  | ILE  | CA-C-O  | -5.72 | 115.97      | 121.63   |
| 8   | A     | 164 | VAL  | CA-C-O  | 5.71  | 125.78      | 121.09   |
| 14  | G     | 192 | VAL  | CA-C-N  | 5.71  | 127.87      | 120.44   |
| 14  | G     | 192 | VAL  | C-N-CA  | 5.71  | 127.87      | 120.44   |
| 16  | I     | 338 | LEU  | N-CA-C  | -5.71 | 106.47      | 113.50   |
| 19  | L     | 230 | LEU  | CA-C-N  | 5.71  | 128.21      | 120.44   |
| 19  | L     | 230 | LEU  | C-N-CA  | 5.71  | 128.21      | 120.44   |
| 3   | 3     | -2  | ASN  | CA-C-O  | 5.71  | 126.12      | 119.32   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 18  | K     | 89  | ILE  | N-CA-C | 5.71  | 116.45      | 110.62   |
| 33  | Z     | 102 | ILE  | CA-C-N | 5.71  | 127.94      | 120.28   |
| 33  | Z     | 102 | ILE  | C-N-CA | 5.71  | 127.94      | 120.28   |
| 29  | V     | 199 | LEU  | CA-C-O | -5.71 | 114.95      | 121.58   |
| 29  | V     | 284 | ALA  | O-C-N  | -5.71 | 116.07      | 122.12   |
| 27  | T     | 145 | PRO  | N-CA-C | 5.71  | 121.36      | 113.65   |
| 15  | H     | 252 | PRO  | CA-C-O | -5.71 | 114.53      | 121.03   |
| 17  | J     | 129 | LYS  | CA-C-N | 5.71  | 129.90      | 120.94   |
| 17  | J     | 129 | LYS  | C-N-CA | 5.71  | 129.90      | 120.94   |
| 23  | P     | 343 | LYS  | CA-C-N | 5.71  | 127.92      | 120.28   |
| 23  | P     | 343 | LYS  | C-N-CA | 5.71  | 127.92      | 120.28   |
| 22  | O     | 286 | PHE  | N-CA-C | 5.70  | 117.50      | 111.28   |
| 23  | P     | 118 | VAL  | CA-C-O | 5.70  | 126.88      | 120.95   |
| 22  | O     | 189 | TYR  | CA-C-N | 5.70  | 127.85      | 120.44   |
| 22  | O     | 189 | TYR  | C-N-CA | 5.70  | 127.85      | 120.44   |
| 27  | T     | 150 | ARG  | CA-C-O | 5.70  | 126.81      | 120.82   |
| 2   | 2     | 175 | VAL  | N-CA-C | -5.70 | 99.57       | 108.86   |
| 10  | C     | 136 | ILE  | CA-C-N | 5.70  | 130.58      | 122.72   |
| 10  | C     | 136 | ILE  | C-N-CA | 5.70  | 130.58      | 122.72   |
| 16  | I     | 260 | GLY  | CA-C-O | -5.70 | 113.37      | 121.52   |
| 20  | M     | 305 | MET  | CA-C-N | 5.70  | 127.92      | 120.28   |
| 20  | M     | 305 | MET  | C-N-CA | 5.70  | 127.92      | 120.28   |
| 21  | N     | 136 | ILE  | O-C-N  | 5.70  | 127.40      | 121.87   |
| 24  | Q     | 29  | SER  | CA-C-O | 5.70  | 126.54      | 120.10   |
| 33  | Z     | 267 | THR  | N-CA-C | 5.70  | 117.57      | 111.36   |
| 7   | 7     | 22  | TYR  | N-CA-C | -5.70 | 99.09       | 108.49   |
| 8   | A     | 157 | THR  | N-CA-C | -5.70 | 101.77      | 110.14   |
| 15  | H     | 278 | GLU  | O-C-N  | -5.70 | 115.26      | 122.27   |
| 28  | U     | 167 | GLU  | CA-C-O | -5.70 | 114.51      | 120.55   |
| 8   | A     | 222 | ASP  | N-CA-C | -5.69 | 106.32      | 113.72   |
| 25  | R     | 155 | GLY  | N-CA-C | 5.69  | 120.84      | 113.27   |
| 33  | Z     | 85  | VAL  | O-C-N  | -5.69 | 114.99      | 121.14   |
| 33  | Z     | 396 | ASN  | O-C-N  | -5.69 | 115.15      | 122.21   |
| 11  | D     | 106 | VAL  | CA-C-N | 5.69  | 128.22      | 120.54   |
| 11  | D     | 106 | VAL  | C-N-CA | 5.69  | 128.22      | 120.54   |
| 16  | I     | 79  | SER  | CA-C-O | -5.69 | 114.52      | 120.55   |
| 25  | R     | 127 | GLU  | N-CA-C | -5.69 | 104.89      | 113.89   |
| 33  | Z     | 388 | GLY  | N-CA-C | 5.69  | 119.56      | 112.73   |
| 1   | 1     | 46  | SER  | O-C-N  | 5.69  | 129.74      | 123.25   |
| 2   | 2     | 64  | GLU  | CA-C-O | 5.69  | 126.53      | 120.10   |
| 4   | 4     | 30  | SER  | O-C-N  | -5.69 | 115.35      | 122.24   |
| 17  | J     | 156 | GLN  | CA-C-O | -5.69 | 114.39      | 120.42   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 464 | GLU  | N-CA-C | 5.69  | 117.56      | 111.36   |
| 33  | Z     | 205 | LEU  | CA-C-N | 5.69  | 127.91      | 120.28   |
| 33  | Z     | 205 | LEU  | C-N-CA | 5.69  | 127.91      | 120.28   |
| 33  | Z     | 472 | LEU  | CA-C-O | -5.69 | 114.52      | 120.55   |
| 10  | C     | 189 | ALA  | O-C-N  | -5.69 | 116.09      | 122.12   |
| 17  | J     | 186 | ILE  | O-C-N  | -5.69 | 117.04      | 123.18   |
| 21  | N     | 519 | VAL  | CA-C-O | -5.69 | 115.04      | 120.95   |
| 23  | P     | 395 | ARG  | CA-C-N | -5.69 | 112.73      | 119.84   |
| 23  | P     | 395 | ARG  | C-N-CA | -5.69 | 112.73      | 119.84   |
| 4   | 4     | 119 | ASP  | O-C-N  | -5.68 | 116.37      | 122.85   |
| 10  | C     | 69  | LEU  | N-CA-C | -5.68 | 106.47      | 113.41   |
| 15  | H     | 417 | ALA  | CA-C-N | 5.68  | 128.36      | 120.29   |
| 15  | H     | 417 | ALA  | C-N-CA | 5.68  | 128.36      | 120.29   |
| 20  | M     | 368 | MET  | CA-C-N | 5.68  | 129.98      | 122.42   |
| 20  | M     | 368 | MET  | C-N-CA | 5.68  | 129.98      | 122.42   |
| 21  | N     | 441 | VAL  | CA-C-N | 5.68  | 127.83      | 120.44   |
| 21  | N     | 441 | VAL  | C-N-CA | 5.68  | 127.83      | 120.44   |
| 16  | I     | 86  | GLU  | N-CA-C | 5.68  | 117.15      | 111.07   |
| 19  | L     | 221 | TYR  | N-CA-C | -5.68 | 100.67      | 109.14   |
| 22  | O     | 188 | PHE  | CA-C-N | 5.68  | 127.89      | 120.28   |
| 22  | O     | 188 | PHE  | C-N-CA | 5.68  | 127.89      | 120.28   |
| 33  | Z     | 419 | VAL  | CA-C-N | 5.68  | 128.46      | 120.28   |
| 33  | Z     | 419 | VAL  | C-N-CA | 5.68  | 128.46      | 120.28   |
| 2   | 2     | 141 | HIS  | N-CA-C | -5.68 | 106.22      | 114.12   |
| 6   | 6     | 64  | LYS  | CA-C-O | -5.68 | 114.86      | 120.82   |
| 7   | 7     | 75  | ALA  | CA-C-O | 5.68  | 124.73      | 118.65   |
| 18  | K     | 423 | LYS  | CA-C-N | 5.68  | 132.39      | 121.54   |
| 18  | K     | 423 | LYS  | C-N-CA | 5.68  | 132.39      | 121.54   |
| 19  | L     | 399 | GLY  | CA-C-O | -5.68 | 114.05      | 120.30   |
| 23  | P     | 200 | SER  | CA-C-N | 5.68  | 127.82      | 120.44   |
| 23  | P     | 200 | SER  | C-N-CA | 5.68  | 127.82      | 120.44   |
| 24  | Q     | 101 | ILE  | N-CA-C | -5.68 | 104.98      | 110.72   |
| 16  | I     | 422 | ARG  | N-CA-C | 5.68  | 117.27      | 111.14   |
| 2   | 2     | 167 | LEU  | N-CA-C | -5.68 | 105.56      | 112.88   |
| 8   | A     | 124 | LEU  | CA-C-O | -5.68 | 114.53      | 120.55   |
| 18  | K     | 156 | SER  | CA-C-O | -5.68 | 115.29      | 121.87   |
| 33  | Z     | 783 | VAL  | N-CA-C | -5.68 | 105.19      | 110.53   |
| 6   | 6     | 54  | ALA  | CA-C-N | 5.67  | 127.88      | 120.28   |
| 6   | 6     | 54  | ALA  | C-N-CA | 5.67  | 127.88      | 120.28   |
| 8   | A     | 235 | THR  | N-CA-C | -5.67 | 100.45      | 109.76   |
| 25  | R     | 62  | TYR  | CA-C-O | 5.67  | 126.24      | 119.60   |
| 25  | R     | 65  | TYR  | O-C-N  | 5.67  | 128.13      | 122.12   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | T     | 69  | SER  | CA-C-O  | -5.67 | 114.53      | 120.55   |
| 20  | M     | 206 | LYS  | CA-C-O  | -5.67 | 114.86      | 120.70   |
| 6   | 6     | 210 | LEU  | CA-C-O  | -5.67 | 114.80      | 121.44   |
| 17  | J     | 380 | GLU  | CA-C-N  | 5.67  | 127.88      | 120.28   |
| 17  | J     | 380 | GLU  | C-N-CA  | 5.67  | 127.88      | 120.28   |
| 6   | 6     | 203 | VAL  | N-CA-C  | -5.67 | 100.23      | 108.17   |
| 6   | 6     | 175 | VAL  | CA-C-N  | 5.67  | 127.88      | 120.28   |
| 6   | 6     | 175 | VAL  | C-N-CA  | 5.67  | 127.88      | 120.28   |
| 12  | E     | 182 | GLU  | O-C-N   | 5.67  | 128.13      | 122.12   |
| 20  | M     | 355 | ASP  | N-CA-C  | -5.67 | 105.10      | 111.28   |
| 23  | P     | 45  | LYS  | CB-CA-C | -5.67 | 101.94      | 110.90   |
| 31  | X     | 117 | LYS  | O-C-N   | -5.67 | 117.31      | 123.26   |
| 13  | F     | 159 | THR  | N-CA-C  | -5.67 | 99.89       | 107.88   |
| 27  | T     | 1   | MET  | CA-C-N  | 5.67  | 125.62      | 119.78   |
| 27  | T     | 1   | MET  | C-N-CA  | 5.67  | 125.62      | 119.78   |
| 12  | E     | 195 | GLU  | CA-C-N  | 5.67  | 127.87      | 120.28   |
| 12  | E     | 195 | GLU  | C-N-CA  | 5.67  | 127.87      | 120.28   |
| 17  | J     | 199 | ALA  | N-CA-C  | 5.66  | 117.45      | 111.28   |
| 7   | 7     | -4  | ILE  | CA-C-O  | 5.66  | 123.88      | 118.90   |
| 9   | B     | 94  | HIS  | O-C-N   | -5.66 | 114.66      | 122.30   |
| 19  | L     | 196 | VAL  | CA-C-N  | -5.66 | 117.36      | 123.08   |
| 19  | L     | 196 | VAL  | C-N-CA  | -5.66 | 117.36      | 123.08   |
| 23  | P     | 126 | THR  | CA-C-N  | 5.66  | 131.46      | 122.74   |
| 23  | P     | 126 | THR  | C-N-CA  | 5.66  | 131.46      | 122.74   |
| 15  | H     | 215 | LYS  | CA-C-N  | 5.66  | 128.14      | 120.44   |
| 15  | H     | 215 | LYS  | C-N-CA  | 5.66  | 128.14      | 120.44   |
| 23  | P     | 93  | ILE  | N-CA-C  | 5.66  | 115.85      | 110.42   |
| 25  | R     | 84  | LYS  | CA-C-O  | 5.66  | 126.18      | 119.56   |
| 7   | 7     | 47  | GLY  | CA-C-N  | 5.66  | 128.79      | 120.82   |
| 7   | 7     | 47  | GLY  | C-N-CA  | 5.66  | 128.79      | 120.82   |
| 24  | Q     | 172 | PRO  | CA-C-N  | 5.66  | 128.91      | 120.31   |
| 24  | Q     | 172 | PRO  | C-N-CA  | 5.66  | 128.91      | 120.31   |
| 24  | Q     | 427 | PHE  | N-CA-C  | 5.66  | 117.44      | 111.28   |
| 11  | D     | 160 | SER  | CA-C-O  | 5.65  | 125.89      | 119.27   |
| 21  | N     | 10  | LEU  | CA-C-N  | 5.65  | 127.86      | 120.28   |
| 21  | N     | 10  | LEU  | C-N-CA  | 5.65  | 127.86      | 120.28   |
| 12  | E     | 34  | GLY  | O-C-N   | -5.65 | 118.30      | 122.71   |
| 21  | N     | 43  | LEU  | CA-C-N  | 5.65  | 125.32      | 119.05   |
| 21  | N     | 43  | LEU  | C-N-CA  | 5.65  | 125.32      | 119.05   |
| 10  | C     | 231 | LYS  | CA-C-N  | 5.65  | 126.90      | 119.84   |
| 10  | C     | 231 | LYS  | C-N-CA  | 5.65  | 126.90      | 119.84   |
| 17  | J     | 345 | LYS  | O-C-N   | -5.65 | 115.71      | 122.15   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | Z     | 832 | ARG  | N-CA-C | 5.65  | 117.44      | 111.28   |
| 15  | H     | 218 | ILE  | O-C-N  | -5.65 | 116.39      | 121.87   |
| 19  | L     | 387 | ASN  | N-CA-C | -5.65 | 101.16      | 109.18   |
| 22  | O     | 317 | THR  | CA-C-O | -5.65 | 113.47      | 119.97   |
| 4   | 4     | 38  | SER  | CA-C-O | -5.65 | 115.80      | 120.71   |
| 19  | L     | 276 | CYS  | CA-C-N | 5.65  | 130.05      | 122.93   |
| 19  | L     | 276 | CYS  | C-N-CA | 5.65  | 130.05      | 122.93   |
| 20  | M     | 320 | ARG  | N-CA-C | -5.65 | 105.20      | 111.36   |
| 20  | M     | 360 | ILE  | CA-C-O | -5.65 | 115.08      | 120.95   |
| 23  | P     | 64  | ASP  | CA-C-N | 5.65  | 127.85      | 120.28   |
| 23  | P     | 64  | ASP  | C-N-CA | 5.65  | 127.85      | 120.28   |
| 30  | W     | 47  | ASN  | N-CA-C | -5.65 | 98.77       | 110.80   |
| 24  | Q     | 429 | LYS  | N-CA-C | 5.65  | 117.11      | 111.07   |
| 1   | 1     | 42  | TRP  | N-CA-C | -5.64 | 101.56      | 109.69   |
| 24  | Q     | 319 | LYS  | O-C-N  | 5.64  | 129.57      | 122.23   |
| 14  | G     | 193 | LYS  | CA-C-O | -5.64 | 114.89      | 120.82   |
| 15  | H     | 156 | VAL  | N-CA-C | -5.64 | 99.51       | 107.75   |
| 23  | P     | 407 | ASN  | N-CA-C | -5.64 | 100.48      | 109.23   |
| 19  | L     | 312 | MET  | CA-C-O | -5.64 | 114.89      | 120.70   |
| 23  | P     | 415 | TRP  | CA-C-N | 5.64  | 130.14      | 120.72   |
| 23  | P     | 415 | TRP  | C-N-CA | 5.64  | 130.14      | 120.72   |
| 23  | P     | 384 | VAL  | O-C-N  | 5.64  | 127.64      | 121.83   |
| 33  | Z     | 236 | PHE  | N-CA-C | 5.64  | 117.43      | 111.28   |
| 21  | N     | 224 | THR  | O-C-N  | 5.64  | 128.58      | 122.15   |
| 21  | N     | 320 | SER  | N-CA-C | 5.64  | 117.10      | 111.07   |
| 21  | N     | 574 | VAL  | CA-C-N | 5.64  | 127.83      | 120.28   |
| 21  | N     | 574 | VAL  | C-N-CA | 5.64  | 127.83      | 120.28   |
| 28  | U     | 25  | THR  | CA-C-N | 5.64  | 130.37      | 122.08   |
| 28  | U     | 25  | THR  | C-N-CA | 5.64  | 130.37      | 122.08   |
| 9   | B     | 9   | LEU  | N-CA-C | -5.64 | 105.75      | 113.30   |
| 15  | H     | 185 | LEU  | O-C-N  | -5.64 | 114.84      | 121.32   |
| 21  | N     | 107 | GLU  | CA-C-O | 5.64  | 126.93      | 120.90   |
| 33  | Z     | 388 | GLY  | O-C-N  | 5.64  | 127.60      | 122.19   |
| 33  | Z     | 344 | LYS  | CA-C-N | 5.63  | 127.83      | 120.28   |
| 33  | Z     | 344 | LYS  | C-N-CA | 5.63  | 127.83      | 120.28   |
| 33  | Z     | 203 | LEU  | O-C-N  | -5.63 | 115.73      | 122.15   |
| 15  | H     | 265 | ASN  | CA-C-N | 5.63  | 128.39      | 120.28   |
| 15  | H     | 265 | ASN  | C-N-CA | 5.63  | 128.39      | 120.28   |
| 31  | X     | 62  | ASP  | O-C-N  | -5.63 | 116.53      | 121.32   |
| 33  | Z     | 114 | SER  | CA-C-N | 5.63  | 127.82      | 120.28   |
| 33  | Z     | 114 | SER  | C-N-CA | 5.63  | 127.82      | 120.28   |
| 14  | G     | 169 | GLN  | CA-C-N | 5.63  | 127.76      | 120.44   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | G     | 169 | GLN  | C-N-CA  | 5.63  | 127.76      | 120.44   |
| 33  | Z     | 414 | GLY  | O-C-N   | -5.63 | 116.79      | 122.19   |
| 21  | N     | 106 | ILE  | CA-C-N  | 5.63  | 128.14      | 120.54   |
| 21  | N     | 106 | ILE  | C-N-CA  | 5.63  | 128.14      | 120.54   |
| 7   | 7     | 113 | SER  | CA-C-N  | 5.62  | 130.38      | 121.44   |
| 7   | 7     | 113 | SER  | C-N-CA  | 5.62  | 130.38      | 121.44   |
| 22  | O     | 70  | TYR  | CA-C-N  | 5.62  | 128.28      | 120.29   |
| 22  | O     | 70  | TYR  | C-N-CA  | 5.62  | 128.28      | 120.29   |
| 26  | S     | 208 | ILE  | O-C-N   | 5.62  | 127.33      | 121.87   |
| 29  | V     | 94  | MET  | CA-C-N  | 5.62  | 128.13      | 120.54   |
| 29  | V     | 94  | MET  | C-N-CA  | 5.62  | 128.13      | 120.54   |
| 9   | B     | 48  | GLU  | CA-C-O  | -5.62 | 114.30      | 120.43   |
| 13  | F     | 187 | ASP  | CA-C-O  | -5.62 | 114.59      | 120.55   |
| 14  | G     | 44  | GLY  | CA-C-N  | 5.62  | 130.90      | 122.58   |
| 14  | G     | 44  | GLY  | C-N-CA  | 5.62  | 130.90      | 122.58   |
| 15  | H     | 248 | LEU  | N-CA-C  | -5.62 | 99.74       | 108.90   |
| 15  | H     | 447 | VAL  | O-C-N   | 5.62  | 127.42      | 121.91   |
| 33  | Z     | 740 | VAL  | O-C-N   | 5.62  | 127.62      | 121.83   |
| 12  | E     | 125 | GLU  | N-CA-C  | -5.62 | 105.11      | 112.41   |
| 15  | H     | 282 | LYS  | CB-CA-C | -5.62 | 102.06      | 110.88   |
| 21  | N     | 293 | LEU  | CA-C-N  | 5.62  | 125.72      | 119.32   |
| 21  | N     | 293 | LEU  | C-N-CA  | 5.62  | 125.72      | 119.32   |
| 28  | U     | 164 | GLU  | CA-C-N  | 5.62  | 128.58      | 120.38   |
| 28  | U     | 164 | GLU  | C-N-CA  | 5.62  | 128.58      | 120.38   |
| 15  | H     | 363 | PRO  | CA-C-N  | 5.62  | 127.81      | 120.28   |
| 15  | H     | 363 | PRO  | C-N-CA  | 5.62  | 127.81      | 120.28   |
| 23  | P     | 248 | ASP  | CA-C-N  | 5.62  | 127.74      | 120.44   |
| 23  | P     | 248 | ASP  | C-N-CA  | 5.62  | 127.74      | 120.44   |
| 20  | M     | 193 | LEU  | N-CA-C  | 5.62  | 117.08      | 111.07   |
| 26  | S     | 408 | CYS  | CA-C-N  | 5.62  | 127.74      | 120.44   |
| 26  | S     | 408 | CYS  | C-N-CA  | 5.62  | 127.74      | 120.44   |
| 16  | I     | 278 | ILE  | CA-C-O  | 5.61  | 126.58      | 120.57   |
| 19  | L     | 339 | ARG  | CA-C-N  | 5.61  | 126.86      | 119.84   |
| 19  | L     | 339 | ARG  | C-N-CA  | 5.61  | 126.86      | 119.84   |
| 11  | D     | 184 | PRO  | CA-C-O  | -5.61 | 112.42      | 120.56   |
| 28  | U     | 155 | LEU  | CA-C-N  | 5.61  | 128.68      | 120.71   |
| 28  | U     | 155 | LEU  | C-N-CA  | 5.61  | 128.68      | 120.71   |
| 17  | J     | 48  | ARG  | CA-C-O  | -5.61 | 114.60      | 120.55   |
| 22  | O     | 104 | ALA  | CA-C-N  | 5.61  | 130.54      | 122.35   |
| 22  | O     | 104 | ALA  | C-N-CA  | 5.61  | 130.54      | 122.35   |
| 25  | R     | 56  | GLU  | CA-C-N  | 5.61  | 133.10      | 121.32   |
| 25  | R     | 56  | GLU  | C-N-CA  | 5.61  | 133.10      | 121.32   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 31  | X     | 130 | ASN  | CA-C-N | 5.61  | 129.67      | 121.31   |
| 31  | X     | 130 | ASN  | C-N-CA | 5.61  | 129.67      | 121.31   |
| 21  | N     | 67  | LYS  | CA-C-N | 5.61  | 127.74      | 120.56   |
| 21  | N     | 67  | LYS  | C-N-CA | 5.61  | 127.74      | 120.56   |
| 21  | N     | 353 | LEU  | O-C-N  | -5.61 | 114.87      | 121.32   |
| 28  | U     | 12  | PRO  | CA-C-N | 5.61  | 127.79      | 120.28   |
| 28  | U     | 12  | PRO  | C-N-CA | 5.61  | 127.79      | 120.28   |
| 28  | U     | 140 | ILE  | N-CA-C | -5.61 | 100.52      | 108.65   |
| 20  | M     | 171 | GLU  | N-CA-C | -5.61 | 100.57      | 109.76   |
| 21  | N     | 689 | LYS  | N-CA-C | -5.61 | 105.04      | 112.94   |
| 33  | Z     | 92  | LEU  | CA-C-O | -5.61 | 114.61      | 120.55   |
| 2   | 2     | 60  | GLY  | N-CA-C | -5.60 | 106.00      | 112.73   |
| 1   | 1     | 38  | HIS  | N-CA-C | -5.60 | 100.22      | 108.79   |
| 18  | K     | 297 | ILE  | O-C-N  | -5.60 | 116.08      | 121.90   |
| 3   | 3     | 165 | ALA  | CA-C-N | 5.60  | 127.78      | 120.28   |
| 3   | 3     | 165 | ALA  | C-N-CA | 5.60  | 127.78      | 120.28   |
| 21  | N     | 141 | ILE  | CA-C-O | -5.60 | 115.24      | 121.17   |
| 24  | Q     | 23  | ALA  | CA-C-N | 5.60  | 127.78      | 120.28   |
| 24  | Q     | 23  | ALA  | C-N-CA | 5.60  | 127.78      | 120.28   |
| 13  | F     | 79  | PRO  | CA-C-N | 5.60  | 128.24      | 120.29   |
| 13  | F     | 79  | PRO  | C-N-CA | 5.60  | 128.24      | 120.29   |
| 3   | 3     | 102 | GLY  | O-C-N  | -5.59 | 117.12      | 123.61   |
| 6   | 6     | 9   | GLU  | CA-C-O | -5.59 | 113.69      | 119.51   |
| 19  | L     | 359 | GLU  | CA-C-N | 5.59  | 128.12      | 120.46   |
| 19  | L     | 359 | GLU  | C-N-CA | 5.59  | 128.12      | 120.46   |
| 24  | Q     | 295 | GLY  | CA-C-N | 5.59  | 128.36      | 120.42   |
| 24  | Q     | 295 | GLY  | C-N-CA | 5.59  | 128.36      | 120.42   |
| 29  | V     | 258 | GLU  | CA-C-N | 5.59  | 127.77      | 120.28   |
| 29  | V     | 258 | GLU  | C-N-CA | 5.59  | 127.77      | 120.28   |
| 18  | K     | 224 | LYS  | CA-C-N | 5.59  | 128.23      | 120.29   |
| 18  | K     | 224 | LYS  | C-N-CA | 5.59  | 128.23      | 120.29   |
| 18  | K     | 241 | GLU  | CA-C-N | 5.59  | 130.92      | 121.14   |
| 18  | K     | 241 | GLU  | C-N-CA | 5.59  | 130.92      | 121.14   |
| 9   | B     | 169 | VAL  | CA-C-N | 5.58  | 128.22      | 120.29   |
| 9   | B     | 169 | VAL  | C-N-CA | 5.58  | 128.22      | 120.29   |
| 7   | 7     | 21  | SER  | CA-C-N | 5.58  | 130.51      | 123.03   |
| 7   | 7     | 21  | SER  | C-N-CA | 5.58  | 130.51      | 123.03   |
| 18  | K     | 245 | LYS  | O-C-N  | 5.58  | 129.39      | 122.19   |
| 27  | T     | 186 | ARG  | CA-C-N | 5.58  | 127.76      | 120.28   |
| 27  | T     | 186 | ARG  | C-N-CA | 5.58  | 127.76      | 120.28   |
| 18  | K     | 232 | ALA  | N-CA-C | -5.58 | 101.49      | 110.14   |
| 21  | N     | 449 | GLY  | CA-C-N | 5.58  | 128.35      | 120.42   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 449 | GLY  | C-N-CA | 5.58  | 128.35      | 120.42   |
| 25  | R     | 269 | LYS  | N-CA-C | -5.58 | 107.72      | 114.75   |
| 18  | K     | 318 | THR  | O-C-N  | -5.58 | 117.03      | 123.33   |
| 26  | S     | 142 | VAL  | N-CA-C | 5.58  | 115.78      | 110.42   |
| 1   | 1     | 21  | THR  | N-CA-C | -5.58 | 100.59      | 109.23   |
| 8   | A     | 11  | GLY  | N-CA-C | -5.58 | 107.55      | 115.30   |
| 17  | J     | 260 | GLY  | O-C-N  | -5.57 | 117.96      | 122.64   |
| 20  | M     | 421 | GLU  | CA-C-N | 5.57  | 130.03      | 122.90   |
| 20  | M     | 421 | GLU  | C-N-CA | 5.57  | 130.03      | 122.90   |
| 25  | R     | 351 | LYS  | CA-C-N | 5.57  | 127.75      | 120.28   |
| 25  | R     | 351 | LYS  | C-N-CA | 5.57  | 127.75      | 120.28   |
| 11  | D     | 175 | LEU  | N-CA-C | 5.57  | 117.35      | 111.28   |
| 14  | G     | 22  | GLN  | N-CA-C | 5.57  | 118.11      | 111.71   |
| 29  | V     | 83  | VAL  | O-C-N  | -5.57 | 115.87      | 122.77   |
| 10  | C     | 38  | ILE  | N-CA-C | -5.57 | 100.11      | 108.12   |
| 18  | K     | 160 | VAL  | CA-C-O | -5.57 | 113.82      | 120.78   |
| 27  | T     | 86  | LYS  | N-CA-C | 5.57  | 121.06      | 113.16   |
| 21  | N     | 645 | THR  | CA-C-N | 5.56  | 131.69      | 122.73   |
| 21  | N     | 645 | THR  | C-N-CA | 5.56  | 131.69      | 122.73   |
| 10  | C     | 14  | SER  | CA-C-N | 5.56  | 125.18      | 119.56   |
| 10  | C     | 14  | SER  | C-N-CA | 5.56  | 125.18      | 119.56   |
| 10  | C     | 20  | TYR  | CA-C-N | 5.56  | 128.29      | 120.28   |
| 10  | C     | 20  | TYR  | C-N-CA | 5.56  | 128.29      | 120.28   |
| 26  | S     | 216 | LYS  | CA-C-N | 5.56  | 127.73      | 120.28   |
| 26  | S     | 216 | LYS  | C-N-CA | 5.56  | 127.73      | 120.28   |
| 31  | X     | 31  | GLY  | N-CA-C | -5.56 | 103.12      | 110.74   |
| 6   | 6     | 117 | ASP  | CA-C-N | 5.56  | 125.40      | 119.28   |
| 6   | 6     | 117 | ASP  | C-N-CA | 5.56  | 125.40      | 119.28   |
| 6   | 6     | 152 | GLU  | N-CA-C | -5.56 | 102.64      | 109.65   |
| 9   | B     | 105 | PRO  | CA-C-O | -5.56 | 112.50      | 120.56   |
| 16  | I     | 90  | GLU  | CA-C-O | -5.56 | 114.98      | 120.82   |
| 33  | Z     | 67  | SER  | N-CA-C | 5.56  | 117.14      | 111.14   |
| 15  | H     | 320 | ASP  | CA-C-N | 5.56  | 130.07      | 122.34   |
| 15  | H     | 320 | ASP  | C-N-CA | 5.56  | 130.07      | 122.34   |
| 20  | M     | 272 | GLU  | N-CA-C | 5.56  | 117.34      | 111.28   |
| 27  | T     | 210 | PHE  | CA-C-N | 5.56  | 132.86      | 122.74   |
| 27  | T     | 210 | PHE  | C-N-CA | 5.56  | 132.86      | 122.74   |
| 10  | C     | 196 | THR  | N-CA-C | 5.56  | 117.34      | 111.28   |
| 22  | O     | 261 | GLY  | N-CA-C | -5.56 | 105.97      | 115.08   |
| 26  | S     | 238 | LEU  | CA-C-N | 5.56  | 127.67      | 120.44   |
| 26  | S     | 238 | LEU  | C-N-CA | 5.56  | 127.67      | 120.44   |
| 30  | W     | 129 | ALA  | O-C-N  | -5.56 | 116.23      | 122.12   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | W     | 163 | ASN  | CB-CA-C | 5.56  | 118.58      | 109.97   |
| 33  | Z     | 874 | ASN  | CA-C-N  | 5.56  | 128.18      | 120.29   |
| 33  | Z     | 874 | ASN  | C-N-CA  | 5.56  | 128.18      | 120.29   |
| 24  | Q     | 118 | CYS  | CA-C-O  | 5.56  | 126.44      | 120.55   |
| 7   | 7     | 29  | ASN  | O-C-N   | -5.55 | 115.79      | 123.12   |
| 9   | B     | 99  | ARG  | N-CA-C  | -5.55 | 106.40      | 114.12   |
| 21  | N     | 315 | ASN  | CA-C-N  | 5.55  | 128.18      | 120.29   |
| 21  | N     | 315 | ASN  | C-N-CA  | 5.55  | 128.18      | 120.29   |
| 25  | R     | 403 | LEU  | CA-C-N  | 5.55  | 128.07      | 120.46   |
| 25  | R     | 403 | LEU  | C-N-CA  | 5.55  | 128.07      | 120.46   |
| 28  | U     | 189 | ARG  | O-C-N   | 5.55  | 127.79      | 122.07   |
| 29  | V     | 111 | HIS  | CA-C-O  | -5.55 | 113.77      | 119.49   |
| 7   | 7     | 163 | GLN  | CA-C-N  | 5.55  | 127.56      | 120.56   |
| 7   | 7     | 163 | GLN  | C-N-CA  | 5.55  | 127.56      | 120.56   |
| 17  | J     | 238 | ARG  | O-C-N   | 5.55  | 128.48      | 122.15   |
| 21  | N     | 687 | THR  | N-CA-C  | -5.55 | 105.31      | 111.36   |
| 26  | S     | 253 | PHE  | CA-C-N  | 5.55  | 128.30      | 120.42   |
| 26  | S     | 253 | PHE  | C-N-CA  | 5.55  | 128.30      | 120.42   |
| 27  | T     | 133 | ILE  | N-CA-C  | 5.55  | 115.75      | 110.53   |
| 4   | 4     | 142 | LEU  | N-CA-C  | -5.55 | 104.63      | 111.40   |
| 15  | H     | 55  | ASP  | O-C-N   | -5.55 | 116.24      | 122.12   |
| 16  | I     | 168 | VAL  | N-CA-C  | -5.55 | 99.81       | 108.86   |
| 11  | D     | 173 | GLU  | CA-C-N  | 5.55  | 127.65      | 120.44   |
| 11  | D     | 173 | GLU  | C-N-CA  | 5.55  | 127.65      | 120.44   |
| 13  | F     | 17  | GLY  | CA-C-O  | 5.55  | 123.98      | 118.77   |
| 23  | P     | 346 | ILE  | CA-C-N  | 5.55  | 127.71      | 120.28   |
| 23  | P     | 346 | ILE  | C-N-CA  | 5.55  | 127.71      | 120.28   |
| 27  | T     | 26  | LEU  | CA-C-O  | -5.55 | 113.83      | 120.10   |
| 27  | T     | 75  | PHE  | CA-C-N  | 5.55  | 127.71      | 120.28   |
| 27  | T     | 75  | PHE  | C-N-CA  | 5.55  | 127.71      | 120.28   |
| 11  | D     | 79  | ASN  | CA-C-N  | 5.54  | 127.65      | 120.44   |
| 11  | D     | 79  | ASN  | C-N-CA  | 5.54  | 127.65      | 120.44   |
| 16  | I     | 131 | SER  | N-CA-C  | -5.54 | 101.50      | 110.32   |
| 15  | H     | 55  | ASP  | CA-C-N  | 5.54  | 127.71      | 120.28   |
| 15  | H     | 55  | ASP  | C-N-CA  | 5.54  | 127.71      | 120.28   |
| 16  | I     | 263 | LEU  | CA-C-N  | 5.54  | 128.16      | 120.29   |
| 16  | I     | 263 | LEU  | C-N-CA  | 5.54  | 128.16      | 120.29   |
| 9   | B     | 230 | ASP  | CA-C-O  | -5.54 | 115.14      | 121.40   |
| 11  | D     | 47  | GLU  | CA-C-N  | 5.54  | 130.91      | 122.65   |
| 11  | D     | 47  | GLU  | C-N-CA  | 5.54  | 130.91      | 122.65   |
| 21  | N     | 264 | SER  | N-CA-C  | 5.54  | 117.12      | 111.14   |
| 22  | O     | 189 | TYR  | O-C-N   | -5.54 | 116.25      | 122.12   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | R     | 122 | GLU  | N-CA-C | 5.54  | 117.12      | 111.14   |
| 3   | 3     | 12  | VAL  | O-C-N  | -5.54 | 116.80      | 122.95   |
| 27  | T     | 2   | PRO  | CA-C-N | 5.54  | 128.97      | 121.05   |
| 27  | T     | 2   | PRO  | C-N-CA | 5.54  | 128.97      | 121.05   |
| 1   | 1     | 114 | PRO  | CA-C-N | 5.54  | 128.73      | 120.31   |
| 1   | 1     | 114 | PRO  | C-N-CA | 5.54  | 128.73      | 120.31   |
| 10  | C     | 151 | SER  | N-CA-C | -5.54 | 100.65      | 109.23   |
| 20  | M     | 55  | ASN  | N-CA-C | -5.54 | 105.24      | 111.28   |
| 26  | S     | 212 | SER  | O-C-N  | 5.54  | 127.78      | 122.07   |
| 21  | N     | 415 | PHE  | CA-C-O | 5.54  | 128.43      | 120.51   |
| 14  | G     | 22  | GLN  | CA-C-N | 5.54  | 129.38      | 120.30   |
| 14  | G     | 22  | GLN  | C-N-CA | 5.54  | 129.38      | 120.30   |
| 27  | T     | 89  | TYR  | O-C-N  | 5.54  | 127.77      | 122.07   |
| 18  | K     | 67  | TYR  | CA-C-N | 5.53  | 128.04      | 120.46   |
| 18  | K     | 67  | TYR  | C-N-CA | 5.53  | 128.04      | 120.46   |
| 29  | V     | 23  | THR  | CA-C-N | 5.53  | 128.57      | 120.71   |
| 29  | V     | 23  | THR  | C-N-CA | 5.53  | 128.57      | 120.71   |
| 14  | G     | 185 | GLY  | CA-C-N | 5.53  | 132.11      | 121.54   |
| 14  | G     | 185 | GLY  | C-N-CA | 5.53  | 132.11      | 121.54   |
| 21  | N     | 157 | ALA  | O-C-N  | 5.53  | 127.98      | 122.12   |
| 30  | W     | 155 | ASP  | CA-C-N | 5.53  | 128.15      | 120.29   |
| 30  | W     | 155 | ASP  | C-N-CA | 5.53  | 128.15      | 120.29   |
| 14  | G     | 238 | ALA  | CA-C-N | 5.53  | 128.04      | 120.46   |
| 14  | G     | 238 | ALA  | C-N-CA | 5.53  | 128.04      | 120.46   |
| 16  | I     | 186 | GLY  | CA-C-N | 5.53  | 131.46      | 122.67   |
| 16  | I     | 186 | GLY  | C-N-CA | 5.53  | 131.46      | 122.67   |
| 22  | O     | 33  | TYR  | CA-C-O | 5.53  | 126.40      | 120.70   |
| 17  | J     | 266 | SER  | CA-C-N | 5.53  | 127.69      | 120.28   |
| 17  | J     | 266 | SER  | C-N-CA | 5.53  | 127.69      | 120.28   |
| 17  | J     | 103 | ASN  | N-CA-C | -5.53 | 100.41      | 109.80   |
| 22  | O     | 364 | THR  | CA-C-N | 5.53  | 127.69      | 120.28   |
| 22  | O     | 364 | THR  | C-N-CA | 5.53  | 127.69      | 120.28   |
| 26  | S     | 232 | MET  | CA-C-O | 5.53  | 126.35      | 120.10   |
| 31  | X     | 17  | TYR  | CA-C-N | 5.53  | 129.20      | 121.02   |
| 31  | X     | 17  | TYR  | C-N-CA | 5.53  | 129.20      | 121.02   |
| 12  | E     | 36  | THR  | O-C-N  | 5.53  | 129.69      | 123.06   |
| 33  | Z     | 386 | VAL  | CA-C-N | 5.53  | 128.00      | 120.54   |
| 33  | Z     | 386 | VAL  | C-N-CA | 5.53  | 128.00      | 120.54   |
| 33  | Z     | 417 | SER  | N-CA-C | 5.53  | 116.98      | 111.07   |
| 33  | Z     | 841 | GLU  | CA-C-N | 5.53  | 128.71      | 120.31   |
| 33  | Z     | 841 | GLU  | C-N-CA | 5.53  | 128.71      | 120.31   |
| 2   | 2     | 87  | LEU  | CA-C-N | 5.52  | 127.62      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | 2     | 87  | LEU  | C-N-CA | 5.52  | 127.62      | 120.44   |
| 3   | 3     | 90  | ARG  | O-C-N  | 5.52  | 129.41      | 122.23   |
| 17  | J     | 105 | LYS  | CA-C-N | 5.52  | 131.65      | 122.54   |
| 17  | J     | 105 | LYS  | C-N-CA | 5.52  | 131.65      | 122.54   |
| 18  | K     | 402 | ILE  | N-CA-C | -5.52 | 97.94       | 106.72   |
| 21  | N     | 182 | ASN  | O-C-N  | -5.52 | 116.27      | 122.12   |
| 21  | N     | 539 | MET  | CA-C-N | 5.52  | 128.70      | 120.31   |
| 21  | N     | 539 | MET  | C-N-CA | 5.52  | 128.70      | 120.31   |
| 22  | O     | 231 | GLY  | CA-C-N | 5.52  | 128.13      | 120.29   |
| 22  | O     | 231 | GLY  | C-N-CA | 5.52  | 128.13      | 120.29   |
| 33  | Z     | 898 | HIS  | N-CA-C | -5.52 | 105.41      | 111.82   |
| 24  | Q     | 93  | THR  | CA-C-O | -5.52 | 114.57      | 120.42   |
| 25  | R     | 139 | GLU  | CA-C-N | 5.52  | 129.10      | 120.82   |
| 25  | R     | 139 | GLU  | C-N-CA | 5.52  | 129.10      | 120.82   |
| 3   | 3     | 27  | VAL  | CA-C-O | -5.52 | 115.11      | 120.30   |
| 22  | O     | 270 | ILE  | O-C-N  | 5.52  | 129.23      | 122.72   |
| 7   | 7     | 192 | ILE  | CA-C-N | 5.52  | 130.87      | 122.65   |
| 7   | 7     | 192 | ILE  | C-N-CA | 5.52  | 130.87      | 122.65   |
| 17  | J     | 361 | VAL  | CA-C-N | 5.52  | 128.12      | 120.29   |
| 17  | J     | 361 | VAL  | C-N-CA | 5.52  | 128.12      | 120.29   |
| 23  | P     | 36  | LEU  | CA-C-N | 5.52  | 127.61      | 120.44   |
| 23  | P     | 36  | LEU  | C-N-CA | 5.52  | 127.61      | 120.44   |
| 33  | Z     | 434 | GLN  | CA-C-N | 5.52  | 127.67      | 120.28   |
| 33  | Z     | 434 | GLN  | C-N-CA | 5.52  | 127.67      | 120.28   |
| 4   | 4     | 44  | SER  | N-CA-C | -5.51 | 101.87      | 110.42   |
| 13  | F     | 163 | ALA  | CA-C-O | -5.51 | 114.63      | 120.92   |
| 14  | G     | 129 | ARG  | CA-C-O | -5.51 | 114.85      | 119.76   |
| 21  | N     | 447 | SER  | N-CA-C | 5.51  | 118.47      | 111.69   |
| 27  | T     | 70  | ILE  | CA-C-N | 5.51  | 127.67      | 120.28   |
| 27  | T     | 70  | ILE  | C-N-CA | 5.51  | 127.67      | 120.28   |
| 25  | R     | 126 | GLY  | CA-C-N | 5.51  | 130.59      | 121.99   |
| 25  | R     | 126 | GLY  | C-N-CA | 5.51  | 130.59      | 121.99   |
| 29  | V     | 143 | PRO  | N-CA-C | -5.51 | 106.93      | 114.98   |
| 21  | N     | 347 | SER  | O-C-N  | 5.51  | 127.96      | 122.12   |
| 25  | R     | 100 | ASN  | N-CA-C | -5.51 | 105.85      | 113.18   |
| 33  | Z     | 149 | TRP  | N-CA-C | -5.51 | 105.28      | 112.23   |
| 2   | 2     | 186 | TYR  | CA-C-O | 5.51  | 126.88      | 120.49   |
| 26  | S     | 416 | GLU  | N-CA-C | -5.51 | 106.60      | 113.38   |
| 27  | T     | 156 | SER  | N-CA-C | -5.51 | 101.29      | 109.11   |
| 2   | 2     | 107 | GLY  | CA-C-O | -5.51 | 116.97      | 121.76   |
| 3   | 3     | 90  | ARG  | CA-C-O | -5.51 | 114.13      | 120.24   |
| 5   | 5     | 120 | THR  | CA-C-O | -5.51 | 114.64      | 120.92   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 18  | K     | 370 | SER  | CA-C-N | 5.51  | 127.66      | 120.28   |
| 18  | K     | 370 | SER  | C-N-CA | 5.51  | 127.66      | 120.28   |
| 27  | T     | 127 | GLN  | N-CA-C | 5.51  | 117.36      | 111.36   |
| 33  | Z     | 383 | SER  | CA-C-N | 5.51  | 127.66      | 120.28   |
| 33  | Z     | 383 | SER  | C-N-CA | 5.51  | 127.66      | 120.28   |
| 1   | 1     | 79  | ALA  | CA-C-N | 5.51  | 127.66      | 120.28   |
| 1   | 1     | 79  | ALA  | C-N-CA | 5.51  | 127.66      | 120.28   |
| 5   | 5     | 163 | ALA  | CA-C-N | 5.51  | 128.11      | 120.29   |
| 5   | 5     | 163 | ALA  | C-N-CA | 5.51  | 128.11      | 120.29   |
| 17  | J     | 390 | MET  | CA-C-N | 5.51  | 127.66      | 120.28   |
| 17  | J     | 390 | MET  | C-N-CA | 5.51  | 127.66      | 120.28   |
| 25  | R     | 387 | ILE  | CA-C-O | 5.51  | 126.82      | 120.76   |
| 16  | I     | 145 | CYS  | CA-C-O | 5.50  | 127.56      | 121.56   |
| 17  | J     | 309 | ARG  | N-CA-C | -5.50 | 99.08       | 110.80   |
| 30  | W     | 184 | ASN  | CA-C-N | 5.50  | 128.00      | 120.46   |
| 30  | W     | 184 | ASN  | C-N-CA | 5.50  | 128.00      | 120.46   |
| 21  | N     | 655 | ALA  | CA-C-N | 5.50  | 128.10      | 120.29   |
| 21  | N     | 655 | ALA  | C-N-CA | 5.50  | 128.10      | 120.29   |
| 23  | P     | 391 | ALA  | N-CA-C | -5.50 | 100.71      | 109.07   |
| 22  | O     | 265 | LYS  | N-CA-C | -5.50 | 105.36      | 111.36   |
| 10  | C     | 136 | ILE  | O-C-N  | 5.50  | 129.03      | 123.20   |
| 14  | G     | 128 | VAL  | CA-C-O | -5.50 | 114.44      | 120.43   |
| 17  | J     | 40  | ASN  | CA-C-O | -5.50 | 115.05      | 120.82   |
| 21  | N     | 661 | SER  | N-CA-C | 5.50  | 118.20      | 111.82   |
| 25  | R     | 176 | ARG  | N-CA-C | -5.50 | 104.98      | 110.97   |
| 19  | L     | 246 | SER  | N-CA-C | -5.49 | 100.61      | 109.40   |
| 26  | S     | 476 | LEU  | CA-C-O | -5.49 | 115.05      | 120.82   |
| 17  | J     | 129 | LYS  | O-C-N  | -5.49 | 116.47      | 123.06   |
| 20  | M     | 208 | LYS  | CA-C-N | 5.49  | 128.09      | 120.29   |
| 20  | M     | 208 | LYS  | C-N-CA | 5.49  | 128.09      | 120.29   |
| 33  | Z     | 221 | VAL  | O-C-N  | 5.49  | 127.48      | 121.83   |
| 14  | G     | 168 | ARG  | O-C-N  | -5.49 | 116.30      | 122.12   |
| 16  | I     | 397 | THR  | N-CA-C | 5.49  | 117.34      | 111.36   |
| 23  | P     | 106 | SER  | CA-C-O | -5.49 | 115.06      | 120.82   |
| 33  | Z     | 350 | GLY  | CA-C-N | 5.49  | 125.80      | 119.93   |
| 33  | Z     | 350 | GLY  | C-N-CA | 5.49  | 125.80      | 119.93   |
| 5   | 5     | 76  | VAL  | CA-C-O | 5.49  | 126.44      | 120.57   |
| 6   | 6     | 9   | GLU  | N-CA-C | -5.49 | 104.26      | 112.54   |
| 11  | D     | 188 | VAL  | N-CA-C | -5.49 | 105.03      | 110.62   |
| 20  | M     | 295 | LYS  | CA-C-N | 5.48  | 129.04      | 120.82   |
| 20  | M     | 295 | LYS  | C-N-CA | 5.48  | 129.04      | 120.82   |
| 21  | N     | 214 | LEU  | N-CA-C | -5.48 | 105.46      | 111.82   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 29  | V     | 289 | GLU  | CA-C-N | 5.48  | 127.62      | 120.28   |
| 29  | V     | 289 | GLU  | C-N-CA | 5.48  | 127.62      | 120.28   |
| 7   | 7     | 12  | VAL  | N-CA-C | -5.48 | 99.81       | 108.90   |
| 9   | B     | 88  | LYS  | CA-C-N | 5.48  | 128.07      | 120.29   |
| 9   | B     | 88  | LYS  | C-N-CA | 5.48  | 128.07      | 120.29   |
| 18  | K     | 141 | ARG  | O-C-N  | 5.48  | 128.40      | 122.15   |
| 25  | R     | 59  | MET  | CA-C-N | 5.48  | 126.94      | 120.09   |
| 25  | R     | 59  | MET  | C-N-CA | 5.48  | 126.94      | 120.09   |
| 26  | S     | 380 | CYS  | CA-C-N | 5.48  | 127.57      | 120.56   |
| 26  | S     | 380 | CYS  | C-N-CA | 5.48  | 127.57      | 120.56   |
| 8   | A     | 26  | TYR  | CA-C-O | -5.47 | 114.75      | 120.55   |
| 33  | Z     | 229 | SER  | N-CA-C | 5.47  | 118.17      | 110.23   |
| 4   | 4     | 86  | GLU  | CA-C-N | 5.47  | 127.61      | 120.28   |
| 4   | 4     | 86  | GLU  | C-N-CA | 5.47  | 127.61      | 120.28   |
| 6   | 6     | 188 | GLN  | N-CA-C | -5.47 | 106.65      | 113.38   |
| 14  | G     | 192 | VAL  | CA-C-O | -5.47 | 115.26      | 120.95   |
| 21  | N     | 105 | SER  | CA-C-N | 5.47  | 127.46      | 120.56   |
| 21  | N     | 105 | SER  | C-N-CA | 5.47  | 127.46      | 120.56   |
| 21  | N     | 350 | LYS  | CA-C-N | 5.47  | 127.88      | 120.44   |
| 21  | N     | 350 | LYS  | C-N-CA | 5.47  | 127.88      | 120.44   |
| 22  | O     | 171 | PHE  | CA-C-N | 5.47  | 127.55      | 120.44   |
| 22  | O     | 171 | PHE  | C-N-CA | 5.47  | 127.55      | 120.44   |
| 18  | K     | 76  | LYS  | CA-C-O | -5.47 | 114.62      | 120.42   |
| 18  | K     | 322 | ASP  | CA-C-N | 5.47  | 128.60      | 120.17   |
| 18  | K     | 322 | ASP  | C-N-CA | 5.47  | 128.60      | 120.17   |
| 33  | Z     | 83  | THR  | CA-C-N | 5.47  | 127.61      | 120.28   |
| 33  | Z     | 83  | THR  | C-N-CA | 5.47  | 127.61      | 120.28   |
| 33  | Z     | 147 | GLU  | O-C-N  | -5.47 | 117.35      | 123.48   |
| 4   | 4     | 61  | ALA  | O-C-N  | -5.47 | 116.44      | 122.07   |
| 4   | 4     | 179 | ILE  | O-C-N  | -5.47 | 117.44      | 123.18   |
| 7   | 7     | 172 | ALA  | N-CA-C | 5.47  | 116.92      | 111.07   |
| 19  | L     | 317 | ASN  | CA-C-O | 5.47  | 126.14      | 120.40   |
| 18  | K     | 71  | GLU  | N-CA-C | 5.47  | 117.24      | 111.28   |
| 9   | B     | 190 | HIS  | N-CA-C | -5.47 | 105.32      | 111.28   |
| 18  | K     | 315 | ILE  | O-C-N  | -5.47 | 117.17      | 123.07   |
| 1   | 1     | 83  | LYS  | CA-C-N | 5.46  | 127.92      | 120.54   |
| 1   | 1     | 83  | LYS  | C-N-CA | 5.46  | 127.92      | 120.54   |
| 6   | 6     | 29  | ARG  | N-CA-C | -5.46 | 105.98      | 113.30   |
| 20  | M     | 371 | ASP  | CA-C-N | 5.46  | 131.98      | 121.54   |
| 20  | M     | 371 | ASP  | C-N-CA | 5.46  | 131.98      | 121.54   |
| 21  | N     | 292 | GLY  | N-CA-C | -5.46 | 107.56      | 115.27   |
| 23  | P     | 243 | GLU  | O-C-N  | -5.46 | 115.92      | 122.15   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 26  | S     | 472 | HIS  | CA-C-O | -5.46 | 114.76      | 120.55   |
| 7   | 7     | 125 | LEU  | N-CA-C | -5.46 | 106.46      | 113.23   |
| 22  | O     | 309 | SER  | CA-C-N | 5.46  | 127.60      | 120.28   |
| 22  | O     | 309 | SER  | C-N-CA | 5.46  | 127.60      | 120.28   |
| 28  | U     | 262 | GLN  | N-CA-C | 5.46  | 119.05      | 112.38   |
| 14  | G     | 190 | GLU  | N-CA-C | 5.46  | 117.23      | 111.28   |
| 33  | Z     | 153 | TYR  | N-CA-C | 5.46  | 117.66      | 111.11   |
| 8   | A     | 116 | VAL  | CA-C-N | 5.46  | 127.60      | 120.28   |
| 8   | A     | 116 | VAL  | C-N-CA | 5.46  | 127.60      | 120.28   |
| 14  | G     | 239 | ILE  | CA-C-N | 5.46  | 127.54      | 120.44   |
| 14  | G     | 239 | ILE  | C-N-CA | 5.46  | 127.54      | 120.44   |
| 11  | D     | 89  | ALA  | CA-C-N | 5.46  | 127.59      | 120.28   |
| 11  | D     | 89  | ALA  | C-N-CA | 5.46  | 127.59      | 120.28   |
| 18  | K     | 183 | GLU  | O-C-N  | 5.46  | 127.69      | 122.07   |
| 21  | N     | 140 | MET  | CA-C-N | 5.46  | 127.44      | 120.56   |
| 21  | N     | 140 | MET  | C-N-CA | 5.46  | 127.44      | 120.56   |
| 23  | P     | 217 | LYS  | N-CA-C | 5.46  | 117.23      | 111.28   |
| 26  | S     | 375 | ASP  | O-C-N  | 5.46  | 129.85      | 122.59   |
| 5   | 5     | 33  | ARG  | N-CA-C | -5.46 | 104.88      | 112.03   |
| 5   | 5     | 195 | GLU  | CA-C-N | 5.46  | 128.14      | 120.28   |
| 5   | 5     | 195 | GLU  | C-N-CA | 5.46  | 128.14      | 120.28   |
| 6   | 6     | 140 | PHE  | CA-C-O | 5.46  | 126.20      | 120.42   |
| 21  | N     | 289 | ILE  | CA-C-N | 5.46  | 131.96      | 121.54   |
| 21  | N     | 289 | ILE  | C-N-CA | 5.46  | 131.96      | 121.54   |
| 24  | Q     | 362 | ILE  | N-CA-C | -5.46 | 105.06      | 110.62   |
| 3   | 3     | 20  | LEU  | CA-C-N | -5.45 | 117.24      | 121.82   |
| 3   | 3     | 20  | LEU  | C-N-CA | -5.45 | 117.24      | 121.82   |
| 15  | H     | 299 | ARG  | CA-C-O | -5.45 | 114.64      | 120.42   |
| 17  | J     | 133 | LEU  | CA-C-N | 5.45  | 131.79      | 121.97   |
| 17  | J     | 133 | LEU  | C-N-CA | 5.45  | 131.79      | 121.97   |
| 30  | W     | 180 | LEU  | CA-C-O | 5.45  | 126.40      | 120.95   |
| 33  | Z     | 282 | ILE  | N-CA-C | 5.45  | 116.23      | 110.72   |
| 10  | C     | 173 | GLN  | CA-C-N | 5.45  | 127.59      | 120.28   |
| 10  | C     | 173 | GLN  | C-N-CA | 5.45  | 127.59      | 120.28   |
| 13  | F     | 73  | SER  | CA-C-O | -5.45 | 114.95      | 121.11   |
| 16  | I     | 354 | ASP  | CA-C-N | 5.45  | 127.59      | 120.28   |
| 16  | I     | 354 | ASP  | C-N-CA | 5.45  | 127.59      | 120.28   |
| 21  | N     | 168 | SER  | O-C-N  | -5.45 | 116.45      | 122.07   |
| 29  | V     | 203 | TYR  | CA-C-N | -5.45 | 114.76      | 122.94   |
| 29  | V     | 203 | TYR  | C-N-CA | -5.45 | 114.76      | 122.94   |
| 16  | I     | 231 | LEU  | CA-C-N | 5.45  | 127.58      | 120.28   |
| 16  | I     | 231 | LEU  | C-N-CA | 5.45  | 127.58      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 23  | P     | 217 | LYS  | CA-C-N | 5.45  | 128.03      | 120.29   |
| 23  | P     | 217 | LYS  | C-N-CA | 5.45  | 128.03      | 120.29   |
| 11  | D     | 169 | LYS  | CA-C-N | 5.45  | 127.85      | 120.44   |
| 11  | D     | 169 | LYS  | C-N-CA | 5.45  | 127.85      | 120.44   |
| 15  | H     | 162 | ARG  | CA-C-O | 5.45  | 126.93      | 120.66   |
| 19  | L     | 267 | PHE  | N-CA-C | -5.45 | 105.42      | 111.36   |
| 24  | Q     | 379 | GLN  | CA-C-N | 5.45  | 127.52      | 120.44   |
| 24  | Q     | 379 | GLN  | C-N-CA | 5.45  | 127.52      | 120.44   |
| 33  | Z     | 802 | ASP  | N-CA-C | -5.45 | 102.13      | 110.14   |
| 4   | 4     | 195 | GLN  | CA-C-O | 5.45  | 126.06      | 119.31   |
| 19  | L     | 216 | LYS  | N-CA-C | -5.45 | 107.89      | 114.75   |
| 7   | 7     | 45  | ILE  | CA-C-O | -5.44 | 114.59      | 120.36   |
| 17  | J     | 283 | GLU  | CA-C-O | -5.44 | 113.23      | 119.60   |
| 7   | 7     | 78  | ALA  | CA-C-N | 5.44  | 130.58      | 122.74   |
| 7   | 7     | 78  | ALA  | C-N-CA | 5.44  | 130.58      | 122.74   |
| 13  | F     | 106 | GLU  | CA-C-N | 5.44  | 128.02      | 120.29   |
| 13  | F     | 106 | GLU  | C-N-CA | 5.44  | 128.02      | 120.29   |
| 19  | L     | 329 | ARG  | O-C-N  | 5.44  | 127.61      | 122.06   |
| 21  | N     | 423 | LEU  | CA-C-N | 5.44  | 128.32      | 120.38   |
| 21  | N     | 423 | LEU  | C-N-CA | 5.44  | 128.32      | 120.38   |
| 23  | P     | 400 | VAL  | CA-C-O | 5.44  | 126.05      | 120.39   |
| 25  | R     | 302 | ALA  | CA-C-N | 5.44  | 131.72      | 122.36   |
| 25  | R     | 302 | ALA  | C-N-CA | 5.44  | 131.72      | 122.36   |
| 11  | D     | 197 | ARG  | CA-C-O | 5.44  | 126.32      | 120.55   |
| 14  | G     | 178 | LEU  | CA-C-N | 5.44  | 127.91      | 120.46   |
| 14  | G     | 178 | LEU  | C-N-CA | 5.44  | 127.91      | 120.46   |
| 26  | S     | 307 | LEU  | CA-C-N | 5.44  | 127.13      | 120.22   |
| 26  | S     | 307 | LEU  | C-N-CA | 5.44  | 127.13      | 120.22   |
| 33  | Z     | 482 | ASP  | N-CA-C | -5.44 | 99.21       | 110.80   |
| 3   | 3     | 90  | ARG  | N-CA-C | -5.44 | 105.00      | 111.69   |
| 6   | 6     | 67  | HIS  | CA-C-O | -5.44 | 115.11      | 120.82   |
| 24  | Q     | 71  | LYS  | CA-C-N | 5.44  | 128.01      | 120.29   |
| 24  | Q     | 71  | LYS  | C-N-CA | 5.44  | 128.01      | 120.29   |
| 19  | L     | 264 | ARG  | N-CA-C | 5.44  | 116.89      | 111.07   |
| 33  | Z     | 304 | PRO  | CA-C-N | 5.44  | 127.41      | 120.56   |
| 33  | Z     | 304 | PRO  | C-N-CA | 5.44  | 127.41      | 120.56   |
| 33  | Z     | 427 | GLN  | N-CA-C | 5.44  | 118.36      | 110.42   |
| 2   | 2     | 10  | ASN  | O-C-N  | 5.43  | 127.45      | 121.85   |
| 17  | J     | 344 | ARG  | N-CA-C | 5.43  | 117.20      | 111.28   |
| 33  | Z     | 283 | ALA  | CA-C-N | 5.43  | 127.56      | 120.28   |
| 33  | Z     | 283 | ALA  | C-N-CA | 5.43  | 127.56      | 120.28   |
| 33  | Z     | 796 | LEU  | O-C-N  | -5.43 | 115.58      | 122.27   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13  | F     | 28  | ALA  | CA-C-N | 5.43  | 127.52      | 120.56   |
| 13  | F     | 28  | ALA  | C-N-CA | 5.43  | 127.52      | 120.56   |
| 33  | Z     | 741 | LEU  | CA-C-N | 5.43  | 126.93      | 120.14   |
| 33  | Z     | 741 | LEU  | C-N-CA | 5.43  | 126.93      | 120.14   |
| 5   | 5     | 12  | ILE  | O-C-N  | 5.43  | 128.91      | 123.10   |
| 8   | A     | 35  | THR  | N-CA-C | -5.43 | 99.23       | 110.80   |
| 30  | W     | 60  | ARG  | N-CA-C | -5.43 | 100.17      | 109.24   |
| 15  | H     | 217 | GLN  | CA-C-N | 5.43  | 127.90      | 120.46   |
| 15  | H     | 217 | GLN  | C-N-CA | 5.43  | 127.90      | 120.46   |
| 9   | B     | 214 | ILE  | N-CA-C | -5.43 | 98.65       | 107.28   |
| 18  | K     | 192 | LEU  | CA-C-N | 5.43  | 127.50      | 120.56   |
| 18  | K     | 192 | LEU  | C-N-CA | 5.43  | 127.50      | 120.56   |
| 21  | N     | 588 | VAL  | CA-C-N | 5.43  | 127.89      | 120.46   |
| 21  | N     | 588 | VAL  | C-N-CA | 5.43  | 127.89      | 120.46   |
| 12  | E     | 93  | ARG  | CA-C-O | -5.42 | 114.67      | 120.42   |
| 20  | M     | 411 | LYS  | CA-C-N | 5.42  | 127.55      | 120.28   |
| 20  | M     | 411 | LYS  | C-N-CA | 5.42  | 127.55      | 120.28   |
| 21  | N     | 581 | ASP  | N-CA-C | 5.42  | 117.27      | 111.36   |
| 8   | A     | 178 | ILE  | N-CA-C | -5.42 | 105.09      | 110.62   |
| 28  | U     | 78  | GLU  | O-C-N  | -5.42 | 116.37      | 122.12   |
| 31  | X     | 38  | ASN  | CA-C-N | 5.42  | 127.49      | 120.44   |
| 31  | X     | 38  | ASN  | C-N-CA | 5.42  | 127.49      | 120.44   |
| 14  | G     | 186 | LEU  | CA-C-N | 5.42  | 132.71      | 121.32   |
| 14  | G     | 186 | LEU  | C-N-CA | 5.42  | 132.71      | 121.32   |
| 20  | M     | 261 | LYS  | CA-C-N | 5.42  | 127.49      | 120.44   |
| 20  | M     | 261 | LYS  | C-N-CA | 5.42  | 127.49      | 120.44   |
| 28  | U     | 93  | TYR  | CA-C-N | 5.42  | 130.99      | 122.21   |
| 28  | U     | 93  | TYR  | C-N-CA | 5.42  | 130.99      | 122.21   |
| 5   | 5     | 3   | THR  | O-C-N  | -5.42 | 116.77      | 123.33   |
| 26  | S     | 273 | PHE  | CA-C-N | 5.42  | 127.49      | 120.44   |
| 26  | S     | 273 | PHE  | C-N-CA | 5.42  | 127.49      | 120.44   |
| 2   | 2     | 222 | ASP  | N-CA-C | -5.42 | 99.49       | 108.75   |
| 12  | E     | 110 | GLU  | N-CA-C | 5.42  | 116.87      | 111.07   |
| 22  | O     | 85  | SER  | O-C-N  | 5.42  | 127.86      | 122.12   |
| 26  | S     | 128 | ILE  | N-CA-C | 5.42  | 115.62      | 110.42   |
| 30  | W     | 141 | ILE  | N-CA-C | -5.42 | 100.58      | 108.17   |
| 3   | 3     | -4  | SER  | CA-C-O | 5.42  | 126.34      | 119.95   |
| 4   | 4     | 54  | GLN  | CA-C-O | -5.42 | 115.13      | 120.82   |
| 23  | P     | 306 | ASN  | CA-C-N | 5.42  | 130.74      | 122.29   |
| 23  | P     | 306 | ASN  | C-N-CA | 5.42  | 130.74      | 122.29   |
| 24  | Q     | 252 | HIS  | CA-C-O | 5.42  | 125.83      | 119.28   |
| 21  | N     | 511 | GLY  | CA-C-N | 5.42  | 127.54      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 511 | GLY  | C-N-CA | 5.42  | 127.54      | 120.28   |
| 6   | 6     | 59  | PHE  | CA-C-N | 5.41  | 128.08      | 120.28   |
| 6   | 6     | 59  | PHE  | C-N-CA | 5.41  | 128.08      | 120.28   |
| 8   | A     | 226 | GLY  | CA-C-O | -5.41 | 116.72      | 120.94   |
| 14  | G     | 108 | ILE  | CA-C-N | 5.41  | 125.23      | 119.28   |
| 14  | G     | 108 | ILE  | C-N-CA | 5.41  | 125.23      | 119.28   |
| 21  | N     | 443 | LEU  | O-C-N  | -5.41 | 115.18      | 122.43   |
| 22  | O     | 379 | LYS  | CA-C-N | 5.41  | 127.48      | 120.44   |
| 22  | O     | 379 | LYS  | C-N-CA | 5.41  | 127.48      | 120.44   |
| 24  | Q     | 362 | ILE  | CA-C-N | 5.41  | 127.53      | 120.28   |
| 24  | Q     | 362 | ILE  | C-N-CA | 5.41  | 127.53      | 120.28   |
| 25  | R     | 187 | VAL  | CA-C-N | 5.41  | 127.53      | 120.28   |
| 25  | R     | 187 | VAL  | C-N-CA | 5.41  | 127.53      | 120.28   |
| 30  | W     | 9   | VAL  | N-CA-C | -5.41 | 99.95       | 107.80   |
| 10  | C     | 46  | LEU  | N-CA-C | -5.41 | 99.62       | 108.76   |
| 22  | O     | 41  | LEU  | N-CA-C | -5.41 | 101.08      | 109.14   |
| 15  | H     | 362 | ASP  | CA-C-N | 5.41  | 125.23      | 119.28   |
| 15  | H     | 362 | ASP  | C-N-CA | 5.41  | 125.23      | 119.28   |
| 21  | N     | 556 | ALA  | CA-C-N | 5.41  | 129.64      | 120.88   |
| 21  | N     | 556 | ALA  | C-N-CA | 5.41  | 129.64      | 120.88   |
| 33  | Z     | 869 | ASP  | CA-C-N | 5.41  | 129.51      | 120.70   |
| 33  | Z     | 869 | ASP  | C-N-CA | 5.41  | 129.51      | 120.70   |
| 10  | C     | 204 | SER  | N-CA-C | 5.41  | 118.07      | 110.23   |
| 15  | H     | 382 | LEU  | CA-C-N | 5.41  | 127.53      | 120.28   |
| 15  | H     | 382 | LEU  | C-N-CA | 5.41  | 127.53      | 120.28   |
| 19  | L     | 240 | GLY  | N-CA-C | -5.41 | 107.81      | 115.43   |
| 23  | P     | 237 | VAL  | CA-C-O | -5.41 | 115.33      | 120.95   |
| 33  | Z     | 542 | ILE  | CA-C-O | 5.41  | 126.90      | 121.17   |
| 33  | Z     | 604 | GLY  | O-C-N  | 5.41  | 127.44      | 122.19   |
| 7   | 7     | 213 | PHE  | N-CA-C | 5.41  | 117.93      | 111.71   |
| 21  | N     | 346 | ASN  | N-CA-C | -5.41 | 106.88      | 112.93   |
| 18  | K     | 188 | VAL  | CA-C-N | 5.40  | 127.79      | 120.44   |
| 18  | K     | 188 | VAL  | C-N-CA | 5.40  | 127.79      | 120.44   |
| 20  | M     | 401 | ILE  | CA-C-O | 5.40  | 126.58      | 120.85   |
| 8   | A     | 130 | GLN  | CA-C-O | 5.40  | 126.59      | 120.00   |
| 12  | E     | 106 | ASP  | CA-C-O | 5.40  | 127.09      | 121.15   |
| 31  | X     | 25  | THR  | O-C-N  | -5.40 | 116.58      | 121.39   |
| 13  | F     | 25  | ALA  | CA-C-O | 5.40  | 126.14      | 120.42   |
| 15  | H     | 220 | LYS  | CA-C-N | 5.40  | 127.51      | 120.28   |
| 15  | H     | 220 | LYS  | C-N-CA | 5.40  | 127.51      | 120.28   |
| 21  | N     | 22  | THR  | CA-C-N | 5.40  | 127.51      | 120.28   |
| 21  | N     | 22  | THR  | C-N-CA | 5.40  | 127.51      | 120.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | N     | 143 | LYS  | N-CA-C  | 5.40  | 117.59      | 111.11   |
| 21  | N     | 57  | ASP  | CA-C-O  | 5.40  | 127.03      | 119.80   |
| 6   | 6     | 110 | LYS  | CA-C-N  | 5.39  | 125.22      | 120.10   |
| 6   | 6     | 110 | LYS  | C-N-CA  | 5.39  | 125.22      | 120.10   |
| 8   | A     | 140 | ILE  | N-CA-C  | -5.39 | 99.88       | 107.75   |
| 17  | J     | 347 | ALA  | CA-C-N  | 5.39  | 128.51      | 120.31   |
| 17  | J     | 347 | ALA  | C-N-CA  | 5.39  | 128.51      | 120.31   |
| 21  | N     | 731 | VAL  | N-CA-C  | 5.39  | 116.77      | 110.62   |
| 33  | Z     | 618 | GLN  | O-C-N   | 5.39  | 128.30      | 122.15   |
| 23  | P     | 196 | ALA  | N-CA-C  | 5.39  | 117.24      | 111.36   |
| 12  | E     | 224 | LYS  | CA-C-O  | 5.39  | 125.66      | 119.35   |
| 18  | K     | 79  | LEU  | CA-C-N  | 5.39  | 127.95      | 120.29   |
| 18  | K     | 79  | LEU  | C-N-CA  | 5.39  | 127.95      | 120.29   |
| 1   | 1     | 107 | LYS  | CB-CA-C | -5.39 | 108.78      | 115.89   |
| 21  | N     | 612 | SER  | CA-C-O  | 5.39  | 127.12      | 121.19   |
| 33  | Z     | 750 | GLU  | CA-C-N  | 5.39  | 127.77      | 120.44   |
| 33  | Z     | 750 | GLU  | C-N-CA  | 5.39  | 127.77      | 120.44   |
| 33  | Z     | 843 | ASP  | N-CA-C  | -5.39 | 105.32      | 111.14   |
| 33  | Z     | 875 | LYS  | N-CA-C  | -5.39 | 105.48      | 111.36   |
| 13  | F     | 29  | ILE  | CA-C-N  | 5.39  | 129.22      | 120.60   |
| 13  | F     | 29  | ILE  | C-N-CA  | 5.39  | 129.22      | 120.60   |
| 20  | M     | 413 | GLU  | N-CA-C  | -5.39 | 105.49      | 111.36   |
| 21  | N     | 719 | ASN  | CA-C-N  | 5.39  | 128.99      | 121.02   |
| 21  | N     | 719 | ASN  | C-N-CA  | 5.39  | 128.99      | 121.02   |
| 24  | Q     | 105 | GLU  | N-CA-C  | -5.39 | 106.71      | 113.28   |
| 26  | S     | 323 | LEU  | N-CA-C  | 5.39  | 116.83      | 111.07   |
| 10  | C     | 145 | GLY  | CA-C-O  | -5.38 | 114.99      | 121.67   |
| 16  | I     | 222 | TYR  | CA-C-N  | 5.38  | 131.96      | 121.41   |
| 16  | I     | 222 | TYR  | C-N-CA  | 5.38  | 131.96      | 121.41   |
| 22  | O     | 216 | ASP  | N-CA-C  | -5.38 | 105.49      | 111.36   |
| 28  | U     | 36  | VAL  | N-CA-C  | -5.38 | 100.72      | 108.53   |
| 33  | Z     | 905 | ASN  | CA-C-O  | -5.38 | 114.81      | 120.63   |
| 10  | C     | 119 | LYS  | O-C-N   | 5.38  | 127.83      | 122.12   |
| 16  | I     | 228 | GLY  | N-CA-C  | -5.38 | 100.42      | 113.18   |
| 23  | P     | 416 | SER  | CA-C-N  | 5.38  | 127.76      | 120.44   |
| 23  | P     | 416 | SER  | C-N-CA  | 5.38  | 127.76      | 120.44   |
| 24  | Q     | 226 | HIS  | O-C-N   | -5.38 | 113.75      | 122.42   |
| 3   | 3     | 170 | ALA  | N-CA-C  | -5.38 | 106.59      | 114.39   |
| 20  | M     | 141 | LYS  | O-C-N   | -5.38 | 115.13      | 121.32   |
| 21  | N     | 569 | LYS  | CA-C-N  | 5.38  | 128.03      | 120.28   |
| 21  | N     | 569 | LYS  | C-N-CA  | 5.38  | 128.03      | 120.28   |
| 26  | S     | 417 | GLN  | CA-C-O  | 5.38  | 124.41      | 118.65   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | C     | 84  | ALA  | O-C-N  | 5.38  | 127.82      | 122.12   |
| 14  | G     | 63  | ASN  | N-CA-C | -5.38 | 105.35      | 112.94   |
| 22  | O     | 244 | ASN  | N-CA-C | -5.38 | 106.72      | 113.28   |
| 29  | V     | 193 | ASN  | CA-C-N | 5.38  | 131.81      | 121.54   |
| 29  | V     | 193 | ASN  | C-N-CA | 5.38  | 131.81      | 121.54   |
| 5   | 5     | 203 | GLU  | N-CA-C | 5.38  | 117.22      | 111.36   |
| 13  | F     | 59  | TYR  | CA-C-N | 5.38  | 131.01      | 122.62   |
| 13  | F     | 59  | TYR  | C-N-CA | 5.38  | 131.01      | 122.62   |
| 20  | M     | 339 | ARG  | CA-C-N | 5.38  | 129.69      | 120.71   |
| 20  | M     | 339 | ARG  | C-N-CA | 5.38  | 129.69      | 120.71   |
| 28  | U     | 303 | GLU  | CA-C-N | 5.38  | 127.48      | 120.28   |
| 28  | U     | 303 | GLU  | C-N-CA | 5.38  | 127.48      | 120.28   |
| 2   | 2     | 138 | LEU  | O-C-N  | -5.38 | 116.42      | 122.12   |
| 24  | Q     | 164 | GLU  | N-CA-C | 5.38  | 116.82      | 111.07   |
| 29  | V     | 165 | ILE  | N-CA-C | -5.38 | 106.62      | 112.80   |
| 33  | Z     | 189 | ALA  | CA-C-N | 5.38  | 129.77      | 122.19   |
| 33  | Z     | 189 | ALA  | C-N-CA | 5.38  | 129.77      | 122.19   |
| 6   | 6     | 79  | SER  | N-CA-C | -5.37 | 105.08      | 111.69   |
| 33  | Z     | 485 | ILE  | CA-C-N | 5.37  | 129.20      | 120.60   |
| 33  | Z     | 485 | ILE  | C-N-CA | 5.37  | 129.20      | 120.60   |
| 6   | 6     | 145 | VAL  | CA-C-O | -5.37 | 115.05      | 120.69   |
| 6   | 6     | 197 | ILE  | N-CA-C | -5.37 | 100.65      | 108.17   |
| 14  | G     | 223 | THR  | CA-C-O | -5.37 | 112.83      | 120.51   |
| 24  | Q     | 418 | GLN  | O-C-N  | 5.37  | 127.60      | 122.07   |
| 19  | L     | 222 | GLY  | CA-C-O | -5.37 | 113.84      | 121.52   |
| 3   | 3     | 174 | TRP  | O-C-N  | 5.37  | 129.21      | 122.55   |
| 5   | 5     | 133 | GLN  | CA-C-O | -5.37 | 114.83      | 120.63   |
| 11  | D     | 200 | LEU  | O-C-N  | 5.37  | 127.81      | 122.12   |
| 23  | P     | 89  | LEU  | O-C-N  | -5.37 | 117.68      | 123.42   |
| 30  | W     | 137 | VAL  | CA-C-O | -5.37 | 114.23      | 121.32   |
| 16  | I     | 131 | SER  | CA-C-N | 5.37  | 128.61      | 120.13   |
| 16  | I     | 131 | SER  | C-N-CA | 5.37  | 128.61      | 120.13   |
| 17  | J     | 235 | VAL  | O-C-N  | -5.37 | 116.65      | 121.91   |
| 33  | Z     | 169 | VAL  | CA-C-N | 5.37  | 127.42      | 120.44   |
| 33  | Z     | 169 | VAL  | C-N-CA | 5.37  | 127.42      | 120.44   |
| 1   | 1     | 139 | ASP  | O-C-N  | -5.37 | 116.03      | 122.15   |
| 10  | C     | 136 | ILE  | N-CA-C | -5.37 | 99.92       | 107.75   |
| 13  | F     | 145 | LEU  | N-CA-C | -5.37 | 101.02      | 109.50   |
| 15  | H     | 52  | THR  | CA-C-O | -5.37 | 114.86      | 120.55   |
| 15  | H     | 164 | SER  | O-C-N  | -5.37 | 115.15      | 121.32   |
| 21  | N     | 188 | TYR  | N-CA-C | -5.37 | 105.43      | 111.28   |
| 25  | R     | 26  | VAL  | CA-C-O | 5.37  | 126.53      | 120.95   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | R     | 348 | LEU  | CA-C-O  | 5.37  | 126.16      | 120.36   |
| 4   | 4     | 176 | LYS  | CA-C-O  | -5.36 | 112.84      | 120.51   |
| 14  | G     | 201 | LEU  | N-CA-C  | -5.36 | 105.52      | 111.36   |
| 17  | J     | 195 | LYS  | CA-C-N  | 5.36  | 127.91      | 120.29   |
| 17  | J     | 195 | LYS  | C-N-CA  | 5.36  | 127.91      | 120.29   |
| 14  | G     | 93  | GLU  | CA-C-O  | 5.36  | 126.23      | 120.55   |
| 8   | A     | 246 | VAL  | N-CA-C  | 5.36  | 116.09      | 110.62   |
| 14  | G     | 136 | ILE  | CA-C-O  | 5.36  | 126.16      | 120.48   |
| 19  | L     | 138 | SER  | CA-C-O  | 5.36  | 125.56      | 119.18   |
| 11  | D     | 107 | GLU  | CA-C-O  | -5.36 | 115.17      | 120.90   |
| 15  | H     | 227 | LEU  | CA-C-O  | -5.36 | 112.82      | 120.16   |
| 21  | N     | 513 | ILE  | O-C-N   | -5.36 | 116.31      | 121.83   |
| 4   | 4     | 72  | TYR  | N-CA-C  | -5.36 | 98.84       | 108.48   |
| 21  | N     | 639 | ASP  | N-CA-C  | 5.36  | 117.12      | 111.28   |
| 24  | Q     | 171 | LYS  | CA-C-N  | 5.36  | 124.97      | 119.56   |
| 24  | Q     | 171 | LYS  | C-N-CA  | 5.36  | 124.97      | 119.56   |
| 10  | C     | 110 | ILE  | CB-CA-C | -5.36 | 105.11      | 111.97   |
| 15  | H     | 379 | LEU  | CA-C-O  | -5.36 | 114.26      | 119.51   |
| 24  | Q     | 231 | ASP  | CA-C-N  | 5.36  | 128.45      | 120.31   |
| 24  | Q     | 231 | ASP  | C-N-CA  | 5.36  | 128.45      | 120.31   |
| 25  | R     | 383 | ARG  | CA-C-N  | 5.36  | 128.22      | 121.85   |
| 25  | R     | 383 | ARG  | C-N-CA  | 5.36  | 128.22      | 121.85   |
| 21  | N     | 557 | LEU  | CA-C-N  | 5.35  | 127.72      | 120.38   |
| 21  | N     | 557 | LEU  | C-N-CA  | 5.35  | 127.72      | 120.38   |
| 17  | J     | 71  | TYR  | CA-C-N  | 5.35  | 131.06      | 122.50   |
| 17  | J     | 71  | TYR  | C-N-CA  | 5.35  | 131.06      | 122.50   |
| 33  | Z     | 545 | SER  | O-C-N   | 5.35  | 127.58      | 122.07   |
| 21  | N     | 90  | ASP  | CA-C-O  | -5.35 | 114.58      | 120.36   |
| 21  | N     | 734 | VAL  | N-CA-C  | -5.35 | 105.17      | 111.00   |
| 30  | W     | 178 | PRO  | CA-C-O  | -5.35 | 114.89      | 121.31   |
| 15  | H     | 340 | LEU  | CA-C-O  | -5.35 | 115.39      | 120.90   |
| 24  | Q     | 36  | SER  | N-CA-C  | -5.35 | 101.28      | 109.41   |
| 27  | T     | 141 | LEU  | CA-C-N  | 5.35  | 127.89      | 120.29   |
| 27  | T     | 141 | LEU  | C-N-CA  | 5.35  | 127.89      | 120.29   |
| 29  | V     | 77  | GLY  | N-CA-C  | -5.35 | 107.41      | 114.95   |
| 1   | 1     | 75  | THR  | CA-C-N  | 5.35  | 128.44      | 120.31   |
| 1   | 1     | 75  | THR  | C-N-CA  | 5.35  | 128.44      | 120.31   |
| 6   | 6     | 195 | ILE  | CA-C-O  | 5.35  | 126.00      | 120.39   |
| 13  | F     | 120 | THR  | N-CA-C  | -5.35 | 106.43      | 113.17   |
| 21  | N     | 56  | SER  | CA-C-O  | 5.35  | 125.90      | 119.59   |
| 27  | T     | 271 | GLU  | CA-C-N  | -5.35 | 112.07      | 121.70   |
| 27  | T     | 271 | GLU  | C-N-CA  | -5.35 | 112.07      | 121.70   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33  | Z     | 434 | GLN  | N-CA-C  | 5.35  | 116.79      | 111.07   |
| 23  | P     | 153 | ILE  | O-C-N   | 5.34  | 127.46      | 121.90   |
| 30  | W     | 139 | VAL  | N-CA-C  | 5.34  | 115.41      | 108.35   |
| 26  | S     | 280 | ASN  | CA-C-N  | 5.34  | 127.44      | 120.28   |
| 26  | S     | 280 | ASN  | C-N-CA  | 5.34  | 127.44      | 120.28   |
| 14  | G     | 27  | VAL  | CB-CA-C | -5.34 | 105.05      | 112.04   |
| 25  | R     | 143 | GLN  | N-CA-C  | 5.34  | 117.18      | 111.36   |
| 17  | J     | 178 | GLY  | CA-C-N  | 5.34  | 127.73      | 120.63   |
| 17  | J     | 178 | GLY  | C-N-CA  | 5.34  | 127.73      | 120.63   |
| 12  | E     | 182 | GLU  | CA-C-N  | 5.34  | 127.43      | 120.28   |
| 12  | E     | 182 | GLU  | C-N-CA  | 5.34  | 127.43      | 120.28   |
| 22  | O     | 250 | TRP  | CA-C-N  | 5.34  | 127.70      | 120.44   |
| 22  | O     | 250 | TRP  | C-N-CA  | 5.34  | 127.70      | 120.44   |
| 15  | H     | 58  | ASP  | CA-C-N  | 5.33  | 127.77      | 120.46   |
| 15  | H     | 58  | ASP  | C-N-CA  | 5.33  | 127.77      | 120.46   |
| 23  | P     | 436 | GLU  | CA-C-N  | 5.33  | 127.38      | 120.44   |
| 23  | P     | 436 | GLU  | C-N-CA  | 5.33  | 127.38      | 120.44   |
| 25  | R     | 111 | LYS  | N-CA-C  | 5.33  | 117.09      | 111.28   |
| 27  | T     | 213 | ASN  | CA-C-O  | 5.33  | 126.24      | 120.32   |
| 26  | S     | 234 | ILE  | CA-C-N  | 5.33  | 127.37      | 120.44   |
| 26  | S     | 234 | ILE  | C-N-CA  | 5.33  | 127.37      | 120.44   |
| 19  | L     | 327 | THR  | CA-C-N  | 5.33  | 127.42      | 120.28   |
| 19  | L     | 327 | THR  | C-N-CA  | 5.33  | 127.42      | 120.28   |
| 22  | O     | 16  | MET  | CA-C-O  | -5.33 | 114.88      | 120.80   |
| 24  | Q     | 142 | ALA  | O-C-N   | 5.33  | 127.77      | 122.12   |
| 24  | Q     | 357 | VAL  | N-CA-C  | -5.33 | 100.18      | 108.44   |
| 17  | J     | 29  | GLU  | CA-C-N  | 5.33  | 127.42      | 120.28   |
| 17  | J     | 29  | GLU  | C-N-CA  | 5.33  | 127.42      | 120.28   |
| 25  | R     | 55  | LYS  | N-CA-C  | -5.33 | 106.71      | 114.12   |
| 8   | A     | 90  | ALA  | O-C-N   | 5.33  | 127.77      | 122.12   |
| 23  | P     | 272 | PRO  | N-CA-C  | -5.33 | 101.50      | 112.47   |
| 24  | Q     | 54  | GLN  | CA-C-N  | 5.33  | 127.42      | 120.28   |
| 24  | Q     | 54  | GLN  | C-N-CA  | 5.33  | 127.42      | 120.28   |
| 2   | 2     | 35  | HIS  | CA-C-O  | -5.33 | 115.06      | 120.71   |
| 15  | H     | 205 | ASP  | N-CA-C  | -5.33 | 106.65      | 112.72   |
| 23  | P     | 70  | ASN  | CA-C-N  | 5.33  | 129.87      | 120.87   |
| 23  | P     | 70  | ASN  | C-N-CA  | 5.33  | 129.87      | 120.87   |
| 26  | S     | 181 | ALA  | CA-C-N  | 5.33  | 127.68      | 120.38   |
| 26  | S     | 181 | ALA  | C-N-CA  | 5.33  | 127.68      | 120.38   |
| 31  | X     | 21  | SER  | N-CA-C  | -5.33 | 105.05      | 112.03   |
| 7   | 7     | 47  | GLY  | N-CA-C  | -5.32 | 105.23      | 112.52   |
| 11  | D     | 95  | SER  | CA-C-N  | 5.32  | 127.68      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 11  | D     | 95  | SER  | C-N-CA | 5.32  | 127.68      | 120.44   |
| 11  | D     | 238 | GLN  | N-CA-C | -5.32 | 105.14      | 111.69   |
| 33  | Z     | 755 | GLU  | CA-C-N | 5.32  | 128.40      | 120.31   |
| 33  | Z     | 755 | GLU  | C-N-CA | 5.32  | 128.40      | 120.31   |
| 13  | F     | 26  | LEU  | O-C-N  | -5.32 | 116.00      | 122.22   |
| 19  | L     | 128 | ILE  | N-CA-C | -5.32 | 100.75      | 108.36   |
| 17  | J     | 44  | LEU  | CA-C-N | 5.32  | 127.84      | 120.29   |
| 17  | J     | 44  | LEU  | C-N-CA | 5.32  | 127.84      | 120.29   |
| 19  | L     | 204 | PRO  | CA-C-N | 5.32  | 127.41      | 120.28   |
| 19  | L     | 204 | PRO  | C-N-CA | 5.32  | 127.41      | 120.28   |
| 33  | Z     | 792 | VAL  | O-C-N  | -5.32 | 116.71      | 121.87   |
| 1   | 1     | -8  | LYS  | O-C-N  | 5.32  | 127.77      | 122.08   |
| 6   | 6     | 168 | VAL  | N-CA-C | 5.32  | 116.04      | 110.62   |
| 19  | L     | 146 | VAL  | O-C-N  | 5.32  | 128.94      | 123.04   |
| 21  | N     | 742 | TRP  | N-CA-C | -5.32 | 99.47       | 110.80   |
| 31  | X     | 98  | PHE  | N-CA-C | -5.32 | 101.21      | 109.72   |
| 33  | Z     | 187 | SER  | CA-C-O | -5.32 | 115.38      | 122.03   |
| 9   | B     | 20  | GLN  | N-CA-C | 5.32  | 117.07      | 111.28   |
| 24  | Q     | 109 | ASP  | CA-C-N | 5.31  | 128.25      | 120.71   |
| 24  | Q     | 109 | ASP  | C-N-CA | 5.31  | 128.25      | 120.71   |
| 1   | 1     | 6   | VAL  | N-CA-C | 5.31  | 115.77      | 108.12   |
| 15  | H     | 276 | GLY  | CA-C-O | 5.31  | 126.01      | 120.80   |
| 19  | L     | 318 | LEU  | N-CA-C | -5.31 | 100.74      | 109.40   |
| 17  | J     | 43  | ARG  | O-C-N  | 5.31  | 127.83      | 122.09   |
| 18  | K     | 401 | VAL  | CA-C-N | -5.31 | 115.88      | 123.10   |
| 18  | K     | 401 | VAL  | C-N-CA | -5.31 | 115.88      | 123.10   |
| 24  | Q     | 33  | LYS  | N-CA-C | 5.31  | 117.34      | 109.69   |
| 6   | 6     | 171 | VAL  | N-CA-C | 5.31  | 116.03      | 110.62   |
| 15  | H     | 359 | ASN  | CA-C-O | -5.31 | 113.06      | 119.27   |
| 14  | G     | 159 | TYR  | CA-C-N | 5.31  | 131.49      | 122.36   |
| 14  | G     | 159 | TYR  | C-N-CA | 5.31  | 131.49      | 122.36   |
| 15  | H     | 313 | ALA  | CA-C-O | 5.31  | 126.05      | 120.42   |
| 18  | K     | 166 | LYS  | CA-C-N | 5.31  | 125.07      | 119.76   |
| 18  | K     | 166 | LYS  | C-N-CA | 5.31  | 125.07      | 119.76   |
| 21  | N     | 632 | LYS  | N-CA-C | -5.31 | 106.57      | 114.64   |
| 25  | R     | 363 | PHE  | CA-C-N | 5.31  | 127.39      | 120.28   |
| 25  | R     | 363 | PHE  | C-N-CA | 5.31  | 127.39      | 120.28   |
| 28  | U     | 207 | VAL  | N-CA-C | 5.31  | 115.52      | 110.42   |
| 33  | Z     | 444 | GLU  | N-CA-C | -5.31 | 102.32      | 110.07   |
| 10  | C     | 223 | GLY  | CA-C-O | -5.31 | 115.58      | 121.05   |
| 4   | 4     | 54  | GLN  | O-C-N  | 5.30  | 127.53      | 122.07   |
| 11  | D     | 121 | THR  | CA-C-O | 5.30  | 126.13      | 120.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | G     | 234 | LEU  | CA-C-N  | 5.30  | 127.82      | 120.29   |
| 14  | G     | 234 | LEU  | C-N-CA  | 5.30  | 127.82      | 120.29   |
| 16  | I     | 418 | GLN  | N-CA-C  | -5.30 | 105.55      | 112.23   |
| 33  | Z     | 591 | ILE  | CA-C-N  | 5.30  | 129.69      | 121.26   |
| 33  | Z     | 591 | ILE  | C-N-CA  | 5.30  | 129.69      | 121.26   |
| 26  | S     | 167 | LEU  | CA-C-N  | 5.30  | 127.39      | 120.28   |
| 26  | S     | 167 | LEU  | C-N-CA  | 5.30  | 127.39      | 120.28   |
| 5   | 5     | 85  | ASN  | O-C-N   | 5.30  | 127.81      | 122.09   |
| 12  | E     | 166 | ARG  | N-CA-C  | -5.30 | 101.05      | 109.96   |
| 20  | M     | 396 | VAL  | CA-C-N  | 5.30  | 127.38      | 120.28   |
| 20  | M     | 396 | VAL  | C-N-CA  | 5.30  | 127.38      | 120.28   |
| 21  | N     | 590 | ALA  | CA-C-N  | 5.30  | 127.38      | 120.28   |
| 21  | N     | 590 | ALA  | C-N-CA  | 5.30  | 127.38      | 120.28   |
| 25  | R     | 256 | THR  | O-C-N   | 5.30  | 127.74      | 122.12   |
| 21  | N     | 254 | SER  | N-CA-C  | -5.30 | 105.62      | 111.71   |
| 31  | X     | 27  | ILE  | N-CA-C  | -5.30 | 101.93      | 107.60   |
| 21  | N     | 293 | LEU  | CA-C-O  | -5.30 | 113.76      | 118.63   |
| 3   | 3     | 146 | GLU  | CA-C-O  | -5.30 | 114.31      | 120.03   |
| 25  | R     | 295 | SER  | N-CA-C  | 5.30  | 116.74      | 111.07   |
| 28  | U     | 164 | GLU  | CB-CA-C | 5.30  | 118.92      | 109.65   |
| 2   | 2     | 13  | VAL  | N-CA-C  | -5.29 | 100.86      | 108.48   |
| 9   | B     | 244 | ASN  | CA-C-O  | -5.29 | 114.91      | 120.63   |
| 12  | E     | 68  | VAL  | O-C-N   | -5.29 | 117.34      | 123.00   |
| 3   | 3     | 195 | GLN  | N-CA-C  | -5.29 | 101.40      | 108.86   |
| 12  | E     | 21  | LEU  | N-CA-C  | 5.29  | 117.55      | 110.35   |
| 22  | O     | 97  | LYS  | O-C-N   | 5.29  | 127.73      | 122.12   |
| 30  | W     | 162 | ASN  | N-CA-C  | 5.29  | 122.07      | 110.80   |
| 33  | Z     | 435 | GLN  | CA-C-N  | 5.29  | 127.90      | 120.28   |
| 33  | Z     | 435 | GLN  | C-N-CA  | 5.29  | 127.90      | 120.28   |
| 9   | B     | 165 | GLY  | CA-C-O  | -5.29 | 118.01      | 122.29   |
| 22  | O     | 270 | ILE  | CA-C-O  | -5.29 | 114.82      | 121.11   |
| 24  | Q     | 347 | LEU  | CA-C-N  | 5.29  | 128.35      | 120.31   |
| 24  | Q     | 347 | LEU  | C-N-CA  | 5.29  | 128.35      | 120.31   |
| 29  | V     | 71  | MET  | CA-C-N  | 5.29  | 126.45      | 119.84   |
| 29  | V     | 71  | MET  | C-N-CA  | 5.29  | 126.45      | 119.84   |
| 1   | 1     | 120 | HIS  | CA-C-N  | 5.29  | 129.64      | 122.19   |
| 1   | 1     | 120 | HIS  | C-N-CA  | 5.29  | 129.64      | 122.19   |
| 16  | I     | 79  | SER  | N-CA-C  | 5.29  | 117.04      | 111.28   |
| 19  | L     | 113 | SER  | N-CA-C  | -5.29 | 101.25      | 108.38   |
| 25  | R     | 82  | ASP  | N-CA-C  | 5.29  | 116.75      | 110.19   |
| 26  | S     | 460 | VAL  | CA-C-N  | 5.29  | 127.31      | 120.44   |
| 26  | S     | 460 | VAL  | C-N-CA  | 5.29  | 127.31      | 120.44   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | T     | 126 | LEU  | CA-C-N  | 5.29  | 127.80      | 120.29   |
| 27  | T     | 126 | LEU  | C-N-CA  | 5.29  | 127.80      | 120.29   |
| 1   | 1     | 149 | GLU  | CA-C-O  | 5.28  | 126.55      | 120.90   |
| 13  | F     | 26  | LEU  | CA-C-N  | 5.28  | 129.62      | 120.58   |
| 13  | F     | 26  | LEU  | C-N-CA  | 5.28  | 129.62      | 120.58   |
| 17  | J     | 25  | GLN  | CA-C-N  | 5.28  | 127.36      | 120.28   |
| 17  | J     | 25  | GLN  | C-N-CA  | 5.28  | 127.36      | 120.28   |
| 19  | L     | 81  | ILE  | O-C-N   | -5.28 | 116.74      | 121.87   |
| 21  | N     | 647 | ASP  | CA-C-O  | -5.28 | 114.94      | 120.70   |
| 29  | V     | 50  | MET  | N-CA-C  | -5.28 | 101.26      | 109.24   |
| 20  | M     | 237 | ALA  | CA-C-N  | 5.28  | 127.79      | 120.29   |
| 20  | M     | 237 | ALA  | C-N-CA  | 5.28  | 127.79      | 120.29   |
| 15  | H     | 56  | LEU  | CA-C-O  | -5.28 | 114.95      | 120.55   |
| 17  | J     | 57  | PHE  | O-C-N   | 5.28  | 127.51      | 122.07   |
| 17  | J     | 132 | PRO  | CA-C-O  | -5.28 | 115.58      | 121.23   |
| 18  | K     | 159 | SER  | N-CA-C  | -5.28 | 106.73      | 114.39   |
| 25  | R     | 240 | SER  | CA-C-N  | 5.28  | 131.47      | 121.97   |
| 25  | R     | 240 | SER  | C-N-CA  | 5.28  | 131.47      | 121.97   |
| 24  | Q     | 338 | LEU  | O-C-N   | 5.28  | 128.17      | 122.15   |
| 21  | N     | 35  | LEU  | CA-C-N  | 5.28  | 127.88      | 120.28   |
| 21  | N     | 35  | LEU  | C-N-CA  | 5.28  | 127.88      | 120.28   |
| 2   | 2     | 195 | VAL  | CA-C-N  | 5.28  | 129.17      | 121.31   |
| 2   | 2     | 195 | VAL  | C-N-CA  | 5.28  | 129.17      | 121.31   |
| 13  | F     | 22  | VAL  | N-CA-C  | -5.28 | 105.25      | 111.00   |
| 20  | M     | 289 | LYS  | N-CA-C  | -5.28 | 106.35      | 114.16   |
| 23  | P     | 258 | LYS  | CA-C-N  | 5.28  | 125.08      | 119.28   |
| 23  | P     | 258 | LYS  | C-N-CA  | 5.28  | 125.08      | 119.28   |
| 24  | Q     | 102 | GLU  | CA-C-N  | 5.28  | 127.35      | 120.28   |
| 24  | Q     | 102 | GLU  | C-N-CA  | 5.28  | 127.35      | 120.28   |
| 29  | V     | 215 | ASN  | N-CA-C  | -5.28 | 106.69      | 113.02   |
| 15  | H     | 246 | ILE  | O-C-N   | -5.27 | 117.36      | 123.00   |
| 16  | I     | 408 | ARG  | CA-C-O  | -5.27 | 114.21      | 120.43   |
| 30  | W     | 119 | SER  | O-C-N   | 5.27  | 129.60      | 122.59   |
| 9   | B     | 137 | ALA  | N-CA-C  | -5.27 | 100.43      | 109.24   |
| 9   | B     | 217 | GLU  | CB-CA-C | 5.27  | 118.88      | 109.65   |
| 12  | E     | 86  | ARG  | CA-C-N  | 5.27  | 127.34      | 120.28   |
| 12  | E     | 86  | ARG  | C-N-CA  | 5.27  | 127.34      | 120.28   |
| 21  | N     | 93  | GLU  | CA-C-N  | 5.27  | 130.22      | 122.63   |
| 21  | N     | 93  | GLU  | C-N-CA  | 5.27  | 130.22      | 122.63   |
| 33  | Z     | 615 | LEU  | O-C-N   | 5.27  | 127.71      | 122.12   |
| 17  | J     | 95  | ILE  | CA-C-O  | -5.27 | 114.93      | 120.57   |
| 21  | N     | 138 | GLU  | CA-C-N  | 5.27  | 128.32      | 120.31   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 138 | GLU  | C-N-CA | 5.27  | 128.32      | 120.31   |
| 22  | O     | 199 | LEU  | CA-C-O | -5.27 | 115.28      | 120.82   |
| 26  | S     | 295 | ALA  | CA-C-N | 5.27  | 127.29      | 120.44   |
| 26  | S     | 295 | ALA  | C-N-CA | 5.27  | 127.29      | 120.44   |
| 16  | I     | 242 | ALA  | N-CA-C | -5.27 | 101.57      | 109.95   |
| 23  | P     | 90  | LYS  | CA-C-N | 5.27  | 127.29      | 120.44   |
| 23  | P     | 90  | LYS  | C-N-CA | 5.27  | 127.29      | 120.44   |
| 1   | 1     | 102 | TYR  | CA-C-O | 5.27  | 126.05      | 120.36   |
| 28  | U     | 135 | ASP  | N-CA-C | -5.27 | 100.44      | 109.24   |
| 31  | X     | 71  | GLY  | CA-C-O | 5.27  | 126.14      | 119.72   |
| 1   | 1     | 144 | GLU  | CA-C-N | 5.27  | 131.60      | 121.54   |
| 1   | 1     | 144 | GLU  | C-N-CA | 5.27  | 131.60      | 121.54   |
| 16  | I     | 411 | VAL  | CA-C-O | -5.26 | 114.77      | 120.67   |
| 30  | W     | 87  | MET  | CA-C-O | 5.26  | 126.35      | 120.82   |
| 30  | W     | 136 | ASN  | CA-C-N | 5.26  | 131.51      | 122.67   |
| 30  | W     | 136 | ASN  | C-N-CA | 5.26  | 131.51      | 122.67   |
| 18  | K     | 254 | VAL  | O-C-N  | -5.26 | 116.68      | 121.94   |
| 21  | N     | 134 | THR  | CA-C-N | 5.26  | 127.64      | 120.54   |
| 21  | N     | 134 | THR  | C-N-CA | 5.26  | 127.64      | 120.54   |
| 13  | F     | 44  | ALA  | CA-C-O | 5.26  | 126.91      | 120.60   |
| 22  | O     | 375 | ASP  | N-CA-C | 5.26  | 117.70      | 111.33   |
| 33  | Z     | 400 | ILE  | CA-C-O | 5.26  | 126.42      | 120.95   |
| 20  | M     | 371 | ASP  | CA-C-O | 5.26  | 125.58      | 119.32   |
| 26  | S     | 249 | SER  | N-CA-C | -5.26 | 106.70      | 113.01   |
| 1   | 1     | 55  | ILE  | O-C-N  | 5.26  | 127.06      | 121.91   |
| 23  | P     | 234 | TYR  | CA-C-O | 5.26  | 126.00      | 119.79   |
| 9   | B     | 27  | ALA  | CA-C-N | 5.26  | 127.66      | 120.46   |
| 9   | B     | 27  | ALA  | C-N-CA | 5.26  | 127.66      | 120.46   |
| 14  | G     | 28  | LYS  | CA-C-N | 5.26  | 128.30      | 120.31   |
| 14  | G     | 28  | LYS  | C-N-CA | 5.26  | 128.30      | 120.31   |
| 13  | F     | 80  | ASP  | CA-C-N | 5.25  | 127.85      | 120.28   |
| 13  | F     | 80  | ASP  | C-N-CA | 5.25  | 127.85      | 120.28   |
| 18  | K     | 223 | VAL  | CA-C-N | 5.25  | 127.32      | 120.28   |
| 18  | K     | 223 | VAL  | C-N-CA | 5.25  | 127.32      | 120.28   |
| 22  | O     | 275 | SER  | N-CA-C | 5.25  | 117.09      | 111.36   |
| 9   | B     | 71  | ILE  | N-CA-C | -5.25 | 100.67      | 108.45   |
| 9   | B     | 221 | LEU  | CA-C-O | 5.25  | 125.79      | 119.59   |
| 19  | L     | 140 | LEU  | CA-C-O | 5.25  | 124.97      | 119.03   |
| 21  | N     | 153 | ALA  | CA-C-O | 5.25  | 126.34      | 120.82   |
| 21  | N     | 672 | ASN  | O-C-N  | 5.25  | 124.42      | 121.27   |
| 25  | R     | 161 | ALA  | O-C-N  | -5.25 | 116.47      | 122.93   |
| 7   | 7     | 131 | SER  | CA-C-N | 5.25  | 124.86      | 119.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | 7     | 131 | SER  | C-N-CA | 5.25  | 124.86      | 119.56   |
| 22  | O     | 151 | ASP  | N-CA-C | 5.25  | 117.00      | 111.28   |
| 33  | Z     | 926 | ASN  | CA-C-N | 5.25  | 130.35      | 122.58   |
| 33  | Z     | 926 | ASN  | C-N-CA | 5.25  | 130.35      | 122.58   |
| 5   | 5     | 35  | ILE  | N-CA-C | -5.25 | 100.85      | 108.36   |
| 5   | 5     | 209 | ASN  | CA-C-N | 5.25  | 130.16      | 123.13   |
| 5   | 5     | 209 | ASN  | C-N-CA | 5.25  | 130.16      | 123.13   |
| 33  | Z     | 407 | VAL  | N-CA-C | 5.25  | 115.97      | 110.62   |
| 4   | 4     | 134 | TYR  | CA-C-O | 5.25  | 125.34      | 119.41   |
| 5   | 5     | 209 | ASN  | CA-C-O | 5.25  | 126.03      | 120.10   |
| 16  | I     | 79  | SER  | CA-C-N | 5.25  | 127.31      | 120.28   |
| 16  | I     | 79  | SER  | C-N-CA | 5.25  | 127.31      | 120.28   |
| 16  | I     | 334 | LEU  | CA-C-N | 5.25  | 127.68      | 120.39   |
| 16  | I     | 334 | LEU  | C-N-CA | 5.25  | 127.68      | 120.39   |
| 19  | L     | 411 | ASN  | N-CA-C | -5.25 | 101.00      | 109.82   |
| 20  | M     | 412 | HIS  | O-C-N  | -5.25 | 116.56      | 122.12   |
| 7   | 7     | -1  | GLY  | N-CA-C | -5.25 | 101.75      | 111.04   |
| 15  | H     | 220 | LYS  | N-CA-C | 5.25  | 117.08      | 111.36   |
| 25  | R     | 331 | ARG  | CA-C-N | 5.25  | 128.29      | 120.31   |
| 25  | R     | 331 | ARG  | C-N-CA | 5.25  | 128.29      | 120.31   |
| 30  | W     | 168 | THR  | CA-C-O | 5.25  | 126.73      | 120.28   |
| 1   | 1     | 136 | GLY  | N-CA-C | -5.25 | 106.14      | 112.49   |
| 4   | 4     | 6   | ILE  | CA-C-O | 5.25  | 126.15      | 120.43   |
| 14  | G     | 177 | LYS  | CA-C-O | -5.25 | 115.31      | 120.82   |
| 19  | L     | 399 | GLY  | O-C-N  | 5.25  | 128.00      | 122.28   |
| 33  | Z     | 354 | PRO  | CA-C-N | 5.25  | 127.31      | 120.28   |
| 33  | Z     | 354 | PRO  | C-N-CA | 5.25  | 127.31      | 120.28   |
| 1   | 1     | -4  | VAL  | O-C-N  | 5.24  | 128.86      | 123.20   |
| 7   | 7     | 103 | TRP  | N-CA-C | 5.24  | 118.83      | 110.70   |
| 21  | N     | 680 | LYS  | CA-C-N | 5.24  | 127.25      | 120.44   |
| 21  | N     | 680 | LYS  | C-N-CA | 5.24  | 127.25      | 120.44   |
| 11  | D     | 218 | ASP  | CA-C-N | 5.24  | 130.29      | 122.74   |
| 11  | D     | 218 | ASP  | C-N-CA | 5.24  | 130.29      | 122.74   |
| 26  | S     | 352 | VAL  | CA-C-N | 5.24  | 127.25      | 120.44   |
| 26  | S     | 352 | VAL  | C-N-CA | 5.24  | 127.25      | 120.44   |
| 2   | 2     | 33  | LYS  | N-CA-C | -5.24 | 106.91      | 113.72   |
| 9   | B     | 46  | ALA  | CA-C-N | 5.24  | 130.47      | 121.87   |
| 9   | B     | 46  | ALA  | C-N-CA | 5.24  | 130.47      | 121.87   |
| 15  | H     | 447 | VAL  | CA-C-O | -5.24 | 115.61      | 121.17   |
| 19  | L     | 135 | VAL  | O-C-N  | -5.24 | 117.14      | 122.54   |
| 28  | U     | 8   | VAL  | N-CA-C | -5.24 | 100.65      | 108.46   |
| 33  | Z     | 567 | ALA  | CA-C-O | -5.24 | 115.50      | 121.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | I     | 307 | LEU  | O-C-N  | -5.24 | 116.18      | 122.15   |
| 26  | S     | 134 | ILE  | CA-C-N | 5.24  | 127.30      | 120.28   |
| 26  | S     | 134 | ILE  | C-N-CA | 5.24  | 127.30      | 120.28   |
| 3   | 3     | 170 | ALA  | CA-C-O | 5.24  | 124.71      | 118.69   |
| 6   | 6     | 114 | TYR  | CA-C-N | -5.24 | 114.25      | 122.73   |
| 6   | 6     | 114 | TYR  | C-N-CA | -5.24 | 114.25      | 122.73   |
| 33  | Z     | 525 | MET  | CA-C-N | 5.24  | 129.06      | 120.63   |
| 33  | Z     | 525 | MET  | C-N-CA | 5.24  | 129.06      | 120.63   |
| 14  | G     | 165 | GLY  | N-CA-C | -5.23 | 105.35      | 112.52   |
| 14  | G     | 240 | ASP  | O-C-N  | 5.23  | 127.46      | 122.07   |
| 24  | Q     | 105 | GLU  | CA-C-N | 5.23  | 128.26      | 120.31   |
| 24  | Q     | 105 | GLU  | C-N-CA | 5.23  | 128.26      | 120.31   |
| 24  | Q     | 278 | VAL  | CA-C-O | 5.23  | 126.39      | 120.95   |
| 15  | H     | 352 | MET  | N-CA-C | -5.23 | 100.37      | 108.90   |
| 16  | I     | 424 | MET  | O-C-N  | 5.23  | 127.46      | 122.07   |
| 19  | L     | 354 | GLU  | CA-C-O | 5.23  | 125.96      | 120.42   |
| 21  | N     | 507 | GLU  | O-C-N  | 5.23  | 127.66      | 122.12   |
| 24  | Q     | 310 | SER  | O-C-N  | 5.23  | 129.39      | 123.27   |
| 32  | Y     | 82  | ASP  | N-CA-C | 5.23  | 116.67      | 111.07   |
| 11  | D     | 7   | ALA  | N-CA-C | 5.23  | 118.22      | 110.48   |
| 25  | R     | 227 | ALA  | CA-C-N | 5.23  | 127.29      | 120.28   |
| 25  | R     | 227 | ALA  | C-N-CA | 5.23  | 127.29      | 120.28   |
| 24  | Q     | 20  | TYR  | N-CA-C | -5.23 | 105.58      | 111.28   |
| 27  | T     | 213 | ASN  | N-CA-C | -5.23 | 99.92       | 108.76   |
| 27  | T     | 261 | GLU  | O-C-N  | -5.23 | 116.44      | 122.09   |
| 3   | 3     | -7  | ASP  | O-C-N  | -5.23 | 116.91      | 121.35   |
| 6   | 6     | 68  | PHE  | CA-C-N | 5.23  | 129.45      | 120.72   |
| 6   | 6     | 68  | PHE  | C-N-CA | 5.23  | 129.45      | 120.72   |
| 25  | R     | 86  | ASP  | N-CA-C | -5.22 | 107.93      | 114.56   |
| 28  | U     | 294 | ASN  | CA-C-N | 5.22  | 127.59      | 120.54   |
| 28  | U     | 294 | ASN  | C-N-CA | 5.22  | 127.59      | 120.54   |
| 33  | Z     | 591 | ILE  | O-C-N  | -5.22 | 117.57      | 121.96   |
| 1   | 1     | 116 | GLY  | CA-C-O | -5.22 | 114.50      | 120.09   |
| 13  | F     | 8   | GLY  | N-CA-C | -5.22 | 107.51      | 115.66   |
| 33  | Z     | 203 | LEU  | CA-C-N | 5.22  | 127.28      | 120.28   |
| 33  | Z     | 203 | LEU  | C-N-CA | 5.22  | 127.28      | 120.28   |
| 11  | D     | 22  | TYR  | CA-C-N | 5.22  | 129.51      | 120.58   |
| 11  | D     | 22  | TYR  | C-N-CA | 5.22  | 129.51      | 120.58   |
| 21  | N     | 194 | ILE  | CA-C-O | 5.22  | 126.30      | 120.71   |
| 16  | I     | 385 | ASP  | N-CA-C | -5.22 | 99.32       | 107.93   |
| 21  | N     | 157 | ALA  | CA-C-N | 5.22  | 127.22      | 120.44   |
| 21  | N     | 157 | ALA  | C-N-CA | 5.22  | 127.22      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 22  | O     | 168 | THR  | CA-C-N | 5.22  | 127.70      | 120.29   |
| 22  | O     | 168 | THR  | C-N-CA | 5.22  | 127.70      | 120.29   |
| 24  | Q     | 29  | SER  | O-C-N  | -5.22 | 116.11      | 122.22   |
| 31  | X     | 69  | ILE  | CA-C-O | -5.22 | 115.49      | 119.98   |
| 33  | Z     | 246 | CYS  | CA-C-N | 5.22  | 127.70      | 120.29   |
| 33  | Z     | 246 | CYS  | C-N-CA | 5.22  | 127.70      | 120.29   |
| 1   | 1     | 113 | ILE  | CA-C-N | 5.22  | 126.36      | 119.84   |
| 1   | 1     | 113 | ILE  | C-N-CA | 5.22  | 126.36      | 119.84   |
| 2   | 2     | 143 | LYS  | N-CA-C | -5.22 | 100.81      | 108.79   |
| 8   | A     | 219 | SER  | N-CA-C | -5.22 | 101.83      | 109.81   |
| 15  | H     | 208 | TYR  | CA-C-O | -5.22 | 115.81      | 121.44   |
| 16  | I     | 100 | ARG  | CA-C-N | 5.22  | 131.63      | 121.41   |
| 16  | I     | 100 | ARG  | C-N-CA | 5.22  | 131.63      | 121.41   |
| 13  | F     | 116 | ALA  | CA-C-N | 5.21  | 127.22      | 120.44   |
| 13  | F     | 116 | ALA  | C-N-CA | 5.21  | 127.22      | 120.44   |
| 16  | I     | 390 | ALA  | N-CA-C | 5.21  | 116.96      | 111.28   |
| 17  | J     | 43  | ARG  | CA-C-O | -5.21 | 115.33      | 120.70   |
| 22  | O     | 26  | PHE  | CA-C-N | 5.21  | 127.70      | 120.29   |
| 22  | O     | 26  | PHE  | C-N-CA | 5.21  | 127.70      | 120.29   |
| 29  | V     | 183 | ALA  | N-CA-C | -5.21 | 105.77      | 111.82   |
| 22  | O     | 141 | ASN  | CA-C-N | 5.21  | 131.50      | 121.54   |
| 22  | O     | 141 | ASN  | C-N-CA | 5.21  | 131.50      | 121.54   |
| 33  | Z     | 871 | HIS  | CA-C-O | -5.21 | 115.79      | 121.84   |
| 15  | H     | 209 | SER  | N-CA-C | -5.21 | 106.45      | 114.16   |
| 10  | C     | 60  | ASP  | N-CA-C | -5.21 | 106.51      | 112.92   |
| 25  | R     | 133 | ALA  | N-CA-C | 5.21  | 117.70      | 111.71   |
| 23  | P     | 74  | ASP  | CA-C-N | 5.21  | 127.21      | 120.44   |
| 23  | P     | 74  | ASP  | C-N-CA | 5.21  | 127.21      | 120.44   |
| 2   | 2     | 101 | ALA  | N-CA-C | -5.21 | 101.38      | 109.24   |
| 9   | B     | 136 | ILE  | CA-C-O | 5.21  | 126.00      | 120.48   |
| 12  | E     | 174 | SER  | N-CA-C | 5.21  | 117.03      | 111.36   |
| 20  | M     | 56  | ASN  | CA-C-O | -5.21 | 114.90      | 120.42   |
| 28  | U     | 38  | LEU  | O-C-N  | -5.21 | 116.84      | 123.24   |
| 17  | J     | 342 | ASN  | N-CA-C | -5.20 | 98.80       | 107.80   |
| 18  | K     | 412 | ALA  | CA-C-N | 5.20  | 127.52      | 120.44   |
| 18  | K     | 412 | ALA  | C-N-CA | 5.20  | 127.52      | 120.44   |
| 10  | C     | 93  | ILE  | CA-C-N | 5.20  | 127.51      | 120.38   |
| 10  | C     | 93  | ILE  | C-N-CA | 5.20  | 127.51      | 120.38   |
| 10  | C     | 237 | ASP  | O-C-N  | 5.20  | 127.43      | 122.07   |
| 16  | I     | 312 | GLN  | O-C-N  | -5.20 | 116.61      | 122.12   |
| 22  | O     | 280 | LEU  | N-CA-C | 5.20  | 116.64      | 111.07   |
| 25  | R     | 294 | ILE  | CA-C-O | 5.20  | 126.36      | 120.95   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | D     | 115 | GLY  | CA-C-N  | 5.20  | 127.80      | 120.42   |
| 11  | D     | 115 | GLY  | C-N-CA  | 5.20  | 127.80      | 120.42   |
| 19  | L     | 260 | ALA  | CA-C-O  | -5.20 | 115.04      | 120.55   |
| 20  | M     | 332 | VAL  | CA-C-N  | 5.20  | 131.61      | 121.63   |
| 20  | M     | 332 | VAL  | C-N-CA  | 5.20  | 131.61      | 121.63   |
| 24  | Q     | 314 | PHE  | O-C-N   | 5.20  | 127.63      | 122.12   |
| 26  | S     | 182 | LYS  | O-C-N   | -5.20 | 116.61      | 122.12   |
| 7   | 7     | 89  | ALA  | N-CA-C  | 5.20  | 117.69      | 111.71   |
| 24  | Q     | 322 | GLU  | O-C-N   | -5.20 | 116.69      | 122.09   |
| 11  | D     | 50  | SER  | CB-CA-C | 5.20  | 119.10      | 109.70   |
| 3   | 3     | 144 | LEU  | CA-C-O  | 5.19  | 125.92      | 120.42   |
| 10  | C     | 237 | ASP  | CA-C-O  | -5.19 | 115.37      | 120.82   |
| 17  | J     | 235 | VAL  | CA-C-N  | 5.19  | 127.24      | 120.28   |
| 17  | J     | 235 | VAL  | C-N-CA  | 5.19  | 127.24      | 120.28   |
| 18  | K     | 127 | ASP  | O-C-N   | 5.19  | 129.69      | 122.78   |
| 19  | L     | 103 | GLN  | CA-C-N  | 5.19  | 130.95      | 122.07   |
| 19  | L     | 103 | GLN  | C-N-CA  | 5.19  | 130.95      | 122.07   |
| 24  | Q     | 58  | ILE  | CA-C-O  | -5.19 | 115.67      | 121.17   |
| 12  | E     | 161 | SER  | CA-C-N  | 5.19  | 129.66      | 122.29   |
| 12  | E     | 161 | SER  | C-N-CA  | 5.19  | 129.66      | 122.29   |
| 24  | Q     | 234 | THR  | CA-C-O  | -5.19 | 114.92      | 120.42   |
| 26  | S     | 444 | GLU  | N-CA-C  | -5.19 | 101.23      | 109.59   |
| 27  | T     | 188 | GLU  | CA-C-N  | 5.19  | 127.79      | 120.42   |
| 27  | T     | 188 | GLU  | C-N-CA  | 5.19  | 127.79      | 120.42   |
| 6   | 6     | 187 | ILE  | O-C-N   | 5.19  | 127.75      | 122.09   |
| 13  | F     | 162 | GLY  | O-C-N   | -5.19 | 116.44      | 122.87   |
| 22  | O     | 282 | GLN  | CA-C-O  | -5.19 | 115.37      | 120.82   |
| 14  | G     | 67  | GLN  | O-C-N   | 5.19  | 129.29      | 123.27   |
| 17  | J     | 101 | ASP  | O-C-N   | 5.19  | 128.52      | 122.24   |
| 17  | J     | 157 | ILE  | N-CA-C  | 5.19  | 115.40      | 110.42   |
| 23  | P     | 262 | SER  | CA-C-N  | 5.19  | 127.23      | 120.28   |
| 23  | P     | 262 | SER  | C-N-CA  | 5.19  | 127.23      | 120.28   |
| 33  | Z     | 254 | PRO  | CA-C-N  | -5.19 | 113.58      | 120.63   |
| 33  | Z     | 254 | PRO  | C-N-CA  | -5.19 | 113.58      | 120.63   |
| 6   | 6     | 78  | ASN  | CA-C-O  | 5.19  | 125.93      | 119.97   |
| 24  | Q     | 78  | ILE  | CA-C-N  | 5.19  | 124.81      | 119.05   |
| 24  | Q     | 78  | ILE  | C-N-CA  | 5.19  | 124.81      | 119.05   |
| 27  | T     | 100 | ASP  | N-CA-C  | 5.19  | 119.88      | 113.50   |
| 1   | 1     | 181 | ALA  | O-C-N   | -5.18 | 115.63      | 122.42   |
| 3   | 3     | 156 | GLU  | CA-C-N  | 5.18  | 127.50      | 120.65   |
| 3   | 3     | 156 | GLU  | C-N-CA  | 5.18  | 127.50      | 120.65   |
| 23  | P     | 135 | GLU  | CA-C-N  | 5.18  | 127.18      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 23  | P     | 135 | GLU  | C-N-CA | 5.18  | 127.18      | 120.44   |
| 11  | D     | 89  | ALA  | N-CA-C | 5.18  | 117.01      | 111.36   |
| 23  | P     | 121 | THR  | CA-C-O | -5.18 | 114.93      | 120.42   |
| 33  | Z     | 533 | VAL  | CA-C-O | -5.18 | 115.68      | 121.17   |
| 6   | 6     | 210 | LEU  | CA-C-N | 5.18  | 131.44      | 121.54   |
| 6   | 6     | 210 | LEU  | C-N-CA | 5.18  | 131.44      | 121.54   |
| 8   | A     | 226 | GLY  | N-CA-C | -5.18 | 102.39      | 111.46   |
| 11  | D     | 153 | SER  | O-C-N  | -5.18 | 116.16      | 122.22   |
| 22  | O     | 285 | SER  | O-C-N  | 5.18  | 128.06      | 122.15   |
| 2   | 2     | 193 | PRO  | CA-C-O | -5.18 | 111.17      | 120.60   |
| 12  | E     | 46  | VAL  | O-C-N  | -5.18 | 117.58      | 123.18   |
| 20  | M     | 232 | ALA  | CA-C-O | 5.18  | 126.26      | 120.82   |
| 24  | Q     | 368 | LEU  | CA-C-O | -5.18 | 115.57      | 121.68   |
| 25  | R     | 52  | ALA  | O-C-N  | 5.18  | 127.41      | 122.07   |
| 25  | R     | 228 | ALA  | N-CA-C | 5.18  | 116.92      | 111.28   |
| 8   | A     | 102 | ALA  | CA-C-N | 5.18  | 127.17      | 120.44   |
| 8   | A     | 102 | ALA  | C-N-CA | 5.18  | 127.17      | 120.44   |
| 21  | N     | 390 | LEU  | N-CA-C | -5.18 | 102.50      | 110.32   |
| 28  | U     | 301 | ILE  | CA-C-N | 5.18  | 127.17      | 120.44   |
| 28  | U     | 301 | ILE  | C-N-CA | 5.18  | 127.17      | 120.44   |
| 15  | H     | 326 | ASP  | N-CA-C | -5.18 | 106.28      | 112.59   |
| 31  | X     | 123 | ASN  | CA-C-O | -5.18 | 115.06      | 120.55   |
| 2   | 2     | 61  | SER  | CA-C-N | 5.17  | 127.73      | 120.28   |
| 2   | 2     | 61  | SER  | C-N-CA | 5.17  | 127.73      | 120.28   |
| 10  | C     | 172 | ALA  | N-CA-C | -5.17 | 105.55      | 111.14   |
| 15  | H     | 407 | ILE  | CA-C-O | -5.17 | 115.57      | 120.95   |
| 17  | J     | 87  | LYS  | O-C-N  | -5.17 | 116.89      | 123.05   |
| 33  | Z     | 373 | GLY  | CA-C-N | 5.17  | 133.09      | 121.76   |
| 33  | Z     | 373 | GLY  | C-N-CA | 5.17  | 133.09      | 121.76   |
| 3   | 3     | 135 | ASP  | CA-C-N | 5.17  | 127.17      | 120.44   |
| 3   | 3     | 135 | ASP  | C-N-CA | 5.17  | 127.17      | 120.44   |
| 7   | 7     | 189 | LEU  | O-C-N  | -5.17 | 116.96      | 123.27   |
| 7   | 7     | 134 | LEU  | N-CA-C | -5.17 | 100.87      | 108.99   |
| 16  | I     | 257 | LEU  | CA-C-O | 5.17  | 126.81      | 120.60   |
| 23  | P     | 187 | SER  | CA-C-O | -5.17 | 114.94      | 120.42   |
| 28  | U     | 231 | ASP  | O-C-N  | 5.17  | 127.40      | 122.07   |
| 13  | F     | 96  | SER  | CA-C-N | 5.17  | 127.47      | 120.44   |
| 13  | F     | 96  | SER  | C-N-CA | 5.17  | 127.47      | 120.44   |
| 22  | O     | 26  | PHE  | CA-C-O | 5.17  | 126.03      | 120.55   |
| 22  | O     | 69  | PHE  | CA-C-O | -5.17 | 115.39      | 120.82   |
| 25  | R     | 145 | GLY  | O-C-N  | 5.17  | 127.89      | 122.51   |
| 23  | P     | 126 | THR  | O-C-N  | -5.17 | 115.28      | 121.64   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | H     | 358 | PRO  | N-CA-C  | -5.17 | 107.44      | 114.98   |
| 17  | J     | 390 | MET  | O-C-N   | -5.17 | 116.64      | 122.12   |
| 21  | N     | 726 | ASP  | CA-C-N  | 5.17  | 127.16      | 120.44   |
| 21  | N     | 726 | ASP  | C-N-CA  | 5.17  | 127.16      | 120.44   |
| 33  | Z     | 848 | THR  | CA-C-N  | 5.17  | 127.16      | 120.44   |
| 33  | Z     | 848 | THR  | C-N-CA  | 5.17  | 127.16      | 120.44   |
| 5   | 5     | 87  | VAL  | N-CA-C  | 5.17  | 116.51      | 110.62   |
| 19  | L     | 349 | ILE  | CA-C-O  | 5.16  | 124.58      | 119.62   |
| 21  | N     | 594 | VAL  | N-CA-C  | -5.16 | 105.35      | 110.62   |
| 25  | R     | 90  | GLU  | N-CA-C  | -5.16 | 104.59      | 111.87   |
| 18  | K     | 330 | ARG  | N-CA-C  | 5.16  | 117.02      | 109.84   |
| 33  | Z     | 926 | ASN  | N-CA-C  | -5.16 | 100.62      | 109.24   |
| 9   | B     | 67  | LEU  | N-CA-C  | -5.16 | 105.82      | 112.68   |
| 24  | Q     | 396 | TRP  | CA-C-N  | 5.16  | 129.84      | 122.72   |
| 24  | Q     | 396 | TRP  | C-N-CA  | 5.16  | 129.84      | 122.72   |
| 1   | 1     | 187 | ILE  | N-CA-C  | -5.16 | 100.69      | 108.12   |
| 5   | 5     | 197 | PHE  | CA-C-N  | 5.16  | 127.19      | 120.28   |
| 5   | 5     | 197 | PHE  | C-N-CA  | 5.16  | 127.19      | 120.28   |
| 13  | F     | 182 | ILE  | N-CA-C  | -5.16 | 99.04       | 106.88   |
| 20  | M     | 214 | ALA  | CB-CA-C | 5.16  | 116.38      | 109.42   |
| 6   | 6     | 22  | THR  | N-CA-C  | -5.16 | 99.26       | 108.13   |
| 12  | E     | 222 | ILE  | CB-CA-C | 5.16  | 118.43      | 110.28   |
| 21  | N     | 870 | ASN  | N-CA-C  | 5.16  | 117.77      | 110.50   |
| 22  | O     | 21  | SER  | N-CA-C  | -5.16 | 106.80      | 114.64   |
| 28  | U     | 193 | GLN  | CA-C-O  | -5.16 | 115.41      | 120.82   |
| 18  | K     | 217 | THR  | CA-C-O  | 5.16  | 124.72      | 119.05   |
| 21  | N     | 123 | PHE  | O-C-N   | 5.16  | 127.58      | 122.12   |
| 24  | Q     | 409 | TYR  | CA-C-N  | 5.16  | 127.14      | 120.44   |
| 24  | Q     | 409 | TYR  | C-N-CA  | 5.16  | 127.14      | 120.44   |
| 8   | A     | 87  | ILE  | N-CA-C  | 5.15  | 120.01      | 108.88   |
| 1   | 1     | 136 | GLY  | CA-C-N  | 5.15  | 127.14      | 120.44   |
| 1   | 1     | 136 | GLY  | C-N-CA  | 5.15  | 127.14      | 120.44   |
| 12  | E     | 188 | HIS  | CA-C-O  | 5.15  | 126.76      | 120.99   |
| 13  | F     | 68  | GLU  | CA-C-O  | 5.15  | 126.70      | 119.80   |
| 18  | K     | 358 | SER  | CA-C-N  | 5.15  | 127.70      | 120.28   |
| 18  | K     | 358 | SER  | C-N-CA  | 5.15  | 127.70      | 120.28   |
| 21  | N     | 683 | LEU  | CA-C-N  | 5.15  | 127.44      | 120.38   |
| 21  | N     | 683 | LEU  | C-N-CA  | 5.15  | 127.44      | 120.38   |
| 23  | P     | 216 | LEU  | CA-C-O  | 5.15  | 125.88      | 120.42   |
| 33  | Z     | 152 | GLU  | O-C-N   | 5.15  | 127.58      | 122.12   |
| 14  | G     | 54  | THR  | CA-C-O  | 5.15  | 124.42      | 118.55   |
| 21  | N     | 242 | PHE  | N-CA-C  | 5.15  | 117.80      | 111.82   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 22  | O     | 328 | VAL  | CA-C-N | 5.15  | 127.18      | 120.28   |
| 22  | O     | 328 | VAL  | C-N-CA | 5.15  | 127.18      | 120.28   |
| 24  | Q     | 293 | SER  | N-CA-C | -5.15 | 101.63      | 108.74   |
| 2   | 2     | 38  | SER  | O-C-N  | -5.15 | 115.40      | 121.32   |
| 15  | H     | 328 | GLU  | CA-C-N | 5.15  | 127.73      | 120.42   |
| 15  | H     | 328 | GLU  | C-N-CA | 5.15  | 127.73      | 120.42   |
| 3   | 3     | 140 | MET  | O-C-N  | -5.15 | 116.77      | 122.07   |
| 4   | 4     | -1  | MET  | CA-C-N | 5.15  | 130.66      | 122.74   |
| 4   | 4     | -1  | MET  | C-N-CA | 5.15  | 130.66      | 122.74   |
| 14  | G     | 203 | HIS  | N-CA-C | -5.15 | 106.26      | 112.54   |
| 4   | 4     | 57  | GLU  | CA-C-N | 5.14  | 127.44      | 120.44   |
| 4   | 4     | 57  | GLU  | C-N-CA | 5.14  | 127.44      | 120.44   |
| 25  | R     | 330 | VAL  | CA-C-N | 5.14  | 127.59      | 120.29   |
| 25  | R     | 330 | VAL  | C-N-CA | 5.14  | 127.59      | 120.29   |
| 28  | U     | 9   | THR  | CA-C-O | -5.14 | 114.80      | 120.36   |
| 7   | 7     | 178 | TYR  | CA-C-O | -5.14 | 115.40      | 120.70   |
| 14  | G     | 118 | TYR  | CA-C-N | 5.14  | 127.72      | 120.42   |
| 14  | G     | 118 | TYR  | C-N-CA | 5.14  | 127.72      | 120.42   |
| 19  | L     | 181 | ASP  | O-C-N  | 5.14  | 129.16      | 122.42   |
| 26  | S     | 257 | LEU  | O-C-N  | -5.14 | 116.67      | 122.12   |
| 17  | J     | 171 | PRO  | CA-C-N | 5.14  | 127.17      | 120.28   |
| 17  | J     | 171 | PRO  | C-N-CA | 5.14  | 127.17      | 120.28   |
| 22  | O     | 165 | LEU  | CA-C-N | 5.14  | 128.53      | 120.82   |
| 22  | O     | 165 | LEU  | C-N-CA | 5.14  | 128.53      | 120.82   |
| 26  | S     | 182 | LYS  | CA-C-O | 5.14  | 126.18      | 120.63   |
| 33  | Z     | 531 | ALA  | O-C-N  | 5.14  | 127.36      | 122.07   |
| 8   | A     | 152 | PRO  | O-C-N  | -5.14 | 116.36      | 122.89   |
| 18  | K     | 152 | PRO  | O-C-N  | 5.14  | 127.92      | 122.93   |
| 18  | K     | 327 | ALA  | CA-C-N | 5.14  | 127.59      | 120.29   |
| 18  | K     | 327 | ALA  | C-N-CA | 5.14  | 127.59      | 120.29   |
| 18  | K     | 387 | MET  | CA-C-N | 5.14  | 127.59      | 120.29   |
| 18  | K     | 387 | MET  | C-N-CA | 5.14  | 127.59      | 120.29   |
| 19  | L     | 91  | THR  | CA-C-N | 5.14  | 127.59      | 120.29   |
| 19  | L     | 91  | THR  | C-N-CA | 5.14  | 127.59      | 120.29   |
| 21  | N     | 25  | LEU  | O-C-N  | 5.14  | 127.44      | 122.09   |
| 19  | L     | 323 | ILE  | O-C-N  | -5.14 | 117.63      | 123.18   |
| 24  | Q     | 91  | SER  | CA-C-N | 5.14  | 127.58      | 120.29   |
| 24  | Q     | 91  | SER  | C-N-CA | 5.14  | 127.58      | 120.29   |
| 28  | U     | 80  | CYS  | CA-C-N | 5.14  | 127.16      | 120.28   |
| 28  | U     | 80  | CYS  | C-N-CA | 5.14  | 127.16      | 120.28   |
| 4   | 4     | 72  | TYR  | CA-C-N | 5.13  | 128.00      | 120.71   |
| 4   | 4     | 72  | TYR  | C-N-CA | 5.13  | 128.00      | 120.71   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | F     | 89  | ARG  | CA-C-N  | 5.13  | 127.16      | 120.28   |
| 13  | F     | 89  | ARG  | C-N-CA  | 5.13  | 127.16      | 120.28   |
| 24  | Q     | 353 | PRO  | CA-C-N  | 5.13  | 131.35      | 121.54   |
| 24  | Q     | 353 | PRO  | C-N-CA  | 5.13  | 131.35      | 121.54   |
| 26  | S     | 136 | CYS  | CA-C-N  | 5.13  | 127.11      | 120.44   |
| 26  | S     | 136 | CYS  | C-N-CA  | 5.13  | 127.11      | 120.44   |
| 12  | E     | 56  | SER  | O-C-N   | 5.13  | 125.40      | 121.65   |
| 15  | H     | 396 | MET  | N-CA-C  | 5.13  | 121.73      | 110.80   |
| 19  | L     | 79  | GLN  | CA-C-N  | 5.13  | 127.11      | 120.44   |
| 19  | L     | 79  | GLN  | C-N-CA  | 5.13  | 127.11      | 120.44   |
| 22  | O     | 166 | ARG  | N-CA-C  | 5.13  | 119.84      | 111.37   |
| 25  | R     | 345 | TYR  | CA-C-O  | -5.13 | 115.63      | 121.58   |
| 19  | L     | 308 | LEU  | CA-C-O  | 5.13  | 126.21      | 120.82   |
| 33  | Z     | 236 | PHE  | CA-C-O  | -5.13 | 115.11      | 120.55   |
| 6   | 6     | 183 | THR  | CA-C-N  | 5.13  | 127.15      | 120.28   |
| 6   | 6     | 183 | THR  | C-N-CA  | 5.13  | 127.15      | 120.28   |
| 14  | G     | 96  | ALA  | O-C-N   | 5.13  | 127.56      | 122.12   |
| 15  | H     | 297 | MET  | CA-C-O  | 5.13  | 125.86      | 120.42   |
| 16  | I     | 270 | VAL  | CA-C-N  | 5.13  | 127.11      | 120.44   |
| 16  | I     | 270 | VAL  | C-N-CA  | 5.13  | 127.11      | 120.44   |
| 19  | L     | 297 | ALA  | N-CA-C  | -5.13 | 104.80      | 112.54   |
| 21  | N     | 646 | LYS  | N-CA-C  | -5.13 | 106.87      | 112.72   |
| 28  | U     | 114 | THR  | N-CA-C  | 5.13  | 118.09      | 110.14   |
| 33  | Z     | 751 | ASP  | CA-C-N  | 5.13  | 127.70      | 120.42   |
| 33  | Z     | 751 | ASP  | C-N-CA  | 5.13  | 127.70      | 120.42   |
| 2   | 2     | 50  | ALA  | N-CA-C  | 5.13  | 116.87      | 111.28   |
| 2   | 2     | 155 | ALA  | O-C-N   | -5.13 | 116.69      | 122.12   |
| 6   | 6     | 92  | ARG  | N-CA-C  | -5.13 | 106.80      | 113.16   |
| 14  | G     | 63  | ASN  | CA-C-N  | 5.13  | 127.37      | 120.50   |
| 14  | G     | 63  | ASN  | C-N-CA  | 5.13  | 127.37      | 120.50   |
| 15  | H     | 385 | ARG  | N-CA-C  | -5.13 | 105.69      | 111.28   |
| 23  | P     | 285 | GLN  | N-CA-C  | -5.13 | 105.71      | 112.94   |
| 24  | Q     | 236 | PHE  | CA-C-N  | 5.13  | 127.57      | 120.29   |
| 24  | Q     | 236 | PHE  | C-N-CA  | 5.13  | 127.57      | 120.29   |
| 33  | Z     | 208 | VAL  | CB-CA-C | -5.13 | 107.28      | 114.00   |
| 11  | D     | 151 | GLU  | CA-C-O  | -5.12 | 115.78      | 120.50   |
| 2   | 2     | 111 | PHE  | N-CA-C  | -5.12 | 101.62      | 109.41   |
| 22  | O     | 97  | LYS  | N-CA-C  | 5.12  | 116.86      | 111.28   |
| 25  | R     | 264 | THR  | O-C-N   | -5.12 | 116.31      | 122.15   |
| 26  | S     | 190 | SER  | CA-C-N  | 5.12  | 129.28      | 120.72   |
| 26  | S     | 190 | SER  | C-N-CA  | 5.12  | 129.28      | 120.72   |
| 26  | S     | 358 | LYS  | O-C-N   | 5.12  | 127.55      | 122.12   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 28  | U     | 165 | GLU  | N-CA-C | 5.12  | 118.31      | 111.75   |
| 3   | 3     | -4  | SER  | O-C-N  | -5.12 | 115.96      | 122.26   |
| 15  | H     | 235 | PHE  | CA-C-N | 5.12  | 127.14      | 120.28   |
| 15  | H     | 235 | PHE  | C-N-CA | 5.12  | 127.14      | 120.28   |
| 16  | I     | 115 | ASP  | N-CA-C | -5.12 | 106.62      | 112.92   |
| 19  | L     | 306 | MET  | CA-C-N | 5.12  | 127.56      | 120.29   |
| 19  | L     | 306 | MET  | C-N-CA | 5.12  | 127.56      | 120.29   |
| 20  | M     | 411 | LYS  | N-CA-C | -5.12 | 101.51      | 109.14   |
| 30  | W     | 4   | GLU  | N-CA-C | 5.12  | 117.51      | 108.75   |
| 33  | Z     | 405 | ASN  | CA-C-N | 5.12  | 127.10      | 120.44   |
| 33  | Z     | 405 | ASN  | C-N-CA | 5.12  | 127.10      | 120.44   |
| 8   | A     | 225 | VAL  | CA-C-O | 5.12  | 125.79      | 120.36   |
| 10  | C     | 41  | SER  | O-C-N  | -5.12 | 115.79      | 122.39   |
| 13  | F     | 43  | HIS  | N-CA-C | -5.12 | 101.59      | 109.52   |
| 17  | J     | 106 | ASP  | N-CA-C | -5.12 | 106.72      | 113.17   |
| 3   | 3     | 56  | GLU  | CA-C-N | 5.12  | 127.55      | 120.29   |
| 3   | 3     | 56  | GLU  | C-N-CA | 5.12  | 127.55      | 120.29   |
| 10  | C     | 140 | TYR  | N-CA-C | -5.12 | 101.42      | 109.50   |
| 33  | Z     | 567 | ALA  | CA-C-N | 5.12  | 127.14      | 120.28   |
| 33  | Z     | 567 | ALA  | C-N-CA | 5.12  | 127.14      | 120.28   |
| 33  | Z     | 117 | ASP  | N-CA-C | 5.11  | 116.85      | 111.28   |
| 33  | Z     | 206 | ASP  | CA-C-N | 5.11  | 127.47      | 120.46   |
| 33  | Z     | 206 | ASP  | C-N-CA | 5.11  | 127.47      | 120.46   |
| 7   | 7     | 194 | LYS  | N-CA-C | -5.11 | 106.55      | 112.89   |
| 9   | B     | 192 | ALA  | CA-C-O | 5.11  | 125.84      | 120.42   |
| 1   | 1     | 51  | ASP  | O-C-N  | 5.11  | 127.33      | 122.07   |
| 16  | I     | 165 | ASP  | CA-C-N | 5.11  | 126.23      | 119.84   |
| 16  | I     | 165 | ASP  | C-N-CA | 5.11  | 126.23      | 119.84   |
| 22  | O     | 324 | VAL  | CA-C-N | 5.11  | 127.13      | 120.28   |
| 22  | O     | 324 | VAL  | C-N-CA | 5.11  | 127.13      | 120.28   |
| 22  | O     | 372 | GLU  | CA-C-N | 5.11  | 127.44      | 120.54   |
| 22  | O     | 372 | GLU  | C-N-CA | 5.11  | 127.44      | 120.54   |
| 23  | P     | 287 | ASP  | CA-C-O | 5.11  | 124.12      | 118.65   |
| 6   | 6     | 116 | PHE  | CA-C-N | 5.11  | 130.75      | 122.48   |
| 6   | 6     | 116 | PHE  | C-N-CA | 5.11  | 130.75      | 122.48   |
| 19  | L     | 312 | MET  | O-C-N  | 5.11  | 127.61      | 122.09   |
| 26  | S     | 338 | MET  | CA-C-N | 5.11  | 127.64      | 120.28   |
| 26  | S     | 338 | MET  | C-N-CA | 5.11  | 127.64      | 120.28   |
| 29  | V     | 261 | LEU  | CA-C-O | -5.11 | 115.46      | 120.82   |
| 33  | Z     | 160 | GLU  | CA-C-N | 5.11  | 127.00      | 120.56   |
| 33  | Z     | 160 | GLU  | C-N-CA | 5.11  | 127.00      | 120.56   |
| 8   | A     | 88  | PRO  | CA-C-N | 5.11  | 128.07      | 120.31   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 8   | A     | 88  | PRO  | C-N-CA     | 5.11  | 128.07      | 120.31   |
| 9   | B     | 78  | MET  | CA-C-N     | 5.11  | 129.88      | 121.87   |
| 9   | B     | 78  | MET  | C-N-CA     | 5.11  | 129.88      | 121.87   |
| 9   | B     | 116 | LYS  | N-CA-C     | -5.11 | 105.80      | 111.36   |
| 11  | D     | 132 | SER  | N-CA-C     | -5.11 | 101.55      | 109.72   |
| 11  | D     | 232 | TYR  | N-CA-C     | -5.11 | 105.41      | 111.69   |
| 12  | E     | 131 | GLU  | CA-C-O     | -5.11 | 115.44      | 121.16   |
| 23  | P     | 166 | GLU  | O-C-N      | -5.11 | 116.71      | 122.12   |
| 30  | W     | 146 | GLU  | N-CA-C     | -5.11 | 107.18      | 113.41   |
| 8   | A     | 20  | SER  | N-CA-C     | -5.10 | 103.52      | 110.36   |
| 21  | N     | 19  | SER  | CA-C-N     | 5.10  | 127.67      | 120.42   |
| 21  | N     | 19  | SER  | C-N-CA     | 5.10  | 127.67      | 120.42   |
| 11  | D     | 170 | THR  | O-C-N      | 5.10  | 127.60      | 122.09   |
| 29  | V     | 162 | GLY  | CA-C-N     | 5.10  | 131.29      | 121.54   |
| 29  | V     | 162 | GLY  | C-N-CA     | 5.10  | 131.29      | 121.54   |
| 1   | 1     | 148 | LYS  | CA-C-O     | -5.10 | 115.44      | 120.90   |
| 21  | N     | 882 | ILE  | CA-C-N     | 5.10  | 130.22      | 122.11   |
| 21  | N     | 882 | ILE  | C-N-CA     | 5.10  | 130.22      | 122.11   |
| 9   | B     | 41  | ASN  | O-C-N      | 5.10  | 128.41      | 122.24   |
| 16  | I     | 380 | LEU  | CA-C-N     | 5.10  | 127.45      | 120.46   |
| 16  | I     | 380 | LEU  | C-N-CA     | 5.10  | 127.45      | 120.46   |
| 25  | R     | 141 | TYR  | CA-C-O     | -5.10 | 113.77      | 119.79   |
| 26  | S     | 242 | LEU  | N-CA-C     | 5.10  | 116.92      | 111.36   |
| 26  | S     | 442 | PHE  | CA-C-O     | 5.10  | 126.87      | 121.11   |
| 28  | U     | 170 | GLY  | CA-C-N     | 5.10  | 127.18      | 120.60   |
| 28  | U     | 170 | GLY  | C-N-CA     | 5.10  | 127.18      | 120.60   |
| 3   | 3     | 82  | VAL  | N-CA-C     | 5.10  | 115.31      | 110.42   |
| 16  | I     | 159 | VAL  | CA-C-O     | -5.10 | 116.22      | 121.93   |
| 21  | N     | 271 | GLU  | O-C-N      | 5.10  | 127.32      | 122.07   |
| 23  | P     | 196 | ALA  | O-C-N      | 5.10  | 127.96      | 122.15   |
| 25  | R     | 221 | VAL  | O-C-N      | 5.10  | 127.56      | 121.80   |
| 18  | K     | 225 | ALA  | CA-C-N     | 5.10  | 127.44      | 120.46   |
| 18  | K     | 225 | ALA  | C-N-CA     | 5.10  | 127.44      | 120.46   |
| 20  | M     | 274 | ALA  | CA-C-O     | -5.10 | 113.18      | 120.16   |
| 21  | N     | 582 | ASP  | O-C-N      | 5.10  | 127.59      | 122.09   |
| 33  | Z     | 599 | ILE  | CA-C-O     | 5.10  | 125.97      | 120.47   |
| 19  | L     | 180 | PHE  | N-CA-C     | -5.09 | 107.06      | 113.28   |
| 22  | O     | 376 | GLN  | CA-C-O     | 5.09  | 126.17      | 120.82   |
| 33  | Z     | 182 | SER  | CA-C-O     | 5.09  | 125.17      | 119.41   |
| 19  | L     | 342 | ARG  | N-CA-C     | -5.09 | 99.95       | 110.80   |
| 20  | M     | 299 | ARG  | NH1-CZ-NH2 | -5.09 | 112.68      | 119.30   |
| 24  | Q     | 266 | LEU  | CA-C-N     | 5.09  | 127.11      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 24  | Q     | 266 | LEU  | C-N-CA | 5.09  | 127.11      | 120.28   |
| 5   | 5     | 145 | LYS  | CA-C-N | 5.09  | 127.52      | 120.29   |
| 5   | 5     | 145 | LYS  | C-N-CA | 5.09  | 127.52      | 120.29   |
| 11  | D     | 125 | GLY  | N-CA-C | -5.09 | 109.02      | 115.08   |
| 15  | H     | 330 | GLN  | CA-C-O | 5.09  | 125.89      | 120.24   |
| 19  | L     | 358 | LEU  | CA-C-N | 5.09  | 127.36      | 120.44   |
| 19  | L     | 358 | LEU  | C-N-CA | 5.09  | 127.36      | 120.44   |
| 3   | 3     | 189 | ARG  | N-CA-C | -5.09 | 100.16      | 108.76   |
| 5   | 5     | 210 | VAL  | CA-C-O | -5.09 | 114.88      | 120.48   |
| 17  | J     | 83  | LYS  | CA-C-O | -5.09 | 115.40      | 121.56   |
| 22  | O     | 357 | ILE  | N-CA-C | -5.09 | 101.14      | 108.42   |
| 11  | D     | 59  | ILE  | N-CA-C | -5.09 | 108.16      | 113.10   |
| 24  | Q     | 332 | ARG  | CA-C-O | -5.09 | 115.16      | 120.55   |
| 6   | 6     | 131 | GLY  | N-CA-C | -5.09 | 104.57      | 112.45   |
| 18  | K     | 64  | GLN  | O-C-N  | 5.09  | 127.95      | 122.15   |
| 20  | M     | 376 | TRP  | CA-C-N | 5.09  | 127.05      | 120.44   |
| 20  | M     | 376 | TRP  | C-N-CA | 5.09  | 127.05      | 120.44   |
| 2   | 2     | 194 | ASN  | CA-C-O | -5.08 | 115.65      | 121.40   |
| 17  | J     | 174 | PHE  | CA-C-O | 5.08  | 125.81      | 120.42   |
| 9   | B     | 69  | PRO  | CA-C-N | 5.08  | 131.58      | 122.38   |
| 9   | B     | 69  | PRO  | C-N-CA | 5.08  | 131.58      | 122.38   |
| 10  | C     | 197 | LEU  | N-CA-C | -5.08 | 105.74      | 111.28   |
| 10  | C     | 202 | ASP  | CA-C-O | 5.08  | 125.83      | 119.78   |
| 11  | D     | 153 | SER  | CA-C-O | 5.08  | 125.84      | 120.10   |
| 16  | I     | 381 | VAL  | N-CA-C | 5.08  | 115.80      | 110.62   |
| 8   | A     | 49  | ASP  | N-CA-C | -5.08 | 106.22      | 114.09   |
| 13  | F     | 136 | GLY  | O-C-N  | -5.08 | 119.03      | 123.76   |
| 21  | N     | 169 | ALA  | N-CA-C | 5.08  | 116.50      | 111.07   |
| 24  | Q     | 199 | THR  | CA-C-N | 5.08  | 127.09      | 120.28   |
| 24  | Q     | 199 | THR  | C-N-CA | 5.08  | 127.09      | 120.28   |
| 2   | 2     | 106 | THR  | CA-C-O | 5.08  | 124.73      | 119.14   |
| 7   | 7     | 159 | LYS  | N-CA-C | -5.08 | 106.67      | 112.92   |
| 13  | F     | 12  | THR  | CA-C-O | -5.08 | 115.98      | 121.36   |
| 20  | M     | 245 | LYS  | N-CA-C | -5.08 | 100.45      | 108.73   |
| 30  | W     | 113 | PHE  | CA-C-N | 5.08  | 130.12      | 123.11   |
| 30  | W     | 113 | PHE  | C-N-CA | 5.08  | 130.12      | 123.11   |
| 11  | D     | 4   | TYR  | N-CA-C | -5.08 | 100.79      | 108.46   |
| 21  | N     | 170 | LEU  | N-CA-C | -5.08 | 105.66      | 111.14   |
| 21  | N     | 613 | HIS  | CA-C-N | 5.08  | 131.24      | 121.54   |
| 21  | N     | 613 | HIS  | C-N-CA | 5.08  | 131.24      | 121.54   |
| 22  | O     | 130 | ASP  | N-CA-C | -5.08 | 105.75      | 111.28   |
| 19  | L     | 191 | ARG  | CA-C-O | 5.08  | 125.80      | 120.42   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 27  | T     | 232 | LYS  | N-CA-C   | 5.08  | 117.43      | 108.75   |
| 33  | Z     | 470 | ALA  | N-CA-C   | 5.08  | 118.57      | 112.38   |
| 14  | G     | 66  | ILE  | N-CA-C   | -5.07 | 101.10      | 108.36   |
| 20  | M     | 277 | ILE  | CB-CA-C  | 5.07  | 118.14      | 110.63   |
| 25  | R     | 170 | VAL  | CA-C-N   | 5.07  | 127.08      | 120.28   |
| 25  | R     | 170 | VAL  | C-N-CA   | 5.07  | 127.08      | 120.28   |
| 26  | S     | 280 | ASN  | N-CA-C   | -5.07 | 105.94      | 111.82   |
| 27  | T     | 264 | MET  | CA-C-O   | -5.07 | 115.50      | 120.82   |
| 8   | A     | 160 | ALA  | O-C-N    | 5.07  | 127.29      | 122.07   |
| 27  | T     | 132 | HIS  | N-CA-C   | -5.07 | 105.40      | 111.03   |
| 30  | W     | 86  | HIS  | N-CA-C   | -5.07 | 101.91      | 109.11   |
| 6   | 6     | 107 | GLU  | N-CA-C   | -5.07 | 107.05      | 113.18   |
| 13  | F     | 144 | LEU  | CA-C-O   | 5.07  | 126.51      | 120.28   |
| 2   | 2     | 44  | ALA  | N-CA-C   | -5.07 | 101.89      | 109.95   |
| 15  | H     | 336 | LEU  | N-CA-C   | 5.07  | 116.80      | 111.28   |
| 10  | C     | 235 | ILE  | CA-C-N   | 5.07  | 127.07      | 120.28   |
| 10  | C     | 235 | ILE  | C-N-CA   | 5.07  | 127.07      | 120.28   |
| 5   | 5     | 86  | LEU  | CA-C-N   | 5.06  | 127.67      | 120.53   |
| 5   | 5     | 86  | LEU  | C-N-CA   | 5.06  | 127.67      | 120.53   |
| 2   | 2     | 142 | TRP  | N-CA-C   | -5.06 | 103.47      | 110.35   |
| 5   | 5     | 9   | GLN  | O-C-N    | 5.06  | 127.36      | 122.09   |
| 10  | C     | 140 | TYR  | O-C-N    | -5.06 | 117.01      | 123.24   |
| 16  | I     | 93  | LYS  | CA-C-N   | 5.06  | 127.02      | 120.44   |
| 16  | I     | 93  | LYS  | C-N-CA   | 5.06  | 127.02      | 120.44   |
| 17  | J     | 83  | LYS  | O-C-N    | 5.06  | 129.63      | 123.10   |
| 19  | L     | 149 | ASP  | N-CA-C   | 5.06  | 117.23      | 110.35   |
| 23  | P     | 362 | LEU  | O-C-N    | 5.06  | 127.92      | 122.15   |
| 25  | R     | 137 | LEU  | O-C-N    | -5.06 | 116.04      | 122.27   |
| 33  | Z     | 888 | LEU  | O-C-N    | 5.06  | 128.14      | 122.32   |
| 9   | B     | 194 | LEU  | O-C-N    | 5.06  | 127.56      | 122.09   |
| 18  | K     | 287 | GLY  | CA-C-N   | 5.06  | 127.90      | 120.71   |
| 18  | K     | 287 | GLY  | C-N-CA   | 5.06  | 127.90      | 120.71   |
| 20  | M     | 335 | PRO  | N-CA-C   | -5.06 | 107.14      | 114.18   |
| 8   | A     | 163 | TYR  | N-CA-C   | -5.06 | 100.77      | 108.76   |
| 8   | A     | 252 | ASP  | CA-CB-CG | 5.06  | 117.66      | 112.60   |
| 25  | R     | 417 | TYR  | O-C-N    | 5.06  | 127.48      | 122.12   |
| 4   | 4     | 60  | GLN  | CA-C-N   | 5.06  | 127.02      | 120.44   |
| 4   | 4     | 60  | GLN  | C-N-CA   | 5.06  | 127.02      | 120.44   |
| 6   | 6     | 71  | ASN  | N-CA-C   | 5.06  | 118.18      | 111.30   |
| 14  | G     | 84  | GLY  | CA-C-N   | 5.06  | 127.06      | 120.28   |
| 14  | G     | 84  | GLY  | C-N-CA   | 5.06  | 127.06      | 120.28   |
| 16  | I     | 96  | LEU  | CA-C-N   | 5.06  | 128.00      | 120.31   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | I     | 96  | LEU  | C-N-CA | 5.06  | 128.00      | 120.31   |
| 16  | I     | 290 | LYS  | CA-C-O | 5.06  | 125.78      | 120.42   |
| 29  | V     | 25  | GLU  | CA-C-O | 5.06  | 126.48      | 120.66   |
| 24  | Q     | 373 | VAL  | O-C-N  | 5.06  | 126.86      | 121.91   |
| 9   | B     | 10  | THR  | CA-C-N | 5.05  | 130.53      | 122.59   |
| 9   | B     | 10  | THR  | C-N-CA | 5.05  | 130.53      | 122.59   |
| 15  | H     | 265 | ASN  | CA-C-O | 5.05  | 126.13      | 120.82   |
| 19  | L     | 73  | GLN  | CA-C-N | 5.05  | 127.05      | 120.28   |
| 19  | L     | 73  | GLN  | C-N-CA | 5.05  | 127.05      | 120.28   |
| 19  | L     | 243 | PHE  | N-CA-C | -5.05 | 101.07      | 109.46   |
| 23  | P     | 233 | GLU  | N-CA-C | -5.05 | 99.02       | 108.02   |
| 6   | 6     | 61  | ASN  | CA-C-O | -5.05 | 113.83      | 119.79   |
| 21  | N     | 208 | ARG  | O-C-N  | 5.05  | 128.13      | 122.22   |
| 23  | P     | 234 | TYR  | O-C-N  | -5.05 | 115.56      | 122.33   |
| 33  | Z     | 85  | VAL  | N-CA-C | -5.05 | 104.32      | 109.02   |
| 3   | 3     | 100 | VAL  | O-C-N  | -5.05 | 117.73      | 123.18   |
| 8   | A     | 104 | PHE  | CA-C-N | 5.05  | 127.05      | 120.28   |
| 8   | A     | 104 | PHE  | C-N-CA | 5.05  | 127.05      | 120.28   |
| 21  | N     | 547 | LEU  | O-C-N  | -5.05 | 116.06      | 122.27   |
| 17  | J     | 115 | LEU  | CA-C-N | 5.05  | 128.04      | 120.87   |
| 17  | J     | 115 | LEU  | C-N-CA | 5.05  | 128.04      | 120.87   |
| 19  | L     | 157 | ARG  | O-C-N  | -5.05 | 117.30      | 123.10   |
| 26  | S     | 137 | PHE  | CA-C-O | -5.05 | 115.52      | 120.82   |
| 1   | 1     | 180 | ALA  | O-C-N  | 5.05  | 128.90      | 122.39   |
| 16  | I     | 140 | LEU  | N-CA-C | -5.05 | 106.71      | 112.92   |
| 21  | N     | 98  | VAL  | N-CA-C | 5.05  | 115.82      | 110.72   |
| 30  | W     | 104 | LYS  | CA-C-N | 5.05  | 128.92      | 120.64   |
| 30  | W     | 104 | LYS  | C-N-CA | 5.05  | 128.92      | 120.64   |
| 5   | 5     | 94  | GLY  | CA-C-O | 5.04  | 124.61      | 119.01   |
| 18  | K     | 124 | SER  | N-CA-C | -5.04 | 107.09      | 113.20   |
| 21  | N     | 311 | ILE  | CA-C-N | 5.04  | 125.58      | 119.98   |
| 21  | N     | 311 | ILE  | C-N-CA | 5.04  | 125.58      | 119.98   |
| 27  | T     | 129 | LEU  | CA-C-N | 5.04  | 127.35      | 120.54   |
| 27  | T     | 129 | LEU  | C-N-CA | 5.04  | 127.35      | 120.54   |
| 1   | 1     | 56  | ALA  | CA-C-O | -5.04 | 114.17      | 119.97   |
| 24  | Q     | 373 | VAL  | CA-C-O | -5.04 | 115.83      | 121.17   |
| 6   | 6     | 143 | ASN  | N-CA-C | 5.04  | 116.58      | 111.14   |
| 12  | E     | 115 | SER  | N-CA-C | 5.04  | 116.78      | 111.28   |
| 15  | H     | 350 | LYS  | N-CA-C | -5.04 | 101.94      | 109.95   |
| 24  | Q     | 335 | PHE  | CA-C-N | 5.04  | 126.99      | 120.44   |
| 24  | Q     | 335 | PHE  | C-N-CA | 5.04  | 126.99      | 120.44   |
| 23  | P     | 401 | ASN  | N-CA-C | -5.04 | 102.31      | 110.32   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 3     | 94  | TYR  | O-C-N    | -5.04 | 117.34      | 123.03   |
| 10  | C     | 211 | LEU  | CA-C-N   | 5.04  | 130.09      | 122.99   |
| 10  | C     | 211 | LEU  | C-N-CA   | 5.04  | 130.09      | 122.99   |
| 19  | L     | 178 | ILE  | CA-C-O   | -5.04 | 116.64      | 121.63   |
| 31  | X     | 86  | ILE  | O-C-N    | -5.04 | 117.60      | 122.99   |
| 32  | Y     | 79  | ALA  | CA-C-O   | 5.04  | 126.29      | 120.90   |
| 12  | E     | 42  | THR  | N-CA-C   | -5.04 | 102.03      | 109.18   |
| 22  | O     | 227 | ILE  | CA-C-N   | 5.04  | 131.16      | 121.54   |
| 22  | O     | 227 | ILE  | C-N-CA   | 5.04  | 131.16      | 121.54   |
| 4   | 4     | 58  | TYR  | CA-C-N   | 5.04  | 127.57      | 120.42   |
| 4   | 4     | 58  | TYR  | C-N-CA   | 5.04  | 127.57      | 120.42   |
| 7   | 7     | 37  | VAL  | CA-C-O   | -5.04 | 114.94      | 120.48   |
| 11  | D     | 242 | GLU  | CA-C-O   | 5.04  | 126.05      | 120.71   |
| 17  | J     | 122 | LEU  | N-CA-C   | -5.04 | 100.86      | 108.67   |
| 19  | L     | 392 | ARG  | CA-C-N   | 5.04  | 127.03      | 120.28   |
| 19  | L     | 392 | ARG  | C-N-CA   | 5.04  | 127.03      | 120.28   |
| 24  | Q     | 252 | HIS  | O-C-N    | -5.04 | 115.42      | 122.37   |
| 25  | R     | 335 | ARG  | CA-C-N   | 5.04  | 127.03      | 120.28   |
| 25  | R     | 335 | ARG  | C-N-CA   | 5.04  | 127.03      | 120.28   |
| 5   | 5     | 58  | TRP  | CA-C-N   | 5.03  | 127.03      | 120.28   |
| 5   | 5     | 58  | TRP  | C-N-CA   | 5.03  | 127.03      | 120.28   |
| 19  | L     | 341 | GLY  | CA-C-O   | 5.03  | 124.61      | 119.02   |
| 22  | O     | 196 | LEU  | O-C-N    | -5.03 | 116.89      | 122.07   |
| 9   | B     | 180 | ASN  | N-CA-C   | -5.03 | 101.64      | 109.14   |
| 17  | J     | 37  | LYS  | CA-C-N   | 5.03  | 127.02      | 120.28   |
| 17  | J     | 37  | LYS  | C-N-CA   | 5.03  | 127.02      | 120.28   |
| 33  | Z     | 439 | TYR  | N-CA-C   | 5.03  | 117.66      | 111.82   |
| 12  | E     | 122 | ARG  | CB-CG-CD | 5.03  | 122.87      | 111.30   |
| 13  | F     | 169 | LYS  | CA-C-N   | 5.03  | 129.18      | 120.58   |
| 13  | F     | 169 | LYS  | C-N-CA   | 5.03  | 129.18      | 120.58   |
| 15  | H     | 321 | ASP  | CA-C-O   | 5.03  | 127.54      | 121.65   |
| 21  | N     | 287 | LEU  | CA-C-O   | 5.03  | 125.78      | 120.10   |
| 21  | N     | 580 | ASN  | N-CA-C   | -5.03 | 102.83      | 110.28   |
| 23  | P     | 440 | HIS  | N-CA-C   | 5.03  | 116.76      | 111.28   |
| 33  | Z     | 267 | THR  | CA-C-N   | 5.03  | 127.02      | 120.28   |
| 33  | Z     | 267 | THR  | C-N-CA   | 5.03  | 127.02      | 120.28   |
| 33  | Z     | 490 | ILE  | CA-C-N   | 5.03  | 127.43      | 120.29   |
| 33  | Z     | 490 | ILE  | C-N-CA   | 5.03  | 127.43      | 120.29   |
| 23  | P     | 341 | LEU  | N-CA-C   | 5.03  | 116.76      | 111.28   |
| 27  | T     | 81  | TYR  | CA-C-N   | 5.03  | 127.02      | 120.28   |
| 27  | T     | 81  | TYR  | C-N-CA   | 5.03  | 127.02      | 120.28   |
| 33  | Z     | 773 | ARG  | CA-C-N   | 5.03  | 127.43      | 120.29   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33  | Z     | 773 | ARG  | C-N-CA  | 5.03  | 127.43      | 120.29   |
| 4   | 4     | 39  | PRO  | O-C-N   | 5.03  | 128.71      | 122.22   |
| 20  | M     | 272 | GLU  | CA-C-N  | 5.03  | 131.38      | 121.58   |
| 20  | M     | 272 | GLU  | C-N-CA  | 5.03  | 131.38      | 121.58   |
| 21  | N     | 21  | LYS  | CA-C-O  | -5.03 | 115.09      | 120.42   |
| 21  | N     | 143 | LYS  | CA-C-N  | 5.03  | 127.02      | 120.28   |
| 21  | N     | 143 | LYS  | C-N-CA  | 5.03  | 127.02      | 120.28   |
| 6   | 6     | 145 | VAL  | N-CA-C  | -5.03 | 106.89      | 111.67   |
| 19  | L     | 106 | GLY  | CA-C-O  | -5.03 | 115.68      | 121.46   |
| 19  | L     | 249 | SER  | N-CA-C  | 5.03  | 121.51      | 110.80   |
| 21  | N     | 473 | ASP  | CA-C-O  | 5.03  | 127.53      | 121.65   |
| 29  | V     | 247 | ILE  | CB-CA-C | -5.03 | 103.05      | 111.29   |
| 30  | W     | 40  | LYS  | CA-C-O  | -5.03 | 115.52      | 120.70   |
| 33  | Z     | 590 | ALA  | CA-C-O  | -5.03 | 115.22      | 120.55   |
| 21  | N     | 549 | TYR  | CA-C-N  | 5.02  | 126.42      | 120.14   |
| 21  | N     | 549 | TYR  | C-N-CA  | 5.02  | 126.42      | 120.14   |
| 21  | N     | 749 | LEU  | CA-C-N  | 5.02  | 127.72      | 120.38   |
| 21  | N     | 749 | LEU  | C-N-CA  | 5.02  | 127.72      | 120.38   |
| 25  | R     | 415 | GLN  | CA-C-N  | 5.02  | 127.01      | 120.28   |
| 25  | R     | 415 | GLN  | C-N-CA  | 5.02  | 127.01      | 120.28   |
| 10  | C     | 133 | VAL  | CA-C-O  | -5.02 | 115.53      | 120.90   |
| 21  | N     | 694 | LEU  | CA-C-N  | 5.02  | 127.51      | 120.28   |
| 21  | N     | 694 | LEU  | C-N-CA  | 5.02  | 127.51      | 120.28   |
| 2   | 2     | 60  | GLY  | CA-C-N  | 5.02  | 126.97      | 120.44   |
| 2   | 2     | 60  | GLY  | C-N-CA  | 5.02  | 126.97      | 120.44   |
| 5   | 5     | 8   | PHE  | N-CA-C  | -5.02 | 101.81      | 108.74   |
| 15  | H     | 286 | GLU  | N-CA-CB | 5.02  | 118.97      | 110.49   |
| 33  | Z     | 762 | GLY  | O-C-N   | 5.02  | 127.04      | 122.17   |
| 33  | Z     | 971 | ILE  | CA-C-N  | 5.02  | 130.50      | 121.06   |
| 33  | Z     | 971 | ILE  | C-N-CA  | 5.02  | 130.50      | 121.06   |
| 15  | H     | 282 | LYS  | CA-C-N  | 5.02  | 128.22      | 121.05   |
| 15  | H     | 282 | LYS  | C-N-CA  | 5.02  | 128.22      | 121.05   |
| 20  | M     | 360 | ILE  | O-C-N   | 5.02  | 126.74      | 121.87   |
| 27  | T     | 200 | LEU  | CA-C-N  | 5.02  | 124.92      | 119.85   |
| 27  | T     | 200 | LEU  | C-N-CA  | 5.02  | 124.92      | 119.85   |
| 28  | U     | 224 | THR  | CA-C-N  | 5.02  | 126.88      | 120.56   |
| 28  | U     | 224 | THR  | C-N-CA  | 5.02  | 126.88      | 120.56   |
| 11  | D     | 52  | LEU  | N-CA-C  | -5.01 | 101.67      | 109.24   |
| 15  | H     | 103 | THR  | CA-C-N  | 5.01  | 131.12      | 121.54   |
| 15  | H     | 103 | THR  | C-N-CA  | 5.01  | 131.12      | 121.54   |
| 15  | H     | 261 | ARG  | CA-C-N  | 5.01  | 126.96      | 120.44   |
| 15  | H     | 261 | ARG  | C-N-CA  | 5.01  | 126.96      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | N     | 106 | ILE  | N-CA-C | -5.01 | 105.61      | 110.42   |
| 22  | O     | 94  | GLU  | CA-C-O | -5.01 | 114.20      | 119.97   |
| 29  | V     | 241 | THR  | CA-C-O | -5.01 | 115.56      | 120.82   |
| 8   | A     | 92  | ASN  | CA-C-N | 5.01  | 127.41      | 120.29   |
| 8   | A     | 92  | ASN  | C-N-CA | 5.01  | 127.41      | 120.29   |
| 21  | N     | 89  | PHE  | O-C-N  | 5.01  | 128.94      | 122.93   |
| 33  | Z     | 780 | MET  | CA-C-O | 5.01  | 125.73      | 120.42   |
| 4   | 4     | 190 | GLN  | CA-C-O | 5.01  | 126.20      | 120.54   |
| 11  | D     | 61  | PRO  | O-C-N  | 5.01  | 128.77      | 123.01   |
| 19  | L     | 278 | ILE  | N-CA-C | -5.01 | 100.68      | 107.99   |
| 17  | J     | 84  | VAL  | CA-C-O | 5.01  | 126.28      | 120.67   |
| 26  | S     | 150 | LYS  | CA-C-O | -5.01 | 113.57      | 119.48   |
| 12  | E     | 94  | THR  | CA-C-N | 5.01  | 127.40      | 120.29   |
| 12  | E     | 94  | THR  | C-N-CA | 5.01  | 127.40      | 120.29   |
| 27  | T     | 36  | LYS  | CA-C-O | 5.01  | 125.86      | 120.55   |
| 11  | D     | 77  | GLY  | N-CA-C | -5.00 | 101.32      | 113.18   |
| 12  | E     | 238 | GLU  | CA-C-O | 5.00  | 125.86      | 120.55   |
| 21  | N     | 185 | ILE  | N-CA-C | 5.00  | 115.22      | 110.42   |
| 25  | R     | 97  | GLU  | CA-C-N | 5.00  | 127.23      | 120.38   |
| 25  | R     | 97  | GLU  | C-N-CA | 5.00  | 127.23      | 120.38   |
| 26  | S     | 335 | GLN  | CA-C-N | 5.00  | 130.09      | 122.29   |
| 26  | S     | 335 | GLN  | C-N-CA | 5.00  | 130.09      | 122.29   |
| 30  | W     | 178 | PRO  | O-C-N  | 5.00  | 129.10      | 123.10   |
| 21  | N     | 519 | VAL  | O-C-N  | 5.00  | 126.72      | 121.87   |
| 23  | P     | 140 | THR  | N-CA-C | -5.00 | 105.91      | 111.36   |
| 28  | U     | 13  | LEU  | N-CA-C | -5.00 | 105.83      | 111.28   |

There are no chirality outliers.

All (44) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | 7     | 100 | ASN  | Peptide   |
| 11  | D     | 104 | VAL  | Peptide   |
| 12  | E     | 122 | ARG  | Sidechain |
| 12  | E     | 132 | ARG  | Sidechain |
| 12  | E     | 136 | ARG  | Sidechain |
| 13  | F     | 47  | VAL  | Mainchain |
| 15  | H     | 101 | ARG  | Peptide   |
| 15  | H     | 145 | TYR  | Sidechain |
| 15  | H     | 162 | ARG  | Peptide   |
| 15  | H     | 170 | GLU  | Peptide   |
| 15  | H     | 283 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 15  | H     | 285 | GLY  | Mainchain |
| 15  | H     | 400 | ARG  | Peptide   |
| 15  | H     | 95  | HIS  | Peptide   |
| 16  | I     | 125 | MET  | Peptide   |
| 16  | I     | 214 | LYS  | Peptide   |
| 16  | I     | 256 | TYR  | Sidechain |
| 16  | I     | 340 | ARG  | Peptide   |
| 18  | K     | 150 | LEU  | Peptide   |
| 18  | K     | 255 | ARG  | Sidechain |
| 19  | L     | 203 | ASN  | Peptide   |
| 19  | L     | 249 | SER  | Peptide   |
| 19  | L     | 253 | ASP  | Peptide   |
| 19  | L     | 257 | GLY  | Mainchain |
| 20  | M     | 299 | ARG  | Sidechain |
| 20  | M     | 75  | LEU  | Peptide   |
| 21  | N     | 774 | ASN  | Peptide   |
| 22  | O     | 125 | GLY  | Peptide   |
| 22  | O     | 140 | LYS  | Peptide   |
| 22  | O     | 19  | ASP  | Peptide   |
| 22  | O     | 240 | GLU  | Peptide   |
| 23  | P     | 53  | ALA  | Peptide   |
| 23  | P     | 69  | ARG  | Sidechain |
| 24  | Q     | 402 | THR  | Peptide   |
| 25  | R     | 184 | GLN  | Peptide   |
| 25  | R     | 381 | ILE  | Peptide   |
| 27  | T     | 237 | ASN  | Peptide   |
| 27  | T     | 247 | ASP  | Peptide   |
| 27  | T     | 252 | GLU  | Peptide   |
| 27  | T     | 253 | GLU  | Peptide   |
| 29  | V     | 110 | SER  | Peptide   |
| 30  | W     | 164 | PRO  | Peptide   |
| 33  | Z     | 317 | GLN  | Peptide   |
| 33  | Z     | 350 | GLY  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 1576  | 0        | 1555     | 173     | 0            |
| 2   | 2     | 1692  | 0        | 1699     | 115     | 0            |
| 3   | 3     | 1581  | 0        | 1574     | 138     | 0            |
| 4   | 4     | 1585  | 0        | 1590     | 112     | 0            |
| 5   | 5     | 1646  | 0        | 1595     | 96      | 0            |
| 6   | 6     | 1757  | 0        | 1708     | 105     | 0            |
| 7   | 7     | 1824  | 0        | 1832     | 111     | 0            |
| 8   | A     | 1921  | 0        | 1910     | 167     | 0            |
| 9   | B     | 1915  | 0        | 1929     | 116     | 0            |
| 10  | C     | 1913  | 0        | 1914     | 146     | 0            |
| 11  | D     | 1899  | 0        | 1908     | 145     | 0            |
| 12  | E     | 1867  | 0        | 1840     | 135     | 0            |
| 13  | F     | 1795  | 0        | 1797     | 192     | 0            |
| 14  | G     | 1900  | 0        | 1888     | 163     | 0            |
| 15  | H     | 2792  | 0        | 2879     | 343     | 0            |
| 16  | I     | 2822  | 0        | 2868     | 291     | 0            |
| 17  | J     | 2928  | 0        | 3054     | 258     | 0            |
| 18  | K     | 3019  | 0        | 3082     | 222     | 0            |
| 19  | L     | 2853  | 0        | 2925     | 255     | 0            |
| 20  | M     | 2866  | 0        | 2936     | 264     | 0            |
| 21  | N     | 6562  | 0        | 6625     | 503     | 0            |
| 22  | O     | 3182  | 0        | 3207     | 262     | 0            |
| 23  | P     | 3401  | 0        | 3482     | 284     | 0            |
| 24  | Q     | 3471  | 0        | 3494     | 280     | 0            |
| 25  | R     | 3218  | 0        | 3216     | 304     | 0            |
| 26  | S     | 2893  | 0        | 2937     | 225     | 0            |
| 27  | T     | 2235  | 0        | 2207     | 175     | 0            |
| 28  | U     | 2061  | 0        | 2115     | 252     | 0            |
| 29  | V     | 1942  | 0        | 1954     | 188     | 0            |
| 30  | W     | 1534  | 0        | 1542     | 148     | 0            |
| 31  | X     | 1032  | 0        | 1017     | 102     | 0            |
| 32  | Y     | 168   | 0        | 153      | 14      | 0            |
| 33  | Z     | 6289  | 0        | 6235     | 809     | 0            |
| All | All   | 80139 | 0        | 80667    | 6199    | 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 39.

All (6199) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 33:Z:574:TYR:CE2 | 33:Z:584:VAL:HG11 | 1.29                     | 1.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:P:131:PHE:CZ   | 23:P:167:THR:HG22 | 1.24                     | 1.65              |
| 15:H:172:MET:HB2  | 16:I:129:TYR:CD2  | 1.26                     | 1.62              |
| 15:H:396:MET:CE   | 15:H:438:ALA:CB   | 1.78                     | 1.57              |
| 15:H:172:MET:CB   | 16:I:129:TYR:CE2  | 1.82                     | 1.57              |
| 33:Z:64:TYR:HD2   | 33:Z:111:LEU:CD1  | 0.97                     | 1.56              |
| 15:H:172:MET:CB   | 16:I:129:TYR:CD2  | 1.75                     | 1.55              |
| 18:K:272:ASP:CB   | 19:L:306:MET:HE1  | 1.34                     | 1.54              |
| 33:Z:89:LEU:CD2   | 33:Z:125:THR:HG21 | 1.08                     | 1.52              |
| 12:E:15:PHE:CE1   | 12:E:21:LEU:HD11  | 1.46                     | 1.51              |
| 28:U:277:TYR:CE1  | 29:V:295:VAL:HG11 | 1.45                     | 1.51              |
| 31:X:79:LYS:HE2   | 31:X:98:PHE:CE2   | 1.44                     | 1.51              |
| 23:P:267:PHE:CE1  | 23:P:329:PHE:HE2  | 1.25                     | 1.51              |
| 31:X:75:TRP:CZ3   | 31:X:125:MET:HE2  | 0.98                     | 1.50              |
| 15:H:396:MET:HE2  | 15:H:438:ALA:CB   | 1.36                     | 1.50              |
| 30:W:21:PHE:CE1   | 30:W:25:ARG:NH1   | 1.79                     | 1.49              |
| 23:P:308:LEU:HD11 | 23:P:349:ASN:CB   | 1.37                     | 1.49              |
| 31:X:75:TRP:CZ2   | 31:X:125:MET:HG3  | 0.99                     | 1.49              |
| 23:P:308:LEU:HD13 | 23:P:349:ASN:CG   | 1.20                     | 1.48              |
| 1:1:14:LEU:HD21   | 1:1:100:ALA:CB    | 1.43                     | 1.48              |
| 15:H:324:GLY:CA   | 20:M:290:ARG:NH2  | 1.76                     | 1.48              |
| 30:W:21:PHE:HE1   | 30:W:25:ARG:NH1   | 1.03                     | 1.48              |
| 8:A:252:ASP:CG    | 23:P:85:LYS:NZ    | 1.73                     | 1.47              |
| 23:P:308:LEU:CD1  | 23:P:349:ASN:CG   | 1.87                     | 1.47              |
| 16:I:204:HIS:CD2  | 16:I:207:LEU:CD1  | 1.98                     | 1.46              |
| 31:X:75:TRP:CZ3   | 31:X:125:MET:CE   | 1.91                     | 1.46              |
| 26:S:184:TRP:CZ2  | 26:S:217:PHE:HE2  | 1.28                     | 1.46              |
| 33:Z:64:TYR:CD2   | 33:Z:111:LEU:HD13 | 0.94                     | 1.46              |
| 17:J:224:GLY:C    | 17:J:225:GLU:N    | 1.73                     | 1.45              |
| 21:N:329:HIS:CB   | 29:V:182:LYS:HZ1  | 1.28                     | 1.45              |
| 30:W:186:ALA:HA   | 30:W:191:ILE:CG2  | 1.43                     | 1.44              |
| 33:Z:188:ALA:H    | 33:Z:201:LEU:CD1  | 1.29                     | 1.44              |
| 31:X:75:TRP:CZ2   | 31:X:125:MET:CG   | 1.95                     | 1.44              |
| 23:P:267:PHE:CE1  | 23:P:329:PHE:CE2  | 2.06                     | 1.44              |
| 1:1:14:LEU:CD2    | 1:1:100:ALA:HB3   | 1.48                     | 1.43              |
| 3:3:129:VAL:HG22  | 3:3:138:PHE:CE1   | 1.54                     | 1.43              |
| 18:K:272:ASP:CB   | 19:L:306:MET:CE   | 1.98                     | 1.42              |
| 30:W:25:ARG:NH1   | 30:W:144:PHE:HE2  | 1.13                     | 1.42              |
| 8:A:252:ASP:OD1   | 23:P:85:LYS:CE    | 1.68                     | 1.40              |
| 18:K:272:ASP:HB3  | 19:L:306:MET:CE   | 1.48                     | 1.40              |
| 16:I:126:PRO:HB3  | 16:I:128:TYR:CE2  | 1.54                     | 1.40              |
| 1:1:83:LYS:NZ     | 1:1:118:SER:HA    | 1.34                     | 1.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:324:GLY:N    | 20:M:290:ARG:HH21 | 1.07                     | 1.40              |
| 24:Q:309:ARG:HH21 | 24:Q:345:SER:CB   | 1.35                     | 1.40              |
| 33:Z:53:VAL:HG13  | 33:Z:95:THR:CG2   | 1.51                     | 1.40              |
| 15:H:173:ARG:CA   | 16:I:129:TYR:OH   | 1.67                     | 1.40              |
| 26:S:461:PHE:CZ   | 28:U:274:MET:O    | 1.75                     | 1.39              |
| 1:1:19:ARG:NH2    | 1:1:171:GLY:N     | 1.68                     | 1.39              |
| 33:Z:474:LEU:CD2  | 33:Z:493:LEU:HD22 | 1.51                     | 1.39              |
| 33:Z:493:LEU:HD11 | 33:Z:497:PHE:CZ   | 1.54                     | 1.37              |
| 24:Q:309:ARG:HH21 | 24:Q:345:SER:CA   | 1.36                     | 1.37              |
| 26:S:461:PHE:CE2  | 28:U:274:MET:O    | 1.77                     | 1.37              |
| 15:H:172:MET:HB2  | 16:I:129:TYR:CE2  | 1.47                     | 1.36              |
| 16:I:395:MET:HE2  | 16:I:420:LYS:NZ   | 1.39                     | 1.36              |
| 33:Z:89:LEU:CD2   | 33:Z:125:THR:CG2  | 2.03                     | 1.36              |
| 29:V:135:ARG:NE   | 29:V:157:ARG:HH12 | 1.23                     | 1.35              |
| 17:J:337:LEU:HD22 | 17:J:382:PHE:CZ   | 1.58                     | 1.35              |
| 22:O:69:PHE:HE2   | 22:O:74:ASN:O     | 1.06                     | 1.35              |
| 1:1:19:ARG:HH21   | 1:1:171:GLY:N     | 1.20                     | 1.35              |
| 16:I:126:PRO:CB   | 16:I:128:TYR:HE2  | 1.40                     | 1.35              |
| 30:W:21:PHE:HE1   | 30:W:25:ARG:CZ    | 1.36                     | 1.35              |
| 25:R:209:ARG:NH2  | 25:R:243:LEU:HD11 | 1.35                     | 1.34              |
| 16:I:204:HIS:HD2  | 16:I:207:LEU:CD1  | 1.33                     | 1.34              |
| 30:W:186:ALA:CA   | 30:W:191:ILE:HG22 | 1.56                     | 1.34              |
| 20:M:47:GLU:OE2   | 20:M:50:ARG:NH2   | 1.61                     | 1.34              |
| 30:W:186:ALA:CA   | 30:W:191:ILE:CG2  | 2.06                     | 1.34              |
| 29:V:135:ARG:HE   | 29:V:157:ARG:NH1  | 1.27                     | 1.33              |
| 28:U:203:LYS:CE   | 28:U:229:LEU:HD21 | 1.59                     | 1.33              |
| 15:H:284:VAL:HG11 | 20:M:253:GLN:C    | 1.54                     | 1.32              |
| 26:S:184:TRP:HZ2  | 26:S:217:PHE:CE2  | 1.46                     | 1.32              |
| 23:P:308:LEU:CD1  | 23:P:349:ASN:CB   | 2.05                     | 1.32              |
| 30:W:25:ARG:NH1   | 30:W:144:PHE:CE2  | 1.96                     | 1.32              |
| 15:H:284:VAL:HB   | 20:M:254:MET:CA   | 1.60                     | 1.31              |
| 26:S:184:TRP:CZ2  | 26:S:217:PHE:CE2  | 2.15                     | 1.31              |
| 33:Z:865:ASP:CG   | 33:Z:909:ARG:HH21 | 1.34                     | 1.31              |
| 21:N:424:LYS:NZ   | 21:N:461:GLU:HB3  | 1.43                     | 1.31              |
| 33:Z:474:LEU:HD23 | 33:Z:493:LEU:CD2  | 1.60                     | 1.31              |
| 16:I:204:HIS:CD2  | 16:I:207:LEU:HD13 | 1.60                     | 1.31              |
| 23:P:308:LEU:CD1  | 23:P:349:ASN:HB2  | 1.61                     | 1.30              |
| 1:1:19:ARG:NH2    | 1:1:171:GLY:H     | 1.18                     | 1.30              |
| 15:H:156:VAL:HG22 | 15:H:181:TYR:OH   | 1.13                     | 1.30              |
| 21:N:329:HIS:CB   | 29:V:182:LYS:NZ   | 1.94                     | 1.30              |
| 28:U:277:TYR:CE1  | 29:V:295:VAL:CG1  | 2.14                     | 1.30              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:52:THR:OG1    | 4:4:84:ARG:NH2    | 1.63                     | 1.30              |
| 29:V:135:ARG:HD2  | 29:V:157:ARG:NH2  | 1.47                     | 1.29              |
| 24:Q:418:GLN:HB3  | 29:V:262:THR:CG2  | 1.60                     | 1.29              |
| 33:Z:562:TRP:CE2  | 33:Z:566:LEU:HD11 | 1.67                     | 1.29              |
| 27:T:86:LYS:CE    | 27:T:128:TYR:HE2  | 1.43                     | 1.29              |
| 8:A:252:ASP:CG    | 23:P:85:LYS:CE    | 2.01                     | 1.29              |
| 14:G:122:HIS:CD2  | 14:G:128:VAL:HG11 | 1.68                     | 1.29              |
| 15:H:173:ARG:N    | 16:I:129:TYR:OH   | 1.66                     | 1.28              |
| 31:X:75:TRP:CH2   | 31:X:125:MET:HE2  | 1.67                     | 1.28              |
| 20:M:251:LEU:O    | 20:M:252:VAL:N    | 1.66                     | 1.28              |
| 33:Z:443:ASP:OD2  | 33:Z:447:VAL:HG11 | 1.26                     | 1.28              |
| 8:A:205:PHE:CZ    | 8:A:209:HIS:CE1   | 2.22                     | 1.27              |
| 22:O:15:ARG:CZ    | 22:O:73:ILE:HD11  | 1.63                     | 1.27              |
| 18:K:212:TYR:CE1  | 18:K:320:ARG:HA   | 1.67                     | 1.27              |
| 8:A:220:LYS:CD    | 8:A:242:GLU:HB2   | 1.64                     | 1.27              |
| 16:I:175:LYS:O    | 17:J:282:PHE:CE1  | 1.88                     | 1.26              |
| 24:Q:146:TYR:CE1  | 24:Q:184:VAL:HA   | 1.70                     | 1.26              |
| 30:W:186:ALA:CB   | 30:W:191:ILE:HG21 | 1.64                     | 1.26              |
| 21:N:406:TYR:OH   | 21:N:748:PHE:CE1  | 1.89                     | 1.26              |
| 21:N:596:LEU:HD22 | 21:N:717:LEU:CD1  | 1.66                     | 1.25              |
| 22:O:250:TRP:O    | 22:O:269:LEU:HD11 | 1.19                     | 1.25              |
| 15:H:172:MET:HB3  | 16:I:129:TYR:CE2  | 1.57                     | 1.25              |
| 15:H:284:VAL:HB   | 20:M:254:MET:CB   | 1.66                     | 1.25              |
| 23:P:203:ILE:HG12 | 23:P:220:TYR:OH   | 1.27                     | 1.25              |
| 26:S:315:LYS:HD3  | 26:S:345:TYR:CE1  | 1.69                     | 1.25              |
| 16:I:384:LYS:NZ   | 16:I:420:LYS:HZ2  | 1.35                     | 1.25              |
| 22:O:342:ASP:OD1  | 23:P:358:SER:HB2  | 1.11                     | 1.25              |
| 33:Z:486:SER:O    | 33:Z:490:ILE:HG12 | 1.29                     | 1.25              |
| 2:2:160:GLN:HE21  | 2:2:164:TRP:NE1   | 1.33                     | 1.25              |
| 24:Q:309:ARG:NH2  | 24:Q:345:SER:CB   | 1.99                     | 1.25              |
| 33:Z:443:ASP:CG   | 33:Z:447:VAL:HG11 | 1.62                     | 1.24              |
| 6:6:91:LYS:HD3    | 6:6:96:TYR:OH     | 1.30                     | 1.24              |
| 13:F:3:ARG:HH21   | 15:H:359:ASN:ND2  | 1.33                     | 1.24              |
| 19:L:336:ALA:HB1  | 19:L:342:ARG:NH1  | 1.53                     | 1.24              |
| 23:P:131:PHE:CZ   | 23:P:167:THR:CG2  | 2.19                     | 1.24              |
| 24:Q:309:ARG:CZ   | 24:Q:345:SER:HB3  | 1.68                     | 1.24              |
| 27:T:2:PRO:O      | 27:T:9:LYS:HD2    | 1.32                     | 1.24              |
| 24:Q:299:MET:HE1  | 24:Q:335:PHE:CZ   | 1.72                     | 1.23              |
| 13:F:120:THR:CB   | 14:G:129:ARG:HH11 | 1.50                     | 1.23              |
| 29:V:107:TRP:CZ3  | 29:V:109:HIS:CD2  | 2.26                     | 1.23              |
| 17:J:167:PRO:HB3  | 17:J:174:PHE:CE2  | 1.73                     | 1.23              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:301:TYR:CE1  | 25:R:305:PHE:CZ   | 2.27                     | 1.23              |
| 15:H:396:MET:CE   | 15:H:438:ALA:HB1  | 1.48                     | 1.22              |
| 31:X:75:TRP:CE2   | 31:X:125:MET:HG3  | 1.74                     | 1.22              |
| 33:Z:428:TRP:CZ3  | 33:Z:461:GLY:HA3  | 1.74                     | 1.22              |
| 33:Z:442:VAL:CG1  | 33:Z:443:ASP:H    | 1.45                     | 1.22              |
| 14:G:173:ALA:CB   | 19:L:420:ARG:HH21 | 1.52                     | 1.22              |
| 15:H:389:PHE:CZ   | 15:H:419:LEU:HD22 | 1.73                     | 1.22              |
| 17:J:337:LEU:HB2  | 25:R:204:TRP:CZ2  | 1.74                     | 1.22              |
| 18:K:212:TYR:HE1  | 18:K:320:ARG:CA   | 1.52                     | 1.22              |
| 27:T:86:LYS:CE    | 27:T:128:TYR:CE2  | 2.23                     | 1.22              |
| 33:Z:865:ASP:OD2  | 33:Z:909:ARG:NH2  | 1.71                     | 1.22              |
| 15:H:324:GLY:HA3  | 20:M:290:ARG:NH2  | 1.34                     | 1.22              |
| 33:Z:64:TYR:OH    | 33:Z:115:LEU:HD21 | 1.39                     | 1.22              |
| 33:Z:217:GLU:CD   | 33:Z:244:ARG:HH21 | 1.47                     | 1.22              |
| 13:F:84:LEU:HD23  | 13:F:132:LEU:CD1  | 1.70                     | 1.21              |
| 27:T:86:LYS:HE3   | 27:T:128:TYR:CE2  | 1.76                     | 1.21              |
| 33:Z:246:CYS:SG   | 33:Z:271:ILE:HG21 | 1.80                     | 1.21              |
| 16:I:384:LYS:HZ3  | 16:I:420:LYS:NZ   | 1.39                     | 1.20              |
| 33:Z:89:LEU:HD21  | 33:Z:125:THR:CG2  | 1.66                     | 1.20              |
| 33:Z:75:ILE:CG2   | 33:Z:121:ILE:HG21 | 1.71                     | 1.20              |
| 33:Z:138:ARG:CZ   | 33:Z:157:LEU:HG   | 1.70                     | 1.20              |
| 33:Z:392:LEU:CD1  | 33:Z:424:SER:O    | 1.90                     | 1.20              |
| 8:A:220:LYS:HD3   | 8:A:242:GLU:CB    | 1.70                     | 1.20              |
| 13:F:159:THR:HA   | 13:F:169:LYS:NZ   | 1.57                     | 1.20              |
| 16:I:207:LEU:HD13 | 33:Z:930:GLY:HA2  | 1.20                     | 1.20              |
| 33:Z:443:ASP:OD2  | 33:Z:447:VAL:CG1  | 1.88                     | 1.20              |
| 31:X:75:TRP:CH2   | 31:X:125:MET:HG3  | 1.76                     | 1.19              |
| 14:G:146:HIS:HB3  | 14:G:148:TYR:CE1  | 1.75                     | 1.19              |
| 33:Z:419:VAL:O    | 33:Z:422:ILE:HG12 | 1.40                     | 1.19              |
| 33:Z:574:TYR:CE2  | 33:Z:584:VAL:CG1  | 2.24                     | 1.19              |
| 13:F:101:ARG:NH1  | 13:F:103:LEU:HA   | 1.55                     | 1.19              |
| 13:F:105:VAL:HG22 | 13:F:145:LEU:CD1  | 1.71                     | 1.19              |
| 25:R:408:ASP:HB2  | 26:S:464:ARG:NH2  | 1.55                     | 1.19              |
| 26:S:315:LYS:HD3  | 26:S:345:TYR:CZ   | 1.78                     | 1.19              |
| 33:Z:823:ASN:HB3  | 33:Z:856:HIS:CE1  | 1.78                     | 1.19              |
| 24:Q:309:ARG:NE   | 24:Q:345:SER:HB3  | 1.57                     | 1.18              |
| 12:E:221:CYS:SG   | 12:E:231:TYR:CE2  | 2.34                     | 1.18              |
| 17:J:337:LEU:CD2  | 17:J:382:PHE:HZ   | 1.56                     | 1.18              |
| 17:J:216:ALA:O    | 17:J:219:VAL:N    | 1.74                     | 1.18              |
| 13:F:84:LEU:HD23  | 13:F:132:LEU:HD11 | 1.26                     | 1.18              |
| 15:H:59:ILE:HG21  | 16:I:92:GLU:OE2   | 1.41                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:301:TYR:HE1  | 25:R:305:PHE:CZ   | 1.60                     | 1.18              |
| 33:Z:574:TYR:CZ   | 33:Z:584:VAL:HG11 | 1.78                     | 1.18              |
| 2:2:50:ALA:CB     | 3:3:118:ILE:HG22  | 1.73                     | 1.17              |
| 21:N:53:ASP:HA    | 21:N:58:ARG:HH21  | 1.08                     | 1.17              |
| 24:Q:418:GLN:CB   | 29:V:262:THR:HG21 | 1.74                     | 1.17              |
| 33:Z:474:LEU:CD2  | 33:Z:493:LEU:CD2  | 2.17                     | 1.17              |
| 33:Z:442:VAL:HG12 | 33:Z:443:ASP:N    | 1.41                     | 1.17              |
| 24:Q:309:ARG:NH2  | 24:Q:345:SER:HB3  | 1.55                     | 1.17              |
| 33:Z:321:PHE:HE2  | 33:Z:351:PRO:HG3  | 1.02                     | 1.17              |
| 33:Z:550:PHE:CZ   | 33:Z:566:LEU:HB3  | 1.77                     | 1.17              |
| 10:C:161:LYS:HD2  | 11:D:56:ASP:HB2   | 1.21                     | 1.17              |
| 33:Z:53:VAL:CG1   | 33:Z:95:THR:CG2   | 2.22                     | 1.17              |
| 33:Z:138:ARG:NE   | 33:Z:157:LEU:HG   | 1.56                     | 1.17              |
| 15:H:324:GLY:N    | 20:M:290:ARG:NH2  | 1.84                     | 1.16              |
| 18:K:272:ASP:HB2  | 19:L:306:MET:CE   | 1.75                     | 1.16              |
| 33:Z:823:ASN:HB3  | 33:Z:856:HIS:HE1  | 1.04                     | 1.16              |
| 30:W:186:ALA:CB   | 30:W:191:ILE:CG2  | 2.24                     | 1.16              |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:CA   | 1.75                     | 1.16              |
| 33:Z:385:PHE:CE2  | 33:Z:389:PHE:CE2  | 2.33                     | 1.15              |
| 8:A:153:SER:HB3   | 8:A:155:TYR:HE1   | 1.05                     | 1.15              |
| 28:U:32:ARG:CB    | 28:U:94:HIS:HE1   | 1.60                     | 1.15              |
| 30:W:9:VAL:HG22   | 30:W:52:ILE:CD1   | 1.76                     | 1.15              |
| 33:Z:863:THR:HG21 | 33:Z:911:LYS:HZ3  | 1.01                     | 1.15              |
| 22:O:69:PHE:CE2   | 22:O:74:ASN:O     | 1.99                     | 1.15              |
| 33:Z:89:LEU:HD22  | 33:Z:125:THR:CG2  | 1.69                     | 1.15              |
| 33:Z:385:PHE:CZ   | 33:Z:389:PHE:CE2  | 2.33                     | 1.15              |
| 16:I:126:PRO:HG2  | 16:I:154:MET:HE3  | 1.26                     | 1.15              |
| 23:P:303:PHE:CE1  | 23:P:345:VAL:HG22 | 1.82                     | 1.15              |
| 15:H:173:ARG:CB   | 16:I:129:TYR:OH   | 1.93                     | 1.15              |
| 15:H:284:VAL:CG1  | 20:M:253:GLN:C    | 2.20                     | 1.15              |
| 17:J:134:VAL:HG12 | 17:J:135:SER:N    | 1.57                     | 1.15              |
| 20:M:251:LEU:C    | 20:M:252:VAL:CA   | 2.18                     | 1.15              |
| 23:P:131:PHE:CE2  | 23:P:167:THR:HG22 | 1.80                     | 1.15              |
| 25:R:266:LEU:HA   | 25:R:270:VAL:HG22 | 1.28                     | 1.15              |
| 27:T:157:TYR:OH   | 27:T:188:GLU:HG2  | 1.46                     | 1.15              |
| 33:Z:205:LEU:HG   | 33:Z:236:PHE:CE1  | 1.80                     | 1.15              |
| 14:G:7:TYR:CE1    | 14:G:13:VAL:HG21  | 1.80                     | 1.14              |
| 11:D:68:ASP:OD2   | 11:D:97:ARG:NH2   | 1.80                     | 1.14              |
| 23:P:303:PHE:HE1  | 23:P:345:VAL:HG22 | 1.06                     | 1.14              |
| 28:U:277:TYR:CZ   | 29:V:295:VAL:HG13 | 1.83                     | 1.14              |
| 16:I:214:LYS:HZ2  | 16:I:318:ASP:C    | 1.54                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:282:TYR:CZ   | 21:N:286:LEU:HD13 | 1.81                     | 1.14              |
| 21:N:329:HIS:HB2  | 29:V:182:LYS:CE   | 1.77                     | 1.14              |
| 23:P:167:THR:OG1  | 23:P:168:TYR:HD1  | 1.27                     | 1.14              |
| 28:U:189:ARG:NH1  | 29:V:296:LEU:HD13 | 1.60                     | 1.14              |
| 14:G:111:PHE:HD1  | 14:G:114:ARG:NH2  | 1.44                     | 1.14              |
| 23:P:267:PHE:CZ   | 23:P:329:PHE:CE2  | 2.35                     | 1.14              |
| 1:1:137:TYR:CZ    | 1:1:157:HIS:HD2   | 1.65                     | 1.14              |
| 30:W:20:ASP:HB3   | 30:W:25:ARG:NH2   | 1.62                     | 1.14              |
| 8:A:252:ASP:CG    | 23:P:85:LYS:HE3   | 1.72                     | 1.13              |
| 21:N:515:ARG:NH2  | 21:N:738:GLN:OE1  | 1.80                     | 1.13              |
| 22:O:250:TRP:HB3  | 22:O:269:LEU:HD21 | 1.25                     | 1.13              |
| 26:S:401:LYS:HE2  | 26:S:444:GLU:OE2  | 1.46                     | 1.13              |
| 30:W:124:GLU:OE1  | 30:W:127:ARG:NH2  | 1.80                     | 1.13              |
| 33:Z:64:TYR:CE2   | 33:Z:111:LEU:HD13 | 1.82                     | 1.13              |
| 23:P:308:LEU:HD22 | 23:P:369:LEU:HD23 | 1.30                     | 1.13              |
| 29:V:131:GLN:NE2  | 29:V:194:ARG:HH21 | 1.47                     | 1.13              |
| 21:N:327:LEU:HD21 | 21:N:743:PHE:HE1  | 1.12                     | 1.13              |
| 28:U:32:ARG:HB3   | 28:U:94:HIS:HE1   | 1.04                     | 1.13              |
| 33:Z:154:ILE:HG22 | 33:Z:211:PHE:CZ   | 1.84                     | 1.13              |
| 33:Z:224:LEU:HD13 | 33:Z:233:LEU:HD23 | 1.22                     | 1.13              |
| 12:E:15:PHE:CD1   | 12:E:21:LEU:HD11  | 1.83                     | 1.12              |
| 13:F:179:PHE:CZ   | 13:F:192:ALA:HB1  | 1.84                     | 1.13              |
| 25:R:107:GLU:HG2  | 25:R:111:LYS:HE2  | 1.30                     | 1.12              |
| 26:S:401:LYS:HG2  | 26:S:444:GLU:HG2  | 1.28                     | 1.13              |
| 13:F:120:THR:HB   | 14:G:129:ARG:HH11 | 1.01                     | 1.12              |
| 30:W:21:PHE:HZ    | 30:W:144:PHE:CD2  | 1.66                     | 1.12              |
| 33:Z:75:ILE:HG21  | 33:Z:121:ILE:CG2  | 1.78                     | 1.12              |
| 33:Z:278:LEU:HD22 | 33:Z:297:VAL:CG1  | 1.79                     | 1.12              |
| 33:Z:188:ALA:H    | 33:Z:201:LEU:HD12 | 1.04                     | 1.12              |
| 5:5:8:PHE:CE1     | 5:5:13:ILE:HG12   | 1.85                     | 1.12              |
| 25:R:209:ARG:HG3  | 25:R:213:TYR:HE2  | 1.11                     | 1.12              |
| 33:Z:138:ARG:NH2  | 33:Z:157:LEU:HD12 | 1.64                     | 1.12              |
| 7:7:129:TYR:HE1   | 7:7:134:LEU:HD22  | 1.02                     | 1.12              |
| 13:F:12:THR:HG23  | 13:F:19:LEU:CD1   | 1.78                     | 1.12              |
| 21:N:329:HIS:HB2  | 29:V:182:LYS:HE3  | 1.23                     | 1.12              |
| 31:X:79:LYS:CE    | 31:X:98:PHE:CE2   | 2.31                     | 1.12              |
| 24:Q:273:ASN:CG   | 24:Q:306:TYR:OH   | 1.92                     | 1.12              |
| 21:N:759:ILE:HG23 | 21:N:871:MET:HE1  | 1.32                     | 1.11              |
| 23:P:131:PHE:HA   | 23:P:136:ARG:NH1  | 1.64                     | 1.11              |
| 30:W:101:ARG:NH1  | 30:W:106:GLN:O    | 1.83                     | 1.11              |
| 1:1:174:ARG:NH1   | 1:1:185:ARG:HH21  | 1.48                     | 1.11              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:135:PHE:HE2   | 5:5:163:ALA:HB1   | 1.08                     | 1.11              |
| 33:Z:188:ALA:N    | 33:Z:201:LEU:CD1  | 2.12                     | 1.11              |
| 33:Z:278:LEU:HD22 | 33:Z:297:VAL:HG13 | 1.12                     | 1.11              |
| 17:J:212:ARG:NH1  | 17:J:246:PHE:CE2  | 2.19                     | 1.11              |
| 4:4:3:ILE:HG22    | 4:4:102:LEU:HD12  | 1.19                     | 1.11              |
| 33:Z:776:VAL:CG1  | 33:Z:777:PRO:HD3  | 1.80                     | 1.11              |
| 33:Z:776:VAL:HG12 | 33:Z:777:PRO:HD3  | 1.32                     | 1.11              |
| 15:H:102:CYS:CB   | 15:H:105:ILE:HD11 | 1.79                     | 1.11              |
| 17:J:305:LEU:HD22 | 17:J:313:LYS:HE3  | 1.17                     | 1.11              |
| 21:N:492:THR:O    | 21:N:528:ARG:NH1  | 1.84                     | 1.11              |
| 22:O:233:LEU:HD22 | 22:O:238:ILE:HD11 | 1.30                     | 1.11              |
| 24:Q:429:LYS:HB2  | 29:V:269:ARG:NH2  | 1.63                     | 1.11              |
| 30:W:9:VAL:CG2    | 30:W:52:ILE:HD11  | 1.79                     | 1.11              |
| 33:Z:574:TYR:CZ   | 33:Z:584:VAL:HG21 | 1.84                     | 1.11              |
| 13:F:105:VAL:HG21 | 13:F:145:LEU:HB2  | 1.32                     | 1.10              |
| 15:H:436:LYS:HE2  | 33:Z:365:SER:HB2  | 1.20                     | 1.10              |
| 33:Z:217:GLU:OE2  | 33:Z:244:ARG:NH2  | 1.85                     | 1.10              |
| 33:Z:748:LEU:CD2  | 33:Z:783:VAL:HG13 | 1.80                     | 1.10              |
| 24:Q:275:ILE:HD11 | 24:Q:306:TYR:CD2  | 1.87                     | 1.10              |
| 28:U:32:ARG:HB3   | 28:U:94:HIS:CE1   | 1.86                     | 1.10              |
| 32:Y:80:GLU:OE2   | 32:Y:83:ARG:NH2   | 1.85                     | 1.10              |
| 13:F:12:THR:HG23  | 13:F:19:LEU:HD13  | 1.14                     | 1.10              |
| 15:H:284:VAL:HG11 | 20:M:253:GLN:O    | 1.50                     | 1.10              |
| 15:H:396:MET:HE2  | 15:H:438:ALA:HB3  | 1.20                     | 1.10              |
| 24:Q:249:LEU:O    | 24:Q:250:THR:HG22 | 1.48                     | 1.10              |
| 11:D:159:TRP:CH2  | 12:E:59:LEU:HD13  | 1.86                     | 1.09              |
| 19:L:177:GLU:OE1  | 19:L:233:LYS:NZ   | 1.84                     | 1.09              |
| 23:P:332:GLU:HB3  | 23:P:337:HIS:CE1  | 1.86                     | 1.09              |
| 24:Q:61:LEU:HD21  | 24:Q:65:TYR:OH    | 1.51                     | 1.09              |
| 30:W:21:PHE:CE1   | 30:W:25:ARG:CZ    | 2.24                     | 1.09              |
| 33:Z:50:GLU:OE2   | 33:Z:55:ARG:NH2   | 1.83                     | 1.09              |
| 33:Z:835:ALA:O    | 33:Z:838:TYR:HD2  | 1.32                     | 1.09              |
| 22:O:15:ARG:HH12  | 22:O:73:ILE:CG1   | 1.63                     | 1.09              |
| 24:Q:418:GLN:HB3  | 29:V:262:THR:HG22 | 1.25                     | 1.09              |
| 25:R:363:PHE:HE1  | 32:Y:78:LYS:HD3   | 1.00                     | 1.09              |
| 33:Z:68:LEU:CD1   | 33:Z:111:LEU:HD22 | 1.83                     | 1.09              |
| 33:Z:748:LEU:HD23 | 33:Z:783:VAL:HG13 | 1.33                     | 1.09              |
| 33:Z:763:HIS:CG   | 33:Z:766:HIS:HE1  | 1.70                     | 1.09              |
| 1:1:83:LYS:CD     | 1:1:119:VAL:HG23  | 1.80                     | 1.09              |
| 23:P:130:ILE:C    | 23:P:136:ARG:HH12 | 1.59                     | 1.09              |
| 25:R:335:ARG:HD2  | 25:R:376:GLN:HB3  | 1.25                     | 1.09              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:409:TYR:HA   | 25:R:403:LEU:HD21 | 1.11                     | 1.09              |
| 29:V:135:ARG:CD   | 29:V:157:ARG:HH22 | 1.64                     | 1.09              |
| 9:B:210:GLU:HG3   | 9:B:237:LYS:HE3   | 1.27                     | 1.09              |
| 13:F:7:ASP:HA     | 13:F:21:GLN:HE21  | 1.11                     | 1.09              |
| 17:J:134:VAL:CG1  | 17:J:135:SER:H    | 1.65                     | 1.09              |
| 17:J:167:PRO:CA   | 17:J:174:PHE:CZ   | 2.35                     | 1.09              |
| 21:N:398:ARG:HD2  | 21:N:438:ASP:HB3  | 1.17                     | 1.09              |
| 23:P:72:TRP:CH2   | 23:P:103:TYR:HB3  | 1.88                     | 1.09              |
| 27:T:89:TYR:CD1   | 27:T:102:LYS:HD3  | 1.87                     | 1.09              |
| 3:3:129:VAL:CG2   | 3:3:138:PHE:CE1   | 2.36                     | 1.08              |
| 28:U:277:TYR:CZ   | 29:V:295:VAL:CG1  | 2.34                     | 1.08              |
| 20:M:74:GLN:O     | 20:M:77:TYR:CE1   | 2.06                     | 1.08              |
| 23:P:72:TRP:HH2   | 23:P:103:TYR:HB3  | 1.16                     | 1.08              |
| 33:Z:304:PRO:HB3  | 33:Z:342:LEU:HD11 | 1.30                     | 1.08              |
| 33:Z:821:GLY:HA2  | 33:Z:863:THR:HG22 | 1.33                     | 1.08              |
| 21:N:221:ASP:CA   | 21:N:894:ARG:HH22 | 1.67                     | 1.08              |
| 21:N:588:VAL:HG11 | 21:N:621:THR:CG2  | 1.83                     | 1.08              |
| 33:Z:71:LEU:O     | 33:Z:75:ILE:HG13  | 1.53                     | 1.08              |
| 33:Z:863:THR:HG21 | 33:Z:911:LYS:NZ   | 1.66                     | 1.08              |
| 14:G:193:LYS:HE2  | 14:G:241:PHE:HB3  | 1.32                     | 1.08              |
| 21:N:327:LEU:CD2  | 21:N:743:PHE:CE1  | 2.37                     | 1.08              |
| 25:R:105:LYS:HE2  | 25:R:109:LYS:HZ2  | 1.18                     | 1.08              |
| 31:X:75:TRP:CE3   | 31:X:125:MET:HE2  | 1.88                     | 1.08              |
| 13:F:120:THR:HB   | 14:G:129:ARG:NH1  | 1.68                     | 1.08              |
| 19:L:88:TYR:HD1   | 20:M:62:ILE:HD13  | 1.17                     | 1.08              |
| 28:U:32:ARG:HE    | 28:U:94:HIS:CE1   | 1.71                     | 1.08              |
| 28:U:275:VAL:O    | 28:U:278:ILE:HG22 | 1.49                     | 1.08              |
| 15:H:323:ALA:C    | 20:M:290:ARG:HH21 | 1.62                     | 1.07              |
| 16:I:248:VAL:HG22 | 17:J:274:GLU:OE1  | 1.54                     | 1.07              |
| 25:R:70:TYR:OH    | 25:R:75:GLY:C     | 1.97                     | 1.07              |
| 25:R:408:ASP:CB   | 26:S:464:ARG:HH22 | 1.66                     | 1.07              |
| 33:Z:562:TRP:NE1  | 33:Z:566:LEU:HD21 | 1.68                     | 1.07              |
| 16:I:204:HIS:HB3  | 16:I:207:LEU:HB2  | 1.36                     | 1.07              |
| 16:I:222:TYR:OH   | 16:I:349:LEU:HB3  | 1.54                     | 1.07              |
| 16:I:253:ILE:CD1  | 16:I:287:ILE:HG22 | 1.84                     | 1.07              |
| 17:J:167:PRO:N    | 17:J:174:PHE:CZ   | 2.22                     | 1.07              |
| 22:O:47:LYS:NZ    | 22:O:62:TYR:OH    | 1.88                     | 1.07              |
| 22:O:235:HIS:HD2  | 22:O:236:HIS:CE1  | 1.72                     | 1.07              |
| 23:P:332:GLU:CB   | 23:P:337:HIS:CE1  | 2.38                     | 1.07              |
| 26:S:315:LYS:CD   | 26:S:345:TYR:CE1  | 2.37                     | 1.07              |
| 33:Z:865:ASP:CG   | 33:Z:909:ARG:NH2  | 2.09                     | 1.07              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:284:VAL:HB   | 20:M:254:MET:HB3  | 1.26                     | 1.07              |
| 21:N:329:HIS:HB3  | 29:V:182:LYS:NZ   | 1.54                     | 1.07              |
| 21:N:596:LEU:HD22 | 21:N:717:LEU:HD11 | 1.17                     | 1.07              |
| 31:X:48:PHE:CE2   | 31:X:68:LEU:HD21  | 1.88                     | 1.07              |
| 33:Z:278:LEU:CD2  | 33:Z:297:VAL:HG13 | 1.85                     | 1.07              |
| 15:H:59:ILE:HD13  | 16:I:92:GLU:OE1   | 1.54                     | 1.07              |
| 16:I:207:LEU:HD22 | 33:Z:930:GLY:HA3  | 1.36                     | 1.07              |
| 21:N:282:TYR:OH   | 21:N:286:LEU:HD13 | 1.52                     | 1.07              |
| 23:P:72:TRP:HH2   | 23:P:103:TYR:CB   | 1.68                     | 1.07              |
| 25:R:63:TYR:HE2   | 25:R:94:PHE:HA    | 1.20                     | 1.07              |
| 25:R:266:LEU:HA   | 25:R:270:VAL:CG2  | 1.85                     | 1.07              |
| 28:U:283:ARG:NH1  | 29:V:291:ASN:ND2  | 2.02                     | 1.07              |
| 33:Z:106:TRP:HA   | 33:Z:112:LYS:HD3  | 1.36                     | 1.07              |
| 11:D:97:ARG:NH1   | 11:D:103:PRO:HG3  | 1.69                     | 1.07              |
| 13:F:84:LEU:CD2   | 13:F:132:LEU:HD12 | 1.85                     | 1.07              |
| 13:F:105:VAL:HG22 | 13:F:145:LEU:HD13 | 1.35                     | 1.07              |
| 14:G:121:ALA:O    | 14:G:125:TYR:HD1  | 1.34                     | 1.07              |
| 21:N:327:LEU:CD2  | 21:N:743:PHE:HE1  | 1.68                     | 1.07              |
| 7:7:88:LEU:HD21   | 7:7:106:ILE:HD13  | 1.36                     | 1.06              |
| 21:N:330:THR:HG21 | 21:N:739:PHE:HE1  | 1.12                     | 1.06              |
| 23:P:144:VAL:HG21 | 23:P:160:LEU:HD21 | 1.33                     | 1.06              |
| 8:A:153:SER:HB3   | 8:A:155:TYR:CE1   | 1.90                     | 1.06              |
| 10:C:40:ALA:HA    | 10:C:184:MET:SD   | 1.95                     | 1.06              |
| 14:G:215:ILE:HG23 | 14:G:230:VAL:HB   | 1.35                     | 1.06              |
| 19:L:365:THR:OG1  | 19:L:376:PHE:HE1  | 1.36                     | 1.06              |
| 21:N:293:LEU:HD22 | 21:N:379:LEU:HD13 | 1.37                     | 1.06              |
| 2:2:50:ALA:HB2    | 3:3:118:ILE:HG22  | 1.35                     | 1.06              |
| 5:5:35:ILE:HD11   | 5:5:45:MET:HE3    | 1.35                     | 1.06              |
| 23:P:203:ILE:CG1  | 23:P:220:TYR:OH   | 2.04                     | 1.06              |
| 30:W:152:GLU:OE1  | 30:W:155:ASP:HB2  | 1.53                     | 1.06              |
| 17:J:337:LEU:HB2  | 25:R:204:TRP:HZ2  | 0.89                     | 1.06              |
| 26:S:192:GLU:HG3  | 26:S:239:ARG:HH12 | 1.13                     | 1.06              |
| 26:S:461:PHE:CE1  | 28:U:278:ILE:HB   | 1.91                     | 1.06              |
| 33:Z:301:THR:HG22 | 33:Z:307:HIS:CE1  | 1.90                     | 1.06              |
| 2:2:8:PHE:CZ      | 2:2:11:GLY:HA3    | 1.91                     | 1.06              |
| 2:2:124:TYR:OH    | 2:2:139:GLU:HB3   | 1.56                     | 1.06              |
| 6:6:91:LYS:HB3    | 6:6:96:TYR:HE1    | 1.15                     | 1.06              |
| 7:7:129:TYR:CE1   | 7:7:134:LEU:HD22  | 1.91                     | 1.06              |
| 12:E:15:PHE:CE1   | 12:E:21:LEU:CD1   | 2.37                     | 1.06              |
| 12:E:165:TYR:HB2  | 12:E:167:TYR:CE1  | 1.89                     | 1.06              |
| 21:N:329:HIS:CB   | 29:V:182:LYS:CE   | 2.34                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:O:62:TYR:CD2   | 22:O:82:LEU:HD13  | 1.91                     | 1.06              |
| 33:Z:89:LEU:HD22  | 33:Z:125:THR:HG21 | 1.08                     | 1.06              |
| 14:G:7:TYR:CE1    | 14:G:13:VAL:CG2   | 2.39                     | 1.05              |
| 15:H:101:ARG:NH2  | 15:H:150:LYS:HE2  | 1.71                     | 1.05              |
| 25:R:137:LEU:HB3  | 25:R:141:TYR:CE2  | 1.90                     | 1.05              |
| 12:E:15:PHE:CD1   | 12:E:21:LEU:CD1   | 2.38                     | 1.05              |
| 14:G:106:ILE:HG12 | 14:G:114:ARG:HH21 | 1.21                     | 1.05              |
| 15:H:174:VAL:CG1  | 15:H:183:ILE:HG21 | 1.87                     | 1.05              |
| 25:R:363:PHE:CE1  | 32:Y:78:LYS:HD3   | 1.91                     | 1.05              |
| 27:T:86:LYS:HE2   | 27:T:128:TYR:CE2  | 1.91                     | 1.05              |
| 2:2:50:ALA:CB     | 3:3:118:ILE:CG2   | 2.35                     | 1.05              |
| 15:H:173:ARG:HB2  | 16:I:129:TYR:OH   | 1.55                     | 1.05              |
| 19:L:125:PRO:HB2  | 19:L:127:TYR:CE2  | 1.91                     | 1.05              |
| 20:M:251:LEU:CA   | 20:M:252:VAL:N    | 2.18                     | 1.05              |
| 27:T:86:LYS:HE3   | 27:T:128:TYR:HE2  | 0.90                     | 1.05              |
| 28:U:189:ARG:HH12 | 29:V:296:LEU:HD13 | 1.12                     | 1.05              |
| 15:H:456:LYS:HE2  | 16:I:332:GLU:O    | 1.57                     | 1.05              |
| 22:O:116:ASN:HB3  | 22:O:127:LEU:HD12 | 1.35                     | 1.05              |
| 25:R:137:LEU:HB3  | 25:R:141:TYR:HE2  | 1.20                     | 1.05              |
| 15:H:156:VAL:HG22 | 15:H:181:TYR:CZ   | 1.90                     | 1.05              |
| 22:O:62:TYR:HD2   | 22:O:82:LEU:HD13  | 1.11                     | 1.05              |
| 22:O:266:PHE:HZ   | 22:O:280:LEU:CD2  | 1.70                     | 1.05              |
| 26:S:286:TYR:CE1  | 26:S:323:LEU:HB3  | 1.92                     | 1.05              |
| 30:W:186:ALA:HB2  | 30:W:191:ILE:HG21 | 1.34                     | 1.05              |
| 31:X:75:TRP:CE2   | 31:X:125:MET:CB   | 2.39                     | 1.05              |
| 6:6:91:LYS:CD     | 6:6:96:TYR:OH     | 2.05                     | 1.04              |
| 21:N:162:ARG:HD3  | 21:N:165:ILE:HG12 | 1.35                     | 1.04              |
| 1:1:83:LYS:HZ3    | 1:1:118:SER:CA    | 1.70                     | 1.04              |
| 9:B:65:SER:HB2    | 9:B:90:ARG:HH21   | 1.18                     | 1.04              |
| 23:P:131:PHE:CA   | 23:P:136:ARG:NH1  | 2.20                     | 1.04              |
| 23:P:259:PRO:HB2  | 23:P:327:LEU:HD12 | 1.37                     | 1.04              |
| 25:R:105:LYS:HE2  | 25:R:109:LYS:NZ   | 1.72                     | 1.04              |
| 13:F:84:LEU:CD2   | 13:F:132:LEU:CD1  | 2.35                     | 1.04              |
| 21:N:584:ARG:NH1  | 21:N:614:ASN:HD22 | 1.54                     | 1.04              |
| 25:R:209:ARG:NH2  | 25:R:243:LEU:CD1  | 2.19                     | 1.04              |
| 15:H:340:LEU:HD13 | 15:H:370:ARG:HG3  | 1.35                     | 1.04              |
| 21:N:293:LEU:CD2  | 21:N:379:LEU:HD13 | 1.87                     | 1.04              |
| 33:Z:321:PHE:CE2  | 33:Z:351:PRO:HG3  | 1.92                     | 1.04              |
| 16:I:175:LYS:O    | 17:J:282:PHE:CD1  | 2.11                     | 1.04              |
| 22:O:250:TRP:CB   | 22:O:269:LEU:HD21 | 1.87                     | 1.04              |
| 31:X:91:PHE:H     | 31:X:96:ARG:HG2   | 1.16                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:124:TYR:OH    | 2:2:139:GLU:CB    | 2.06                     | 1.03              |
| 5:5:135:PHE:CE2   | 5:5:163:ALA:HB1   | 1.92                     | 1.03              |
| 21:N:588:VAL:CG1  | 21:N:621:THR:HG22 | 1.88                     | 1.03              |
| 22:O:185:PHE:CD2  | 22:O:223:LEU:HD13 | 1.93                     | 1.03              |
| 23:P:308:LEU:HD13 | 23:P:349:ASN:ND2  | 1.73                     | 1.03              |
| 28:U:92:TRP:HZ2   | 28:U:120:LEU:HD12 | 1.22                     | 1.03              |
| 11:D:10:ILE:HD11  | 12:E:10:ARG:HD2   | 1.38                     | 1.03              |
| 13:F:120:THR:O    | 14:G:129:ARG:HD2  | 1.56                     | 1.03              |
| 15:H:323:ALA:C    | 20:M:290:ARG:NH2  | 2.14                     | 1.03              |
| 16:I:380:LEU:HD22 | 16:I:420:LYS:HG3  | 1.40                     | 1.03              |
| 24:Q:309:ARG:NH2  | 24:Q:345:SER:CA   | 2.18                     | 1.03              |
| 16:I:320:GLY:HA2  | 16:I:323:LYS:HE2  | 1.39                     | 1.03              |
| 22:O:342:ASP:OD1  | 23:P:358:SER:CB   | 2.06                     | 1.03              |
| 33:Z:805:LEU:HD22 | 33:Z:841:GLU:CD   | 1.83                     | 1.03              |
| 4:4:66:TYR:CE2    | 10:C:102:TYR:OH   | 2.12                     | 1.03              |
| 18:K:242:PHE:C    | 18:K:243:VAL:N    | 2.17                     | 1.03              |
| 21:N:330:THR:HG21 | 21:N:739:PHE:CE1  | 1.91                     | 1.03              |
| 21:N:584:ARG:HH11 | 21:N:614:ASN:ND2  | 1.56                     | 1.03              |
| 25:R:408:ASP:HB2  | 26:S:464:ARG:HH22 | 1.10                     | 1.03              |
| 33:Z:53:VAL:CG1   | 33:Z:95:THR:HG21  | 1.83                     | 1.03              |
| 33:Z:923:ILE:HD11 | 33:Z:985:LYS:HE2  | 1.40                     | 1.03              |
| 15:H:206:VAL:HG21 | 15:H:261:ARG:HE   | 1.23                     | 1.03              |
| 15:H:396:MET:HE3  | 15:H:438:ALA:HB2  | 1.08                     | 1.03              |
| 28:U:203:LYS:CE   | 28:U:229:LEU:CD2  | 2.36                     | 1.03              |
| 15:H:174:VAL:HG13 | 15:H:183:ILE:HG21 | 1.34                     | 1.02              |
| 15:H:329:VAL:HG21 | 16:I:300:ARG:HH12 | 1.20                     | 1.02              |
| 16:I:395:MET:HE2  | 16:I:420:LYS:CE   | 1.90                     | 1.02              |
| 18:K:346:ARG:HG2  | 18:K:349:ARG:NH2  | 1.74                     | 1.02              |
| 29:V:107:TRP:CZ3  | 29:V:109:HIS:HD2  | 1.70                     | 1.02              |
| 7:7:33:ARG:HH21   | 7:7:46:SER:HA     | 1.17                     | 1.02              |
| 14:G:122:HIS:CD2  | 14:G:128:VAL:CG1  | 2.42                     | 1.02              |
| 15:H:156:VAL:CG2  | 15:H:181:TYR:OH   | 2.05                     | 1.02              |
| 15:H:172:MET:C    | 16:I:129:TYR:CE2  | 2.36                     | 1.02              |
| 15:H:324:GLY:CA   | 20:M:290:ARG:HH21 | 1.56                     | 1.02              |
| 19:L:361:PHE:CZ   | 19:L:391:ILE:HD12 | 1.93                     | 1.02              |
| 33:Z:392:LEU:HD12 | 33:Z:424:SER:O    | 1.54                     | 1.02              |
| 19:L:340:PRO:HB3  | 19:L:344:ASP:OD2  | 1.58                     | 1.02              |
| 21:N:327:LEU:HD23 | 21:N:743:PHE:CE1  | 1.94                     | 1.02              |
| 33:Z:443:ASP:CB   | 33:Z:447:VAL:HG11 | 1.89                     | 1.02              |
| 15:H:102:CYS:HB2  | 15:H:105:ILE:HD11 | 1.37                     | 1.02              |
| 16:I:204:HIS:CG   | 16:I:207:LEU:HD12 | 1.94                     | 1.02              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:222:TYR:CZ   | 16:I:349:LEU:HB3  | 1.93                     | 1.02              |
| 27:T:126:LEU:HD22 | 27:T:136:LEU:HD21 | 1.39                     | 1.02              |
| 10:C:115:LEU:CD1  | 10:C:137:TYR:OH   | 2.08                     | 1.02              |
| 21:N:329:HIS:CG   | 29:V:182:LYS:HZ1  | 1.77                     | 1.02              |
| 33:Z:493:LEU:CD1  | 33:Z:497:PHE:CZ   | 2.43                     | 1.02              |
| 4:4:81:SER:HA     | 4:4:124:LYS:HZ3   | 1.24                     | 1.01              |
| 6:6:91:LYS:HB3    | 6:6:96:TYR:CE1    | 1.94                     | 1.01              |
| 15:H:59:ILE:HD13  | 16:I:92:GLU:CD    | 1.85                     | 1.01              |
| 19:L:189:GLN:NE2  | 19:L:350:PRO:HD2  | 1.74                     | 1.01              |
| 15:H:173:ARG:N    | 16:I:129:TYR:CZ   | 2.28                     | 1.01              |
| 18:K:212:TYR:HE1  | 18:K:320:ARG:HA   | 0.99                     | 1.01              |
| 8:A:252:ASP:OXT   | 23:P:44:LYS:NZ    | 1.94                     | 1.01              |
| 15:H:156:VAL:HG13 | 15:H:181:TYR:CE1  | 1.95                     | 1.01              |
| 15:H:284:VAL:CB   | 20:M:254:MET:CA   | 2.38                     | 1.01              |
| 23:P:332:GLU:HB3  | 23:P:337:HIS:NE2  | 1.74                     | 1.01              |
| 30:W:20:ASP:CB    | 30:W:25:ARG:NH2   | 2.23                     | 1.01              |
| 30:W:21:PHE:CZ    | 30:W:144:PHE:CE2  | 2.48                     | 1.01              |
| 33:Z:886:VAL:HA   | 33:Z:893:PHE:CE2  | 1.94                     | 1.01              |
| 3:3:60:TYR:CD2    | 10:C:96:GLN:HB3   | 1.95                     | 1.01              |
| 19:L:290:ARG:HD2  | 19:L:293:GLU:HA   | 1.43                     | 1.01              |
| 21:N:717:LEU:CD2  | 21:N:733:LEU:CD1  | 2.39                     | 1.01              |
| 30:W:20:ASP:CB    | 30:W:25:ARG:HH21  | 1.73                     | 1.01              |
| 10:C:177:GLN:HG2  | 11:D:54:LEU:HD21  | 1.41                     | 1.01              |
| 16:I:174:ASP:OD1  | 17:J:282:PHE:HB2  | 1.61                     | 1.01              |
| 24:Q:36:SER:O     | 24:Q:46:VAL:HG23  | 1.60                     | 1.01              |
| 33:Z:68:LEU:HD12  | 33:Z:111:LEU:HD22 | 1.02                     | 1.01              |
| 33:Z:138:ARG:NH2  | 33:Z:157:LEU:CD1  | 2.24                     | 1.01              |
| 33:Z:863:THR:CG2  | 33:Z:911:LYS:HZ3  | 1.74                     | 1.01              |
| 1:1:137:TYR:CZ    | 1:1:157:HIS:CD2   | 2.49                     | 1.00              |
| 4:4:45:PHE:CD2    | 4:4:101:VAL:HG12  | 1.96                     | 1.00              |
| 16:I:204:HIS:CD2  | 16:I:207:LEU:HD12 | 1.96                     | 1.00              |
| 23:P:366:ASN:ND2  | 23:P:373:GLU:HA   | 1.74                     | 1.00              |
| 28:U:16:LEU:HD23  | 28:U:19:LEU:HD12  | 1.43                     | 1.00              |
| 1:1:-8:LYS:HZ3    | 2:2:117:GLY:HA3   | 1.26                     | 1.00              |
| 28:U:203:LYS:HE3  | 28:U:229:LEU:CD2  | 1.91                     | 1.00              |
| 30:W:21:PHE:CZ    | 30:W:144:PHE:CD2  | 2.48                     | 1.00              |
| 2:2:50:ALA:HB3    | 3:3:118:ILE:CG2   | 1.92                     | 1.00              |
| 7:7:33:ARG:HH21   | 7:7:46:SER:CA     | 1.74                     | 1.00              |
| 17:J:340:GLY:HA2  | 25:R:238:PHE:CE1  | 1.95                     | 1.00              |
| 18:K:272:ASP:HB2  | 19:L:306:MET:HE2  | 1.41                     | 1.00              |
| 19:L:336:ALA:C    | 19:L:342:ARG:HH11 | 1.69                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:O:15:ARG:NH1   | 22:O:73:ILE:CG1   | 2.23                     | 1.00              |
| 29:V:145:GLN:HG2  | 29:V:148:LYS:HE3  | 1.44                     | 1.00              |
| 33:Z:290:GLU:HG3  | 33:Z:293:MET:HE3  | 1.40                     | 1.00              |
| 20:M:50:ARG:NH1   | 20:M:54:GLU:OE2   | 1.95                     | 1.00              |
| 33:Z:385:PHE:CZ   | 33:Z:389:PHE:CZ   | 2.50                     | 1.00              |
| 16:I:204:HIS:CG   | 16:I:207:LEU:CD1  | 2.45                     | 0.99              |
| 28:U:67:PHE:CE1   | 30:W:97:THR:OG1   | 2.13                     | 0.99              |
| 19:L:290:ARG:NH1  | 19:L:293:GLU:HB3  | 1.77                     | 0.99              |
| 26:S:428:ARG:HA   | 27:T:195:LEU:CD2  | 1.91                     | 0.99              |
| 21:N:362:TRP:CZ2  | 29:V:23:THR:HG21  | 1.97                     | 0.99              |
| 14:G:173:ALA:CB   | 19:L:420:ARG:NH2  | 2.23                     | 0.99              |
| 33:Z:154:ILE:CG2  | 33:Z:211:PHE:CZ   | 2.45                     | 0.99              |
| 8:A:54:ILE:HG22   | 8:A:210:MET:HE1   | 1.44                     | 0.99              |
| 19:L:95:ILE:HG23  | 20:M:68:LYS:HZ2   | 1.26                     | 0.99              |
| 25:R:335:ARG:CD   | 25:R:376:GLN:HB3  | 1.90                     | 0.99              |
| 14:G:200:TYR:CE1  | 14:G:246:ILE:CG2  | 2.45                     | 0.99              |
| 31:X:75:TRP:CE2   | 31:X:125:MET:CG   | 2.40                     | 0.99              |
| 33:Z:246:CYS:SG   | 33:Z:271:ILE:CG2  | 2.50                     | 0.99              |
| 15:H:396:MET:HE3  | 15:H:438:ALA:CB   | 1.63                     | 0.99              |
| 21:N:53:ASP:CA    | 21:N:58:ARG:HH21  | 1.75                     | 0.99              |
| 25:R:241:ILE:HG22 | 25:R:242:GLU:HG3  | 1.41                     | 0.99              |
| 28:U:203:LYS:HE3  | 28:U:229:LEU:HD21 | 1.02                     | 0.99              |
| 33:Z:562:TRP:HE1  | 33:Z:566:LEU:HD21 | 1.21                     | 0.99              |
| 14:G:111:PHE:CD1  | 14:G:114:ARG:NH2  | 2.27                     | 0.99              |
| 17:J:62:LEU:HD11  | 18:K:89:ILE:HG13  | 1.41                     | 0.99              |
| 23:P:272:PRO:O    | 23:P:273:TYR:CD1  | 2.15                     | 0.99              |
| 1:1:-8:LYS:NZ     | 2:2:117:GLY:HA3   | 1.78                     | 0.99              |
| 12:E:87:SER:O     | 12:E:91:HIS:ND1   | 1.94                     | 0.99              |
| 14:G:168:ARG:HE   | 14:G:172:LYS:NZ   | 1.59                     | 0.99              |
| 22:O:15:ARG:NH1   | 22:O:73:ILE:HD11  | 1.77                     | 0.99              |
| 22:O:377:VAL:HG21 | 28:U:200:LEU:HD11 | 1.45                     | 0.99              |
| 33:Z:884:THR:O    | 33:Z:888:LEU:HD12 | 1.61                     | 0.99              |
| 19:L:88:TYR:CD1   | 20:M:62:ILE:HB    | 1.97                     | 0.99              |
| 24:Q:418:GLN:HB2  | 29:V:262:THR:HG21 | 1.40                     | 0.99              |
| 22:O:228:TYR:HA   | 22:O:290:LYS:NZ   | 1.76                     | 0.98              |
| 13:F:101:ARG:HH12 | 13:F:103:LEU:HD12 | 1.26                     | 0.98              |
| 18:K:280:LYS:NZ   | 18:K:296:LEU:HD23 | 1.78                     | 0.98              |
| 27:T:126:LEU:HD22 | 27:T:136:LEU:CD2  | 1.93                     | 0.98              |
| 33:Z:64:TYR:CD2   | 33:Z:111:LEU:CD1  | 1.87                     | 0.98              |
| 33:Z:886:VAL:HG13 | 33:Z:893:PHE:CZ   | 1.98                     | 0.98              |
| 15:H:172:MET:HB3  | 16:I:129:TYR:CD2  | 1.66                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:37:TYR:OH     | 3:3:59:ARG:HB2    | 1.64                     | 0.98              |
| 17:J:337:LEU:CB   | 25:R:204:TRP:HZ2  | 1.76                     | 0.98              |
| 21:N:593:PHE:CZ   | 21:N:734:VAL:HG22 | 1.97                     | 0.98              |
| 33:Z:188:ALA:H    | 33:Z:201:LEU:HD11 | 1.24                     | 0.98              |
| 16:I:126:PRO:HG2  | 16:I:154:MET:CE   | 1.93                     | 0.98              |
| 17:J:340:GLY:CA   | 25:R:238:PHE:CE1  | 2.46                     | 0.98              |
| 2:2:160:GLN:NE2   | 2:2:164:TRP:NE1   | 2.10                     | 0.98              |
| 20:M:196:ALA:HB2  | 20:M:345:ARG:HE   | 1.24                     | 0.98              |
| 24:Q:299:MET:CE   | 24:Q:335:PHE:HZ   | 1.77                     | 0.98              |
| 31:X:75:TRP:CE3   | 31:X:125:MET:CE   | 2.43                     | 0.98              |
| 33:Z:74:SER:HB2   | 33:Z:79:THR:HG22  | 1.45                     | 0.98              |
| 8:A:164:VAL:HB    | 9:B:61:LEU:HD21   | 1.44                     | 0.98              |
| 12:E:165:TYR:HB2  | 12:E:167:TYR:HE1  | 1.27                     | 0.98              |
| 19:L:365:THR:OG1  | 19:L:376:PHE:CE1  | 2.11                     | 0.98              |
| 33:Z:929:VAL:O    | 33:Z:955:VAL:HG22 | 1.63                     | 0.98              |
| 1:1:83:LYS:HD2    | 1:1:119:VAL:HG23  | 1.00                     | 0.98              |
| 11:D:10:ILE:H     | 11:D:18:PHE:HE2   | 1.05                     | 0.98              |
| 23:P:344:ARG:O    | 23:P:348:HIS:ND1  | 1.97                     | 0.98              |
| 14:G:7:TYR:HE1    | 14:G:13:VAL:HG21  | 1.26                     | 0.97              |
| 33:Z:68:LEU:HD12  | 33:Z:111:LEU:CD2  | 1.93                     | 0.97              |
| 12:E:15:PHE:HE1   | 12:E:21:LEU:HD11  | 1.21                     | 0.97              |
| 16:I:126:PRO:CG   | 16:I:154:MET:HE3  | 1.93                     | 0.97              |
| 17:J:167:PRO:CB   | 17:J:174:PHE:CE2  | 2.47                     | 0.97              |
| 19:L:336:ALA:HB1  | 19:L:342:ARG:HH12 | 1.05                     | 0.97              |
| 9:B:218:ASN:O     | 9:B:222:LEU:HG    | 1.64                     | 0.97              |
| 26:S:141:LEU:O    | 26:S:145:PHE:HD1  | 1.47                     | 0.97              |
| 15:H:101:ARG:HH22 | 15:H:150:LYS:HE2  | 1.29                     | 0.97              |
| 15:H:379:LEU:CD2  | 15:H:415:THR:HG22 | 1.94                     | 0.97              |
| 17:J:277:ASN:HD21 | 17:J:309:ARG:CZ   | 1.76                     | 0.97              |
| 32:Y:80:GLU:CD    | 32:Y:83:ARG:HH21  | 1.73                     | 0.97              |
| 17:J:134:VAL:HG12 | 17:J:135:SER:H    | 0.82                     | 0.97              |
| 21:N:329:HIS:HB3  | 29:V:182:LYS:HZ1  | 0.80                     | 0.97              |
| 21:N:424:LYS:HZ1  | 21:N:461:GLU:HB3  | 0.82                     | 0.97              |
| 22:O:190:TYR:HD1  | 22:O:227:ILE:HD11 | 1.30                     | 0.97              |
| 26:S:286:TYR:CZ   | 26:S:323:LEU:HB3  | 2.00                     | 0.97              |
| 11:D:193:LYS:HG3  | 11:D:197:ARG:NH1  | 1.80                     | 0.97              |
| 30:W:141:ILE:HD13 | 30:W:154:LEU:HD22 | 1.45                     | 0.97              |
| 3:3:60:TYR:HA     | 10:C:96:GLN:OE1   | 1.65                     | 0.97              |
| 16:I:310:LEU:HD11 | 16:I:337:ALA:O    | 1.65                     | 0.97              |
| 17:J:228:ARG:NH1  | 17:J:232:GLU:OE2  | 1.97                     | 0.97              |
| 24:Q:299:MET:HE1  | 24:Q:335:PHE:HZ   | 1.24                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:418:GLN:CB   | 29:V:262:THR:CG2  | 2.33                     | 0.97              |
| 28:U:32:ARG:CB    | 28:U:94:HIS:CE1   | 2.45                     | 0.97              |
| 33:Z:769:ASN:HB3  | 33:Z:772:ILE:HD12 | 1.47                     | 0.97              |
| 10:C:3:SER:HB3    | 11:D:6:ARG:NH2    | 1.78                     | 0.97              |
| 13:F:179:PHE:CZ   | 13:F:192:ALA:CB   | 2.47                     | 0.96              |
| 16:I:104:LEU:CD2  | 16:I:149:LEU:O    | 2.13                     | 0.96              |
| 20:M:148:VAL:HG22 | 20:M:155:ILE:HG12 | 1.46                     | 0.96              |
| 28:U:21:HIS:CE1   | 28:U:93:TYR:OH    | 2.18                     | 0.96              |
| 30:W:103:ASN:HB2  | 30:W:106:GLN:HE21 | 1.30                     | 0.96              |
| 33:Z:474:LEU:HD23 | 33:Z:493:LEU:HD22 | 0.99                     | 0.96              |
| 33:Z:835:ALA:O    | 33:Z:838:TYR:CD2  | 2.19                     | 0.96              |
| 33:Z:290:GLU:HG3  | 33:Z:293:MET:CE   | 1.95                     | 0.96              |
| 7:7:93:TYR:HE1    | 7:7:96:ARG:HH21   | 1.04                     | 0.96              |
| 18:K:161:MET:HE3  | 18:K:257:VAL:HG21 | 1.46                     | 0.96              |
| 24:Q:309:ARG:HE   | 24:Q:345:SER:HB3  | 1.22                     | 0.96              |
| 24:Q:429:LYS:HB2  | 29:V:269:ARG:HH21 | 1.30                     | 0.96              |
| 30:W:9:VAL:HG22   | 30:W:52:ILE:HD11  | 0.98                     | 0.96              |
| 1:1:83:LYS:NZ     | 1:1:118:SER:CA    | 2.28                     | 0.96              |
| 3:3:129:VAL:HG22  | 3:3:138:PHE:CD1   | 1.99                     | 0.96              |
| 7:7:93:TYR:CE1    | 7:7:96:ARG:NH2    | 2.32                     | 0.96              |
| 20:M:75:LEU:HA    | 20:M:77:TYR:HD1   | 1.30                     | 0.96              |
| 21:N:318:LYS:HA   | 29:V:180:LEU:HG   | 1.46                     | 0.96              |
| 25:R:70:TYR:OH    | 25:R:75:GLY:O     | 1.82                     | 0.96              |
| 33:Z:394:TYR:HD2  | 33:Z:396:ASN:ND2  | 1.62                     | 0.96              |
| 16:I:207:LEU:HD22 | 33:Z:930:GLY:CA   | 1.95                     | 0.96              |
| 21:N:329:HIS:CB   | 29:V:182:LYS:HE3  | 1.93                     | 0.96              |
| 28:U:119:LEU:HD12 | 28:U:137:TYR:O    | 1.65                     | 0.96              |
| 19:L:159:LEU:HD12 | 19:L:160:PRO:O    | 1.64                     | 0.96              |
| 21:N:588:VAL:HG11 | 21:N:621:THR:HG22 | 1.45                     | 0.96              |
| 1:1:14:LEU:HD11   | 1:1:100:ALA:HB1   | 1.48                     | 0.96              |
| 18:K:159:SER:CB   | 18:K:244:HIS:HE2  | 1.79                     | 0.96              |
| 22:O:59:LEU:HD21  | 22:O:85:SER:CB    | 1.95                     | 0.96              |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:HD11 | 1.20                     | 0.96              |
| 33:Z:208:VAL:HG21 | 33:Z:236:PHE:CE2  | 2.01                     | 0.96              |
| 2:2:82:MET:O      | 2:2:86:HIS:ND1    | 1.97                     | 0.96              |
| 28:U:92:TRP:CZ2   | 28:U:120:LEU:HD12 | 2.01                     | 0.96              |
| 15:H:249:TYR:CE1  | 15:H:376:GLU:HA   | 2.01                     | 0.95              |
| 21:N:162:ARG:CD   | 21:N:165:ILE:HG12 | 1.95                     | 0.95              |
| 33:Z:249:MET:HE1  | 33:Z:268:ALA:HB2  | 1.46                     | 0.95              |
| 16:I:172:LYS:HG2  | 17:J:278:GLN:HG3  | 1.49                     | 0.95              |
| 28:U:32:ARG:CG    | 28:U:94:HIS:CE1   | 2.48                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:U:92:TRP:CZ2   | 28:U:120:LEU:CD1  | 2.49                     | 0.95              |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:CE2  | 2.01                     | 0.95              |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:HD22 | 1.49                     | 0.95              |
| 23:P:141:LYS:HB2  | 23:P:179:PHE:HE1  | 1.30                     | 0.95              |
| 2:2:8:PHE:CZ      | 2:2:11:GLY:CA     | 2.49                     | 0.95              |
| 14:G:200:TYR:CE1  | 14:G:246:ILE:HG21 | 2.01                     | 0.95              |
| 15:H:306:ILE:HG22 | 15:H:308:PHE:CE1  | 2.01                     | 0.95              |
| 33:Z:89:LEU:HD22  | 33:Z:125:THR:CB   | 1.94                     | 0.95              |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:HA   | 1.45                     | 0.95              |
| 15:H:172:MET:CB   | 16:I:129:TYR:HD2  | 1.75                     | 0.95              |
| 15:H:324:GLY:CA   | 20:M:290:ARG:HH22 | 1.54                     | 0.95              |
| 25:R:209:ARG:HG3  | 25:R:213:TYR:CE2  | 2.02                     | 0.95              |
| 33:Z:322:GLU:HG2  | 33:Z:464:ASP:OD2  | 1.67                     | 0.95              |
| 7:7:193:ASP:HB3   | 7:7:196:THR:OG1   | 1.64                     | 0.95              |
| 15:H:436:LYS:HE2  | 33:Z:365:SER:CB   | 1.97                     | 0.95              |
| 21:N:346:ASN:HB3  | 21:N:350:LYS:HE3  | 1.47                     | 0.95              |
| 22:O:266:PHE:HZ   | 22:O:280:LEU:HD22 | 1.31                     | 0.95              |
| 23:P:131:PHE:N    | 23:P:136:ARG:HH12 | 1.64                     | 0.95              |
| 25:R:158:LEU:HD11 | 25:R:197:MET:HE1  | 1.46                     | 0.95              |
| 33:Z:64:TYR:CE2   | 33:Z:68:LEU:HD11  | 2.01                     | 0.95              |
| 14:G:53:ILE:HD11  | 14:G:212:GLU:HB2  | 1.46                     | 0.95              |
| 21:N:424:LYS:NZ   | 21:N:461:GLU:CB   | 2.30                     | 0.95              |
| 28:U:67:PHE:CZ    | 30:W:97:THR:HA    | 2.00                     | 0.95              |
| 29:V:131:GLN:HE22 | 29:V:194:ARG:HH21 | 1.12                     | 0.95              |
| 24:Q:309:ARG:HH21 | 24:Q:345:SER:HA   | 1.28                     | 0.95              |
| 33:Z:884:THR:O    | 33:Z:888:LEU:CD1  | 2.13                     | 0.95              |
| 7:7:68:TYR:OH     | 14:G:70:ASP:N     | 1.99                     | 0.95              |
| 23:P:131:PHE:HA   | 23:P:136:ARG:HH11 | 1.25                     | 0.95              |
| 28:U:67:PHE:CE2   | 30:W:97:THR:HA    | 2.02                     | 0.95              |
| 29:V:135:ARG:HA   | 29:V:157:ARG:CZ   | 1.97                     | 0.95              |
| 33:Z:748:LEU:CD2  | 33:Z:783:VAL:CG1  | 2.45                     | 0.95              |
| 14:G:146:HIS:CB   | 14:G:148:TYR:HE1  | 1.79                     | 0.95              |
| 23:P:366:ASN:HD21 | 23:P:373:GLU:HA   | 1.28                     | 0.95              |
| 33:Z:64:TYR:CZ    | 33:Z:68:LEU:HD11  | 2.02                     | 0.95              |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:CG1  | 1.96                     | 0.95              |
| 19:L:336:ALA:CB   | 19:L:342:ARG:HH12 | 1.80                     | 0.94              |
| 24:Q:146:TYR:HE1  | 24:Q:184:VAL:HA   | 1.15                     | 0.94              |
| 16:I:204:HIS:HD2  | 16:I:207:LEU:HD11 | 1.28                     | 0.94              |
| 20:M:197:ILE:HB   | 20:M:322:LYS:HD3  | 1.46                     | 0.94              |
| 16:I:253:ILE:HD13 | 16:I:287:ILE:HG22 | 1.48                     | 0.94              |
| 7:7:145:PRO:HA    | 7:7:148:ARG:HE    | 1.32                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:172:MET:HB2  | 16:I:129:TYR:CG   | 2.01                     | 0.94              |
| 18:K:137:VAL:HB   | 18:K:146:LEU:CD1  | 1.98                     | 0.94              |
| 22:O:59:LEU:HD21  | 22:O:85:SER:HB3   | 1.48                     | 0.94              |
| 15:H:59:ILE:CD1   | 16:I:92:GLU:OE1   | 2.15                     | 0.94              |
| 33:Z:562:TRP:NE1  | 33:Z:566:LEU:CD2  | 2.29                     | 0.94              |
| 14:G:122:HIS:NE2  | 14:G:128:VAL:HG11 | 1.82                     | 0.94              |
| 15:H:284:VAL:CG2  | 20:M:254:MET:HA   | 1.98                     | 0.94              |
| 18:K:135:MET:HG2  | 18:K:259:ARG:HH22 | 1.31                     | 0.94              |
| 33:Z:165:TYR:HE1  | 33:Z:190:THR:HG1  | 0.96                     | 0.94              |
| 33:Z:327:GLN:HG2  | 33:Z:349:THR:HB   | 1.47                     | 0.94              |
| 8:A:205:PHE:CZ    | 8:A:209:HIS:HE1   | 1.82                     | 0.94              |
| 26:S:343:LEU:CD1  | 26:S:347:HIS:HE1  | 1.81                     | 0.94              |
| 30:W:158:ILE:HG13 | 30:W:171:LEU:HB2  | 1.50                     | 0.94              |
| 1:1:83:LYS:HD2    | 1:1:119:VAL:CG2   | 1.95                     | 0.94              |
| 4:4:129:TYR:OH    | 4:4:144:ASP:OD1   | 1.86                     | 0.94              |
| 14:G:173:ALA:HA   | 19:L:420:ARG:NH2  | 1.83                     | 0.94              |
| 16:I:310:LEU:HD13 | 16:I:338:LEU:HA   | 1.50                     | 0.94              |
| 18:K:224:LYS:CE   | 18:K:236:ARG:NH2  | 2.30                     | 0.94              |
| 20:M:74:GLN:O     | 20:M:77:TYR:HE1   | 1.49                     | 0.94              |
| 25:R:411:LEU:CD2  | 26:S:464:ARG:HH11 | 1.81                     | 0.94              |
| 28:U:283:ARG:HH12 | 29:V:291:ASN:ND2  | 1.60                     | 0.94              |
| 33:Z:205:LEU:CG   | 33:Z:236:PHE:HE1  | 1.80                     | 0.94              |
| 33:Z:497:PHE:CE2  | 33:Z:505:VAL:HG12 | 2.02                     | 0.94              |
| 19:L:336:ALA:CB   | 19:L:342:ARG:NH1  | 2.30                     | 0.94              |
| 27:T:47:GLN:O     | 27:T:48:ASN:CG    | 2.10                     | 0.94              |
| 6:6:91:LYS:HD3    | 6:6:96:TYR:HH     | 1.25                     | 0.94              |
| 16:I:214:LYS:NZ   | 16:I:318:ASP:C    | 2.26                     | 0.94              |
| 13:F:13:PHE:HE1   | 14:G:130:PRO:HD2  | 1.32                     | 0.93              |
| 15:H:172:MET:CG   | 16:I:129:TYR:CD2  | 2.51                     | 0.93              |
| 33:Z:863:THR:CG2  | 33:Z:911:LYS:NZ   | 2.31                     | 0.93              |
| 13:F:120:THR:CB   | 14:G:129:ARG:NH1  | 2.27                     | 0.93              |
| 20:M:251:LEU:C    | 20:M:252:VAL:N    | 0.84                     | 0.93              |
| 21:N:536:ILE:HD13 | 21:N:555:ILE:CG1  | 1.98                     | 0.93              |
| 23:P:308:LEU:CD1  | 23:P:349:ASN:OD1  | 2.16                     | 0.93              |
| 30:W:44:ASN:HB2   | 30:W:47:ASN:HD21  | 1.32                     | 0.93              |
| 33:Z:56:LEU:CD2   | 33:Z:68:LEU:HD23  | 1.99                     | 0.93              |
| 33:Z:385:PHE:CE2  | 33:Z:389:PHE:HE2  | 1.79                     | 0.93              |
| 33:Z:562:TRP:CD1  | 33:Z:566:LEU:HG   | 2.02                     | 0.93              |
| 25:R:130:GLN:HE21 | 25:R:134:TRP:HE1  | 1.12                     | 0.93              |
| 22:O:356:ARG:HH12 | 28:U:234:ASN:HB2  | 1.32                     | 0.93              |
| 17:J:337:LEU:HD23 | 17:J:377:VAL:HB   | 1.49                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:427:GLN:HG2  | 33:Z:428:TRP:CD1  | 2.03                     | 0.93              |
| 25:R:50:VAL:HG13  | 25:R:54:ILE:HD12  | 1.50                     | 0.93              |
| 26:S:461:PHE:CD2  | 28:U:277:TYR:HB2  | 2.03                     | 0.93              |
| 7:7:6:MET:HE1     | 7:7:150:VAL:HG11  | 1.49                     | 0.93              |
| 26:S:141:LEU:O    | 26:S:145:PHE:CD1  | 2.21                     | 0.93              |
| 30:W:139:VAL:HG11 | 30:W:157:PHE:CE2  | 2.04                     | 0.93              |
| 1:1:57:ASP:HB3    | 8:A:106:TYR:CE1   | 2.02                     | 0.93              |
| 14:G:121:ALA:O    | 14:G:125:TYR:CD1  | 2.22                     | 0.93              |
| 19:L:88:TYR:CE1   | 20:M:62:ILE:HB    | 2.02                     | 0.93              |
| 21:N:329:HIS:CG   | 29:V:182:LYS:NZ   | 2.34                     | 0.93              |
| 33:Z:546:ILE:CG2  | 33:Z:550:PHE:CE2  | 2.51                     | 0.93              |
| 1:1:19:ARG:HH21   | 1:1:171:GLY:CA    | 1.80                     | 0.93              |
| 7:7:129:TYR:HE1   | 7:7:134:LEU:CD2   | 1.82                     | 0.93              |
| 10:C:44:ILE:HB    | 10:C:216:ILE:HD12 | 1.51                     | 0.93              |
| 14:G:146:HIS:HB3  | 14:G:148:TYR:HE1  | 1.10                     | 0.93              |
| 21:N:536:ILE:HD13 | 21:N:555:ILE:HG12 | 1.48                     | 0.93              |
| 22:O:15:ARG:NH1   | 22:O:73:ILE:CD1   | 2.32                     | 0.93              |
| 1:1:174:ARG:NH1   | 1:1:185:ARG:NH2   | 2.17                     | 0.92              |
| 15:H:65:GLU:O     | 15:H:69:VAL:HG23  | 1.69                     | 0.92              |
| 16:I:75:PHE:HD2   | 16:I:76:VAL:HG23  | 1.33                     | 0.92              |
| 23:P:184:MET:CB   | 23:P:223:LEU:HD13 | 1.98                     | 0.92              |
| 23:P:342:GLN:HE21 | 23:P:346:ILE:HD11 | 1.31                     | 0.92              |
| 33:Z:306:MET:HE3  | 33:Z:310:LEU:HD21 | 1.49                     | 0.92              |
| 16:I:395:MET:CE   | 16:I:420:LYS:NZ   | 2.32                     | 0.92              |
| 13:F:84:LEU:HD21  | 13:F:132:LEU:HD12 | 1.47                     | 0.92              |
| 13:F:105:VAL:CG2  | 13:F:145:LEU:HB2  | 1.99                     | 0.92              |
| 18:K:161:MET:HE1  | 18:K:237:VAL:HG13 | 1.51                     | 0.92              |
| 18:K:212:TYR:CE1  | 18:K:321:ALA:N    | 2.38                     | 0.92              |
| 30:W:21:PHE:CZ    | 30:W:25:ARG:NH1   | 2.36                     | 0.92              |
| 24:Q:309:ARG:NH2  | 24:Q:345:SER:HA   | 1.83                     | 0.92              |
| 31:X:75:TRP:HZ2   | 31:X:125:MET:HG3  | 1.26                     | 0.92              |
| 15:H:173:ARG:HA   | 16:I:129:TYR:OH   | 1.66                     | 0.92              |
| 18:K:224:LYS:HE2  | 18:K:236:ARG:NH2  | 1.84                     | 0.92              |
| 21:N:717:LEU:HD23 | 21:N:733:LEU:CD1  | 1.99                     | 0.92              |
| 22:O:15:ARG:HH12  | 22:O:73:ILE:HG12  | 1.34                     | 0.92              |
| 24:Q:329:GLU:OE1  | 24:Q:332:ARG:NH2  | 2.03                     | 0.92              |
| 33:Z:443:ASP:CB   | 33:Z:447:VAL:CG1  | 2.47                     | 0.92              |
| 20:M:290:ARG:HD3  | 20:M:294:GLU:HB3  | 1.49                     | 0.92              |
| 23:P:308:LEU:HD13 | 23:P:349:ASN:OD1  | 1.70                     | 0.92              |
| 28:U:32:ARG:HH22  | 28:U:106:ILE:HD12 | 1.33                     | 0.92              |
| 33:Z:562:TRP:CD2  | 33:Z:566:LEU:HD11 | 2.05                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:192:VAL:HG13 | 14:G:215:ILE:HD13 | 1.50                     | 0.92              |
| 10:C:13:PHE:CZ    | 11:D:127:ARG:NH1  | 2.37                     | 0.92              |
| 13:F:3:ARG:NH2    | 15:H:359:ASN:ND2  | 2.18                     | 0.92              |
| 16:I:126:PRO:HB3  | 16:I:128:TYR:HE2  | 0.75                     | 0.92              |
| 16:I:204:HIS:CB   | 16:I:207:LEU:HD12 | 1.99                     | 0.92              |
| 21:N:273:LEU:O    | 21:N:277:LEU:HG   | 1.68                     | 0.92              |
| 22:O:15:ARG:NH1   | 22:O:73:ILE:HG12  | 1.82                     | 0.92              |
| 33:Z:53:VAL:HG23  | 33:Z:91:PHE:CE2   | 2.05                     | 0.92              |
| 9:B:65:SER:HB2    | 9:B:90:ARG:NH2    | 1.83                     | 0.92              |
| 12:E:165:TYR:CB   | 12:E:167:TYR:CE1  | 2.53                     | 0.92              |
| 16:I:207:LEU:CD1  | 33:Z:930:GLY:HA2  | 2.00                     | 0.92              |
| 25:R:50:VAL:HG13  | 25:R:54:ILE:CD1   | 2.00                     | 0.92              |
| 26:S:461:PHE:HZ   | 28:U:274:MET:O    | 1.52                     | 0.92              |
| 19:L:88:TYR:CD1   | 20:M:62:ILE:HD13  | 2.04                     | 0.92              |
| 23:P:202:LYS:HE2  | 23:P:206:LYS:NZ   | 1.85                     | 0.92              |
| 25:R:50:VAL:CG1   | 25:R:54:ILE:HD12  | 2.00                     | 0.92              |
| 26:S:461:PHE:HE1  | 28:U:278:ILE:HB   | 1.34                     | 0.92              |
| 33:Z:165:TYR:OH   | 33:Z:188:ALA:HB1  | 1.70                     | 0.92              |
| 9:B:66:LEU:HD11   | 9:B:235:PHE:CE2   | 2.04                     | 0.91              |
| 21:N:221:ASP:HA   | 21:N:894:ARG:HH22 | 1.32                     | 0.91              |
| 25:R:63:TYR:CE2   | 25:R:94:PHE:HA    | 2.04                     | 0.91              |
| 29:V:53:MET:CE    | 29:V:65:VAL:HG11  | 2.00                     | 0.91              |
| 8:A:56:GLN:NE2    | 8:A:214:LEU:HD13  | 1.84                     | 0.91              |
| 11:D:68:ASP:CG    | 11:D:97:ARG:HH21  | 1.77                     | 0.91              |
| 15:H:284:VAL:CB   | 20:M:254:MET:HB3  | 2.00                     | 0.91              |
| 33:Z:53:VAL:HG13  | 33:Z:95:THR:HG21  | 0.92                     | 0.91              |
| 33:Z:188:ALA:N    | 33:Z:201:LEU:HD12 | 1.79                     | 0.91              |
| 4:4:3:ILE:CG2     | 4:4:102:LEU:HD12  | 1.98                     | 0.91              |
| 21:N:207:LEU:HB2  | 21:N:232:LEU:HD21 | 1.51                     | 0.91              |
| 33:Z:574:TYR:OH   | 33:Z:584:VAL:CG2  | 2.19                     | 0.91              |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:C    | 1.95                     | 0.91              |
| 8:A:156:LYS:HB3   | 8:A:166:TYR:CE1   | 2.04                     | 0.91              |
| 14:G:173:ALA:HB1  | 19:L:420:ARG:HH21 | 1.32                     | 0.91              |
| 18:K:70:ASP:OD1   | 18:K:73:ARG:NH2   | 2.03                     | 0.91              |
| 19:L:357:ARG:HH12 | 19:L:386:PHE:HB2  | 1.34                     | 0.91              |
| 29:V:71:MET:HE1   | 29:V:83:VAL:HG13  | 1.48                     | 0.91              |
| 7:7:187:PHE:CZ    | 7:7:204:LEU:HB3   | 2.06                     | 0.91              |
| 11:D:7:ALA:HB2    | 12:E:125:GLU:OE2  | 1.71                     | 0.91              |
| 12:E:208:MET:HG2  | 12:E:210:GLU:H    | 1.36                     | 0.91              |
| 18:K:159:SER:HG   | 18:K:244:HIS:HE2  | 0.96                     | 0.91              |
| 2:2:8:PHE:CE2     | 2:2:11:GLY:N      | 2.37                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:J:167:PRO:HA   | 17:J:174:PHE:CZ   | 2.06                     | 0.91              |
| 33:Z:562:TRP:HE1  | 33:Z:566:LEU:CD2  | 1.84                     | 0.91              |
| 5:5:38:ASN:HD21   | 5:5:41:LEU:HD12   | 1.36                     | 0.91              |
| 10:C:115:LEU:HD12 | 10:C:137:TYR:OH   | 1.71                     | 0.91              |
| 13:F:12:THR:CG2   | 13:F:19:LEU:CD1   | 2.49                     | 0.91              |
| 5:5:55:TRP:NE1    | 6:6:89:TYR:OH     | 2.03                     | 0.91              |
| 15:H:351:VAL:HG12 | 15:H:353:PHE:CE1  | 2.04                     | 0.91              |
| 23:P:267:PHE:HE1  | 23:P:329:PHE:CE2  | 1.65                     | 0.91              |
| 31:X:75:TRP:HZ3   | 31:X:125:MET:HE2  | 1.20                     | 0.91              |
| 31:X:100:TRP:CZ3  | 31:X:102:GLN:HA   | 2.06                     | 0.91              |
| 5:5:159:ARG:HH12  | 5:5:200:VAL:HA    | 1.35                     | 0.91              |
| 14:G:48:ALA:HB1   | 14:G:199:ILE:HD11 | 1.53                     | 0.90              |
| 24:Q:311:LEU:HD22 | 24:Q:343:LEU:CD1  | 1.99                     | 0.90              |
| 28:U:32:ARG:CG    | 28:U:94:HIS:HE1   | 1.84                     | 0.90              |
| 22:O:250:TRP:O    | 22:O:269:LEU:CD1  | 2.16                     | 0.90              |
| 23:P:72:TRP:CH2   | 23:P:103:TYR:CB   | 2.48                     | 0.90              |
| 23:P:332:GLU:HB2  | 23:P:337:HIS:CE1  | 2.06                     | 0.90              |
| 15:H:340:LEU:CD1  | 15:H:370:ARG:HG3  | 2.00                     | 0.90              |
| 17:J:377:VAL:HG12 | 17:J:382:PHE:CE2  | 2.05                     | 0.90              |
| 22:O:266:PHE:CZ   | 22:O:280:LEU:CD2  | 2.54                     | 0.90              |
| 30:W:31:ASP:O     | 30:W:35:PHE:HD1   | 1.55                     | 0.90              |
| 31:X:79:LYS:HE2   | 31:X:98:PHE:HE2   | 1.35                     | 0.90              |
| 8:A:128:TYR:CZ    | 8:A:134:MET:HE1   | 2.07                     | 0.90              |
| 15:H:206:VAL:CG2  | 15:H:261:ARG:HE   | 1.83                     | 0.90              |
| 21:N:211:PHE:CD2  | 21:N:237:LEU:HD22 | 2.07                     | 0.90              |
| 24:Q:146:TYR:OH   | 24:Q:183:LYS:O    | 1.89                     | 0.90              |
| 25:R:411:LEU:HD23 | 26:S:464:ARG:NH1  | 1.87                     | 0.90              |
| 28:U:203:LYS:HE2  | 28:U:229:LEU:CD2  | 1.99                     | 0.90              |
| 5:5:135:PHE:HB2   | 5:5:167:ARG:NH2   | 1.87                     | 0.90              |
| 13:F:101:ARG:HG2  | 13:F:103:LEU:H    | 1.36                     | 0.90              |
| 15:H:284:VAL:HB   | 20:M:254:MET:N    | 1.86                     | 0.90              |
| 24:Q:299:MET:HE1  | 24:Q:335:PHE:CE1  | 2.06                     | 0.90              |
| 22:O:377:VAL:HG11 | 28:U:200:LEU:HD12 | 1.52                     | 0.90              |
| 33:Z:562:TRP:CE2  | 33:Z:566:LEU:CD1  | 2.53                     | 0.90              |
| 4:4:3:ILE:HG22    | 4:4:102:LEU:CD1   | 2.02                     | 0.90              |
| 4:4:26:VAL:HG11   | 4:4:29:ASP:HB3    | 1.49                     | 0.90              |
| 23:P:131:PHE:CA   | 23:P:136:ARG:HH11 | 1.83                     | 0.90              |
| 25:R:130:GLN:HE21 | 25:R:134:TRP:NE1  | 1.69                     | 0.90              |
| 28:U:32:ARG:HG2   | 28:U:94:HIS:CE1   | 2.05                     | 0.90              |
| 29:V:107:TRP:HZ3  | 29:V:109:HIS:CD2  | 1.77                     | 0.90              |
| 21:N:327:LEU:HD21 | 21:N:743:PHE:CE1  | 2.01                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:125:LYS:O     | 3:3:126:ASP:OD1   | 1.89                     | 0.90              |
| 5:5:111:THR:HG21  | 5:5:113:TYR:CZ    | 2.06                     | 0.90              |
| 15:H:172:MET:HB3  | 16:I:129:TYR:HE2  | 1.31                     | 0.90              |
| 15:H:251:PRO:HD2  | 15:H:377:PHE:CD2  | 2.06                     | 0.90              |
| 15:H:284:VAL:CB   | 20:M:254:MET:HA   | 2.02                     | 0.90              |
| 20:M:290:ARG:HD3  | 20:M:294:GLU:CB   | 2.02                     | 0.90              |
| 21:N:75:TYR:OH    | 26:S:223:LEU:HD12 | 1.72                     | 0.90              |
| 33:Z:553:ARG:HH12 | 33:Z:595:MET:HE3  | 1.37                     | 0.90              |
| 33:Z:574:TYR:HE2  | 33:Z:584:VAL:CG1  | 1.70                     | 0.90              |
| 9:B:219:PRO:HA    | 9:B:222:LEU:HD12  | 1.53                     | 0.90              |
| 19:L:222:GLY:HA3  | 19:L:349:ILE:HD12 | 1.51                     | 0.90              |
| 27:T:136:LEU:HD22 | 27:T:146:ILE:HD11 | 1.52                     | 0.90              |
| 33:Z:888:LEU:HB3  | 33:Z:901:PHE:HE1  | 1.35                     | 0.90              |
| 16:I:204:HIS:HB3  | 16:I:207:LEU:CB   | 2.02                     | 0.89              |
| 24:Q:275:ILE:HD11 | 24:Q:306:TYR:HD2  | 1.32                     | 0.89              |
| 26:S:218:LEU:HG   | 26:S:256:LYS:NZ   | 1.87                     | 0.89              |
| 4:4:166:GLU:HB3   | 4:4:170:ARG:HH21  | 1.36                     | 0.89              |
| 18:K:71:GLU:OE2   | 21:N:576:VAL:HG22 | 1.72                     | 0.89              |
| 20:M:119:VAL:HG11 | 20:M:155:ILE:HD11 | 1.55                     | 0.89              |
| 33:Z:64:TYR:OH    | 33:Z:115:LEU:CD2  | 2.19                     | 0.89              |
| 33:Z:154:ILE:HG21 | 33:Z:211:PHE:CE1  | 2.06                     | 0.89              |
| 22:O:228:TYR:HA   | 22:O:290:LYS:HZ1  | 1.35                     | 0.89              |
| 25:R:334:ARG:NH1  | 25:R:363:PHE:HZ   | 1.70                     | 0.89              |
| 26:S:188:TYR:HE2  | 26:S:239:ARG:HH11 | 1.20                     | 0.89              |
| 16:I:395:MET:HE2  | 16:I:420:LYS:HZ3  | 1.13                     | 0.89              |
| 19:L:170:MET:HE1  | 19:L:265:GLU:HB3  | 1.54                     | 0.89              |
| 21:N:585:ARG:NH2  | 21:N:623:PHE:CE2  | 2.39                     | 0.89              |
| 23:P:130:ILE:C    | 23:P:136:ARG:NH1  | 2.30                     | 0.89              |
| 16:I:395:MET:CE   | 16:I:420:LYS:HZ3  | 1.86                     | 0.89              |
| 18:K:137:VAL:HB   | 18:K:146:LEU:HD11 | 1.53                     | 0.89              |
| 24:Q:343:LEU:HD11 | 24:Q:368:LEU:HD11 | 1.54                     | 0.89              |
| 33:Z:813:PHE:CZ   | 33:Z:847:ILE:HG12 | 2.07                     | 0.89              |
| 6:6:196:LEU:CD2   | 6:6:205:LYS:HG2   | 2.02                     | 0.89              |
| 33:Z:74:SER:CB    | 33:Z:79:THR:HG22  | 2.02                     | 0.89              |
| 11:D:11:PHE:HE2   | 12:E:26:TYR:CB    | 1.85                     | 0.89              |
| 14:G:122:HIS:CG   | 14:G:128:VAL:HG12 | 2.07                     | 0.89              |
| 19:L:167:VAL:HG23 | 20:M:142:PRO:HG3  | 1.55                     | 0.89              |
| 24:Q:165:PHE:CZ   | 24:Q:173:SER:OG   | 2.26                     | 0.89              |
| 24:Q:299:MET:CE   | 24:Q:335:PHE:CZ   | 2.52                     | 0.89              |
| 33:Z:138:ARG:HH21 | 33:Z:157:LEU:CD1  | 1.81                     | 0.89              |
| 33:Z:863:THR:CB   | 33:Z:911:LYS:NZ   | 2.35                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:888:LEU:HB3  | 33:Z:901:PHE:CE1  | 2.07                     | 0.89              |
| 13:F:7:ASP:CA     | 13:F:21:GLN:HE21  | 1.86                     | 0.89              |
| 31:X:67:ILE:HD12  | 31:X:69:ILE:HD11  | 1.54                     | 0.89              |
| 33:Z:205:LEU:HG   | 33:Z:236:PHE:HE1  | 1.28                     | 0.89              |
| 33:Z:763:HIS:CG   | 33:Z:766:HIS:CE1  | 2.61                     | 0.89              |
| 13:F:159:THR:HA   | 13:F:169:LYS:HZ3  | 1.25                     | 0.89              |
| 26:S:428:ARG:HA   | 27:T:195:LEU:HD23 | 1.54                     | 0.89              |
| 3:3:155:PHE:CE1   | 3:3:189:ARG:HD2   | 2.08                     | 0.88              |
| 15:H:351:VAL:HG11 | 15:H:353:PHE:CZ   | 2.08                     | 0.88              |
| 21:N:596:LEU:HD13 | 21:N:717:LEU:HD13 | 1.55                     | 0.88              |
| 22:O:116:ASN:CB   | 22:O:127:LEU:HD12 | 2.03                     | 0.88              |
| 23:P:167:THR:CB   | 23:P:168:TYR:CD1  | 2.56                     | 0.88              |
| 33:Z:484:LYS:HB2  | 33:Z:521:GLU:OE1  | 1.71                     | 0.88              |
| 6:6:66:TYR:CE2    | 6:6:73:LYS:O      | 2.25                     | 0.88              |
| 19:L:157:ARG:HH21 | 20:M:128:PHE:HD2  | 1.17                     | 0.88              |
| 30:W:20:ASP:HB3   | 30:W:25:ARG:HH21  | 1.30                     | 0.88              |
| 33:Z:111:LEU:O    | 33:Z:115:LEU:HG   | 1.73                     | 0.88              |
| 16:I:317:ASP:HB3  | 16:I:343:ARG:NH2  | 1.88                     | 0.88              |
| 23:P:131:PHE:HZ   | 23:P:167:THR:HG22 | 1.09                     | 0.88              |
| 33:Z:546:ILE:HG22 | 33:Z:550:PHE:CE2  | 2.08                     | 0.88              |
| 11:D:208:LYS:HE2  | 11:D:226:SER:HB3  | 1.54                     | 0.88              |
| 18:K:212:TYR:CE1  | 18:K:320:ARG:CA   | 2.40                     | 0.88              |
| 25:R:209:ARG:O    | 25:R:213:TYR:HD2  | 1.56                     | 0.88              |
| 27:T:15:PHE:CZ    | 27:T:67:LEU:HB3   | 2.09                     | 0.88              |
| 11:D:92:GLU:OE2   | 11:D:108:TYR:HE2  | 1.55                     | 0.88              |
| 23:P:125:VAL:HG23 | 23:P:126:THR:HG23 | 1.54                     | 0.88              |
| 23:P:245:TYR:CZ   | 23:P:257:TRP:NE1  | 2.40                     | 0.88              |
| 28:U:67:PHE:CZ    | 30:W:97:THR:HG23  | 2.08                     | 0.88              |
| 33:Z:75:ILE:O     | 33:Z:75:ILE:HG22  | 1.72                     | 0.88              |
| 33:Z:138:ARG:CZ   | 33:Z:157:LEU:CG   | 2.52                     | 0.88              |
| 33:Z:387:ASN:HD22 | 33:Z:400:ILE:HD11 | 1.36                     | 0.88              |
| 33:Z:763:HIS:HA   | 33:Z:766:HIS:ND1  | 1.88                     | 0.88              |
| 17:J:337:LEU:HD22 | 17:J:382:PHE:HZ   | 0.73                     | 0.88              |
| 21:N:588:VAL:HG11 | 21:N:621:THR:HG23 | 1.54                     | 0.88              |
| 24:Q:61:LEU:HG    | 24:Q:65:TYR:CZ    | 2.08                     | 0.88              |
| 33:Z:812:ILE:HG12 | 33:Z:834:LEU:HD22 | 1.54                     | 0.88              |
| 20:M:289:LYS:HD3  | 20:M:305:MET:HE1  | 1.56                     | 0.88              |
| 33:Z:473:LEU:O    | 33:Z:477:TYR:CD2  | 2.26                     | 0.88              |
| 7:7:118:PHE:CE2   | 7:7:120:ARG:HD2   | 2.08                     | 0.88              |
| 26:S:461:PHE:HE2  | 28:U:274:MET:CA   | 1.86                     | 0.88              |
| 1:1:66:TYR:CE2    | 1:1:73:PRO:HB3    | 2.08                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:F:105:VAL:HG22 | 13:F:145:LEU:HD12 | 1.55                     | 0.88              |
| 23:P:167:THR:OG1  | 23:P:168:TYR:CD1  | 2.07                     | 0.88              |
| 25:R:316:LEU:HD11 | 25:R:329:PHE:CE1  | 2.09                     | 0.88              |
| 33:Z:154:ILE:HG22 | 33:Z:211:PHE:HZ   | 1.33                     | 0.88              |
| 33:Z:208:VAL:HG11 | 33:Z:236:PHE:CD2  | 2.08                     | 0.88              |
| 33:Z:463:HIS:O    | 33:Z:466:GLU:HG2  | 1.74                     | 0.88              |
| 15:H:249:TYR:CZ   | 15:H:376:GLU:HA   | 2.08                     | 0.87              |
| 19:L:88:TYR:CE1   | 20:M:62:ILE:CB    | 2.55                     | 0.87              |
| 33:Z:750:GLU:HG2  | 33:Z:753:GLY:H    | 1.37                     | 0.87              |
| 1:1:98:ILE:HD11   | 1:1:127:ALA:HB3   | 1.56                     | 0.87              |
| 3:3:60:TYR:CE2    | 10:C:96:GLN:HB3   | 2.09                     | 0.87              |
| 18:K:241:GLU:HA   | 19:L:303:ARG:NH1  | 1.90                     | 0.87              |
| 4:4:109:LYS:HG3   | 4:4:110:LYS:HG3   | 1.55                     | 0.87              |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:HG22 | 1.56                     | 0.87              |
| 17:J:337:LEU:H    | 25:R:204:TRP:HE1  | 1.16                     | 0.87              |
| 21:N:162:ARG:HD3  | 21:N:165:ILE:CG1  | 2.03                     | 0.87              |
| 1:1:30:VAL:HG23   | 1:1:172:VAL:CG2   | 2.03                     | 0.87              |
| 12:E:17:PRO:HA    | 13:F:24:TYR:CE2   | 2.09                     | 0.87              |
| 20:M:331:ASP:OD1  | 20:M:332:VAL:HG23 | 1.75                     | 0.87              |
| 21:N:361:ASN:HB3  | 21:N:399:PHE:CD2  | 2.10                     | 0.87              |
| 24:Q:322:GLU:HG3  | 24:Q:326:MET:CE   | 2.03                     | 0.87              |
| 27:T:11:LEU:HD22  | 27:T:30:ILE:HD13  | 1.56                     | 0.87              |
| 19:L:289:ARG:NH1  | 19:L:333:LEU:O    | 2.07                     | 0.87              |
| 22:O:178:TYR:CZ   | 22:O:182:LYS:NZ   | 2.42                     | 0.87              |
| 25:R:266:LEU:HD21 | 25:R:293:THR:HG23 | 1.56                     | 0.87              |
| 13:F:72:LEU:HD13  | 13:F:132:LEU:HD22 | 1.54                     | 0.87              |
| 19:L:95:ILE:HG23  | 20:M:68:LYS:NZ    | 1.89                     | 0.87              |
| 25:R:158:LEU:HD11 | 25:R:197:MET:CE   | 2.04                     | 0.87              |
| 27:T:206:LYS:NZ   | 27:T:214:GLU:OE2  | 2.07                     | 0.87              |
| 33:Z:795:THR:HG22 | 33:Z:799:PHE:HE2  | 1.38                     | 0.87              |
| 1:1:94:THR:CG2    | 1:1:115:LEU:HD22  | 2.05                     | 0.87              |
| 21:N:207:LEU:CB   | 21:N:232:LEU:HD21 | 2.04                     | 0.87              |
| 33:Z:250:VAL:HG21 | 33:Z:272:TYR:OH   | 1.73                     | 0.87              |
| 8:A:205:PHE:CE2   | 8:A:209:HIS:CE1   | 2.62                     | 0.87              |
| 11:D:8:LEU:O      | 11:D:18:PHE:HZ    | 1.58                     | 0.87              |
| 21:N:444:HIS:ND1  | 21:N:476:THR:O    | 2.08                     | 0.87              |
| 30:W:115:CYS:SG   | 30:W:144:PHE:CZ   | 2.68                     | 0.87              |
| 11:D:11:PHE:HE2   | 12:E:26:TYR:HB3   | 1.40                     | 0.87              |
| 23:P:154:ASP:CG   | 23:P:190:LYS:HZ3  | 1.83                     | 0.87              |
| 23:P:267:PHE:CE1  | 23:P:329:PHE:CD2  | 2.63                     | 0.87              |
| 26:S:461:PHE:CE2  | 28:U:274:MET:C    | 2.52                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:217:GLU:CD   | 33:Z:244:ARG:NH2  | 2.31                     | 0.87              |
| 24:Q:11:ALA:HB2   | 24:Q:26:VAL:HG11  | 1.54                     | 0.86              |
| 16:I:126:PRO:CB   | 16:I:128:TYR:CE2  | 2.30                     | 0.86              |
| 17:J:218:LEU:HD21 | 17:J:230:VAL:HA   | 1.57                     | 0.86              |
| 21:N:770:LYS:HE3  | 21:N:917:ILE:HG21 | 1.55                     | 0.86              |
| 24:Q:382:LEU:HB3  | 25:R:263:ARG:NH1  | 1.90                     | 0.86              |
| 17:J:329:ARG:HH11 | 17:J:333:ARG:CZ   | 1.88                     | 0.86              |
| 21:N:53:ASP:HA    | 21:N:58:ARG:NH2   | 1.90                     | 0.86              |
| 21:N:315:ASN:HA   | 21:N:318:LYS:NZ   | 1.90                     | 0.86              |
| 21:N:596:LEU:CD2  | 21:N:717:LEU:HD11 | 2.05                     | 0.86              |
| 23:P:332:GLU:CB   | 23:P:337:HIS:NE2  | 2.36                     | 0.86              |
| 26:S:461:PHE:HE2  | 28:U:274:MET:O    | 1.56                     | 0.86              |
| 33:Z:221:VAL:HG22 | 33:Z:245:VAL:HG13 | 1.56                     | 0.86              |
| 33:Z:394:TYR:HD2  | 33:Z:396:ASN:HD21 | 0.87                     | 0.86              |
| 15:H:396:MET:HE1  | 15:H:438:ALA:HB1  | 1.56                     | 0.86              |
| 17:J:167:PRO:HA   | 17:J:174:PHE:CE1  | 2.10                     | 0.86              |
| 19:L:263:ILE:O    | 19:L:267:PHE:HD1  | 1.58                     | 0.86              |
| 31:X:79:LYS:HE2   | 31:X:98:PHE:CD2   | 2.10                     | 0.86              |
| 18:K:371:LEU:HD21 | 18:K:407:LEU:HD13 | 1.55                     | 0.86              |
| 26:S:399:TYR:HD2  | 26:S:401:LYS:O    | 1.58                     | 0.86              |
| 2:2:42:TRP:HD1    | 2:2:178:MET:SD    | 1.98                     | 0.86              |
| 15:H:172:MET:CA   | 16:I:129:TYR:CE2  | 2.58                     | 0.86              |
| 16:I:384:LYS:HD3  | 16:I:420:LYS:HD2  | 1.55                     | 0.86              |
| 16:I:331:ILE:HD13 | 16:I:347:LYS:HE2  | 1.56                     | 0.86              |
| 27:T:2:PRO:O      | 27:T:9:LYS:CD     | 2.22                     | 0.86              |
| 13:F:157:TYR:HD2  | 14:G:57:LEU:O     | 1.59                     | 0.86              |
| 15:H:351:VAL:CG1  | 15:H:353:PHE:CE1  | 2.58                     | 0.86              |
| 22:O:253:GLN:HB2  | 22:O:269:LEU:HD12 | 1.55                     | 0.86              |
| 23:P:95:TYR:CD2   | 23:P:96:MET:CE    | 2.59                     | 0.86              |
| 4:4:45:PHE:CD2    | 4:4:101:VAL:CG1   | 2.58                     | 0.86              |
| 16:I:163:ASP:HB2  | 17:J:76:ILE:HD13  | 1.56                     | 0.86              |
| 20:M:236:ALA:HB2  | 20:M:277:ILE:HD12 | 1.57                     | 0.86              |
| 21:N:599:TYR:HE1  | 21:N:634:LEU:HD13 | 1.39                     | 0.86              |
| 23:P:259:PRO:CB   | 23:P:327:LEU:HD12 | 2.06                     | 0.86              |
| 17:J:26:LYS:HE2   | 18:K:51:LEU:HD21  | 1.58                     | 0.85              |
| 24:Q:141:LEU:HD11 | 24:Q:145:HIS:NE2  | 1.91                     | 0.85              |
| 25:R:301:TYR:CE1  | 25:R:305:PHE:CE1  | 2.64                     | 0.85              |
| 28:U:32:ARG:HG2   | 28:U:94:HIS:NE2   | 1.91                     | 0.85              |
| 33:Z:126:TYR:HD2  | 33:Z:128:GLU:HB2  | 1.37                     | 0.85              |
| 33:Z:748:LEU:CD2  | 33:Z:783:VAL:O    | 2.23                     | 0.85              |
| 15:H:97:LEU:HD11  | 15:H:176:VAL:H    | 1.42                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:284:VAL:HG21 | 20:M:254:MET:HA   | 1.57                     | 0.85              |
| 24:Q:10:GLU:O     | 24:Q:14:LEU:HG    | 1.76                     | 0.85              |
| 31:X:37:PRO:HB3   | 31:X:46:TRP:CZ3   | 2.11                     | 0.85              |
| 22:O:178:TYR:OH   | 22:O:182:LYS:NZ   | 2.08                     | 0.85              |
| 23:P:344:ARG:HH21 | 23:P:347:GLU:CD   | 1.85                     | 0.85              |
| 28:U:32:ARG:NH2   | 28:U:106:ILE:HD12 | 1.91                     | 0.85              |
| 10:C:13:PHE:CE2   | 11:D:127:ARG:NH1  | 2.44                     | 0.85              |
| 13:F:7:ASP:HA     | 13:F:21:GLN:NE2   | 1.90                     | 0.85              |
| 20:M:195:GLU:HA   | 20:M:199:LEU:HD12 | 1.56                     | 0.85              |
| 23:P:167:THR:HB   | 23:P:168:TYR:CE1  | 2.11                     | 0.85              |
| 25:R:134:TRP:CH2  | 25:R:156:LYS:NZ   | 2.44                     | 0.85              |
| 15:H:97:LEU:HD21  | 15:H:175:GLY:HA3  | 1.55                     | 0.85              |
| 21:N:326:SER:HA   | 29:V:182:LYS:HE2  | 1.59                     | 0.85              |
| 21:N:717:LEU:HD23 | 21:N:733:LEU:HD11 | 1.57                     | 0.85              |
| 23:P:131:PHE:HZ   | 23:P:167:THR:CG2  | 1.75                     | 0.85              |
| 26:S:461:PHE:HE2  | 28:U:274:MET:C    | 1.85                     | 0.85              |
| 1:1:61:TYR:HE1    | 8:A:103:GLU:HA    | 1.42                     | 0.85              |
| 5:5:81:LYS:HG2    | 11:D:101:GLU:OE2  | 1.77                     | 0.85              |
| 15:H:306:ILE:CG2  | 15:H:308:PHE:CE1  | 2.60                     | 0.85              |
| 19:L:401:PHE:CD1  | 19:L:404:ARG:NH1  | 2.44                     | 0.85              |
| 22:O:235:HIS:CD2  | 22:O:236:HIS:CE1  | 2.63                     | 0.85              |
| 24:Q:311:LEU:HD22 | 24:Q:343:LEU:HD13 | 1.56                     | 0.85              |
| 24:Q:382:LEU:HD13 | 25:R:263:ARG:CZ   | 2.07                     | 0.85              |
| 7:7:42:VAL:HG23   | 7:7:192:ILE:HD11  | 1.59                     | 0.85              |
| 33:Z:205:LEU:CD2  | 33:Z:236:PHE:HE1  | 1.89                     | 0.85              |
| 15:H:389:PHE:CZ   | 15:H:419:LEU:CD2  | 2.59                     | 0.85              |
| 17:J:114:CYS:SG   | 18:K:119:VAL:HG21 | 2.17                     | 0.85              |
| 22:O:15:ARG:NH2   | 22:O:73:ILE:HD11  | 1.91                     | 0.85              |
| 31:X:48:PHE:CZ    | 31:X:68:LEU:HD21  | 2.11                     | 0.85              |
| 33:Z:763:HIS:HA   | 33:Z:766:HIS:CE1  | 2.11                     | 0.85              |
| 12:E:86:ARG:NH1   | 12:E:90:GLU:HB2   | 1.92                     | 0.85              |
| 23:P:184:MET:HB2  | 23:P:223:LEU:HD13 | 1.59                     | 0.85              |
| 24:Q:426:LEU:HD22 | 28:U:293:GLU:OE1  | 1.76                     | 0.85              |
| 14:G:200:TYR:CE1  | 14:G:246:ILE:HG22 | 2.09                     | 0.84              |
| 15:H:101:ARG:NH2  | 15:H:150:LYS:CE   | 2.38                     | 0.84              |
| 15:H:329:VAL:HG21 | 16:I:300:ARG:NH1  | 1.91                     | 0.84              |
| 23:P:101:MET:HE2  | 23:P:139:VAL:HG13 | 1.59                     | 0.84              |
| 33:Z:75:ILE:HG21  | 33:Z:121:ILE:HG21 | 0.89                     | 0.84              |
| 33:Z:763:HIS:O    | 33:Z:766:HIS:CE1  | 2.30                     | 0.84              |
| 18:K:258:PHE:CG   | 18:K:302:GLN:HB3  | 2.12                     | 0.84              |
| 14:G:173:ALA:CA   | 19:L:420:ARG:NH2  | 2.39                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:37:TYR:CE1    | 3:3:59:ARG:HG3    | 2.13                     | 0.84              |
| 15:H:284:VAL:CG1  | 20:M:254:MET:N    | 2.39                     | 0.84              |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:CG2  | 2.07                     | 0.84              |
| 19:L:157:ARG:NH2  | 20:M:128:PHE:CD2  | 2.46                     | 0.84              |
| 23:P:229:LEU:HD22 | 23:P:332:GLU:HG3  | 1.59                     | 0.84              |
| 25:R:167:LYS:HE2  | 25:R:197:MET:HE2  | 1.58                     | 0.84              |
| 25:R:170:VAL:HG12 | 25:R:194:VAL:HG21 | 1.59                     | 0.84              |
| 1:1:-4:VAL:CG1    | 1:1:49:ALA:HB3    | 2.08                     | 0.84              |
| 17:J:219:VAL:HB   | 18:K:281:ARG:HD2  | 1.57                     | 0.84              |
| 30:W:46:GLU:O     | 30:W:47:ASN:CG    | 2.19                     | 0.84              |
| 33:Z:562:TRP:NE1  | 33:Z:566:LEU:CG   | 2.39                     | 0.84              |
| 16:I:208:TYR:CE1  | 16:I:209:GLU:HG3  | 2.12                     | 0.84              |
| 18:K:386:ILE:HA   | 18:K:414:GLN:HE22 | 1.43                     | 0.84              |
| 21:N:282:TYR:CZ   | 21:N:286:LEU:CD1  | 2.59                     | 0.84              |
| 24:Q:289:GLU:HB2  | 24:Q:291:TYR:HD1  | 1.42                     | 0.84              |
| 31:X:48:PHE:CZ    | 31:X:68:LEU:CD2   | 2.61                     | 0.84              |
| 33:Z:493:LEU:HD11 | 33:Z:497:PHE:CE1  | 2.12                     | 0.84              |
| 13:F:105:VAL:HG21 | 13:F:145:LEU:CB   | 2.08                     | 0.84              |
| 15:H:249:TYR:OH   | 15:H:376:GLU:HB2  | 1.78                     | 0.84              |
| 21:N:579:SER:HA   | 21:N:584:ARG:NH2  | 1.92                     | 0.84              |
| 31:X:75:TRP:CH2   | 31:X:125:MET:SD   | 2.70                     | 0.84              |
| 33:Z:53:VAL:CG1   | 33:Z:95:THR:HG22  | 2.06                     | 0.84              |
| 13:F:13:PHE:CE1   | 14:G:130:PRO:HD2  | 2.11                     | 0.84              |
| 20:M:116:ALA:HB1  | 20:M:128:PHE:CE1  | 2.12                     | 0.84              |
| 21:N:749:LEU:HG   | 21:N:753:PHE:CZ   | 2.13                     | 0.84              |
| 23:P:95:TYR:HD2   | 23:P:96:MET:CE    | 1.90                     | 0.84              |
| 26:S:397:LEU:HD22 | 26:S:402:ILE:HG21 | 1.58                     | 0.84              |
| 30:W:139:VAL:HG11 | 30:W:157:PHE:HE2  | 1.43                     | 0.84              |
| 33:Z:574:TYR:CZ   | 33:Z:584:VAL:CG2  | 2.61                     | 0.84              |
| 5:5:111:THR:CG2   | 5:5:113:TYR:CZ    | 2.61                     | 0.84              |
| 12:E:20:ARG:HD3   | 20:M:432:PHE:CZ   | 2.12                     | 0.84              |
| 10:C:161:LYS:CD   | 11:D:56:ASP:HB2   | 2.07                     | 0.84              |
| 24:Q:48:ASP:OD1   | 24:Q:92:LYS:HE3   | 1.77                     | 0.84              |
| 33:Z:574:TYR:CZ   | 33:Z:584:VAL:CG1  | 2.56                     | 0.83              |
| 13:F:159:THR:HA   | 13:F:169:LYS:HZ2  | 1.40                     | 0.83              |
| 21:N:223:LEU:HD11 | 21:N:722:THR:HG22 | 1.59                     | 0.83              |
| 31:X:27:ILE:HB    | 31:X:59:ARG:NH2   | 1.92                     | 0.83              |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:CD2  | 2.14                     | 0.83              |
| 5:5:6:PHE:CZ      | 5:5:13:ILE:HB     | 2.11                     | 0.83              |
| 13:F:120:THR:O    | 14:G:129:ARG:CD   | 2.25                     | 0.83              |
| 20:M:47:GLU:CD    | 20:M:50:ARG:NH2   | 2.37                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:P:144:VAL:HG21 | 23:P:160:LEU:CD2  | 2.08                     | 0.83              |
| 26:S:192:GLU:HG3  | 26:S:239:ARG:NH1  | 1.94                     | 0.83              |
| 28:U:32:ARG:NE    | 28:U:94:HIS:CE1   | 2.45                     | 0.83              |
| 28:U:46:ILE:HD13  | 28:U:119:LEU:HD22 | 1.58                     | 0.83              |
| 5:5:8:PHE:CZ      | 5:5:13:ILE:HD11   | 2.14                     | 0.83              |
| 10:C:4:ARG:HG3    | 11:D:6:ARG:HD2    | 1.59                     | 0.83              |
| 15:H:206:VAL:HG21 | 15:H:261:ARG:NE   | 1.92                     | 0.83              |
| 19:L:145:ARG:HE   | 19:L:162:GLU:HG3  | 1.44                     | 0.83              |
| 12:E:86:ARG:HH12  | 12:E:90:GLU:HB2   | 1.43                     | 0.83              |
| 14:G:217:TRP:HE1  | 14:G:228:LYS:HB2  | 1.42                     | 0.83              |
| 19:L:88:TYR:HE1   | 20:M:62:ILE:HG12  | 1.43                     | 0.83              |
| 33:Z:138:ARG:HH21 | 33:Z:157:LEU:HD12 | 1.38                     | 0.83              |
| 5:5:100:MET:SD    | 5:5:127:PHE:HB2   | 2.19                     | 0.83              |
| 18:K:48:TYR:CZ    | 21:N:156:ILE:HD11 | 2.14                     | 0.83              |
| 19:L:369:LYS:HE3  | 20:M:209:ASP:O    | 1.79                     | 0.83              |
| 25:R:209:ARG:HE   | 25:R:243:LEU:HD22 | 1.41                     | 0.83              |
| 31:X:38:ASN:HD22  | 31:X:42:GLU:H     | 1.25                     | 0.83              |
| 33:Z:443:ASP:HB3  | 33:Z:447:VAL:CB   | 2.08                     | 0.83              |
| 33:Z:463:HIS:NE2  | 33:Z:497:PHE:CD1  | 2.47                     | 0.83              |
| 33:Z:886:VAL:HG13 | 33:Z:893:PHE:CE1  | 2.13                     | 0.83              |
| 11:D:11:PHE:CE2   | 12:E:26:TYR:HB3   | 2.13                     | 0.83              |
| 23:P:426:ILE:O    | 29:V:230:TYR:OH   | 1.97                     | 0.83              |
| 17:J:241:ALA:HB2  | 17:J:288:ILE:HD11 | 1.59                     | 0.83              |
| 17:J:329:ARG:NH1  | 17:J:333:ARG:CZ   | 2.42                     | 0.83              |
| 18:K:98:GLN:HE22  | 18:K:136:SER:CB   | 1.90                     | 0.83              |
| 19:L:290:ARG:NH1  | 19:L:293:GLU:CB   | 2.41                     | 0.83              |
| 21:N:406:TYR:CD1  | 21:N:448:LEU:HB3  | 2.13                     | 0.83              |
| 25:R:137:LEU:O    | 25:R:141:TYR:CD2  | 2.31                     | 0.83              |
| 33:Z:985:LYS:HE3  | 33:Z:991:GLU:HB2  | 1.61                     | 0.83              |
| 15:H:168:ILE:HD12 | 15:H:187:LEU:HD12 | 1.59                     | 0.83              |
| 15:H:246:ILE:HD11 | 15:H:352:MET:HE3  | 1.60                     | 0.83              |
| 19:L:357:ARG:HH22 | 19:L:386:PHE:H    | 1.27                     | 0.83              |
| 22:O:185:PHE:CG   | 22:O:223:LEU:HD13 | 2.13                     | 0.83              |
| 1:1:83:LYS:HZ2    | 1:1:118:SER:HA    | 1.42                     | 0.82              |
| 5:5:40:PHE:HB3    | 5:5:73:ARG:NH2    | 1.94                     | 0.82              |
| 9:B:239:THR:HG22  | 9:B:241:GLN:H     | 1.42                     | 0.82              |
| 21:N:222:TYR:H    | 21:N:894:ARG:CZ   | 1.91                     | 0.82              |
| 21:N:717:LEU:CD2  | 21:N:733:LEU:HD12 | 2.07                     | 0.82              |
| 22:O:253:GLN:CB   | 22:O:269:LEU:HD12 | 2.10                     | 0.82              |
| 1:1:-2:LEU:HD12   | 1:1:1:THR:H       | 1.44                     | 0.82              |
| 19:L:167:VAL:CG2  | 20:M:142:PRO:HG3  | 2.09                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:424:LYS:HZ1  | 21:N:461:GLU:CB   | 1.79                     | 0.82              |
| 4:4:109:LYS:HE3   | 4:4:110:LYS:HE3   | 1.61                     | 0.82              |
| 15:H:299:ARG:NH2  | 15:H:345:PRO:HD3  | 1.94                     | 0.82              |
| 15:H:323:ALA:O    | 20:M:290:ARG:NH2  | 2.12                     | 0.82              |
| 15:H:324:GLY:HA3  | 20:M:290:ARG:HH22 | 0.71                     | 0.82              |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:CG2  | 2.09                     | 0.82              |
| 25:R:408:ASP:CB   | 26:S:464:ARG:NH2  | 2.33                     | 0.82              |
| 31:X:75:TRP:CH2   | 31:X:125:MET:CG   | 2.49                     | 0.82              |
| 33:Z:119:LEU:HB3  | 33:Z:137:TYR:CD2  | 2.14                     | 0.82              |
| 16:I:281:ILE:HG21 | 16:I:284:ILE:HD11 | 1.62                     | 0.82              |
| 18:K:216:GLY:HA3  | 19:L:342:ARG:NH2  | 1.94                     | 0.82              |
| 26:S:425:ARG:NH2  | 27:T:153:MET:O    | 2.12                     | 0.82              |
| 31:X:66:LEU:HD22  | 31:X:97:TYR:CD1   | 2.14                     | 0.82              |
| 3:3:57:MET:HE2    | 3:3:89:ARG:NH2    | 1.94                     | 0.82              |
| 24:Q:311:LEU:CD2  | 24:Q:343:LEU:HD13 | 2.09                     | 0.82              |
| 28:U:203:LYS:HE2  | 28:U:229:LEU:HD21 | 1.54                     | 0.82              |
| 33:Z:53:VAL:HG13  | 33:Z:95:THR:HG22  | 1.61                     | 0.82              |
| 8:A:252:ASP:CG    | 23:P:85:LYS:HZ2   | 1.61                     | 0.82              |
| 9:B:174:PHE:HB3   | 9:B:178:ARG:HH12  | 1.45                     | 0.82              |
| 15:H:102:CYS:HB3  | 15:H:105:ILE:CD1  | 2.10                     | 0.82              |
| 22:O:377:VAL:HG21 | 28:U:200:LEU:CD1  | 2.08                     | 0.82              |
| 23:P:267:PHE:CZ   | 23:P:329:PHE:CD2  | 2.68                     | 0.82              |
| 25:R:266:LEU:CA   | 25:R:270:VAL:HG22 | 2.09                     | 0.82              |
| 4:4:107:ASP:OD1   | 4:4:109:LYS:HG2   | 1.78                     | 0.82              |
| 13:F:201:LEU:O    | 13:F:202:ARG:HG3  | 1.80                     | 0.82              |
| 15:H:59:ILE:CG2   | 16:I:92:GLU:OE2   | 2.27                     | 0.82              |
| 17:J:305:LEU:HD22 | 17:J:313:LYS:CE   | 2.07                     | 0.82              |
| 31:X:36:LYS:NZ    | 31:X:49:GLU:OE1   | 2.12                     | 0.82              |
| 6:6:66:TYR:OH     | 6:6:73:LYS:HG2    | 1.80                     | 0.82              |
| 13:F:65:LYS:HG3   | 13:F:222:PHE:CD2  | 2.15                     | 0.82              |
| 18:K:167:PRO:HG2  | 18:K:228:ASN:HB2  | 1.62                     | 0.82              |
| 22:O:219:ILE:HG23 | 22:O:274:ILE:CD1  | 2.10                     | 0.82              |
| 31:X:100:TRP:HZ3  | 31:X:102:GLN:HA   | 1.43                     | 0.82              |
| 33:Z:900:LEU:HD22 | 33:Z:903:MET:CE   | 2.09                     | 0.82              |
| 10:C:115:LEU:HD13 | 10:C:137:TYR:OH   | 1.80                     | 0.81              |
| 10:C:137:TYR:O    | 10:C:148:LEU:HD12 | 1.80                     | 0.81              |
| 13:F:157:TYR:OH   | 14:G:59:VAL:HG23  | 1.80                     | 0.81              |
| 29:V:135:ARG:HD2  | 29:V:157:ARG:HH22 | 0.73                     | 0.81              |
| 33:Z:89:LEU:HD21  | 33:Z:125:THR:HG21 | 0.82                     | 0.81              |
| 5:5:83:LEU:O      | 5:5:87:VAL:HG23   | 1.79                     | 0.81              |
| 33:Z:64:TYR:HD2   | 33:Z:111:LEU:HD11 | 1.40                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:321:PHE:HE2  | 33:Z:351:PRO:CG   | 1.89                     | 0.81              |
| 33:Z:550:PHE:CZ   | 33:Z:566:LEU:CB   | 2.61                     | 0.81              |
| 33:Z:550:PHE:CE1  | 33:Z:566:LEU:HB3  | 2.14                     | 0.81              |
| 6:6:43:MET:HG3    | 6:6:102:ILE:HG22  | 1.61                     | 0.81              |
| 14:G:122:HIS:CG   | 14:G:128:VAL:CG1  | 2.62                     | 0.81              |
| 17:J:167:PRO:CD   | 17:J:174:PHE:CZ   | 2.64                     | 0.81              |
| 18:K:49:PHE:CE2   | 18:K:53:LYS:HE3   | 2.15                     | 0.81              |
| 21:N:77:SER:O     | 21:N:81:TYR:HD1   | 1.62                     | 0.81              |
| 21:N:615:ALA:HB3  | 21:N:651:PHE:HZ   | 1.44                     | 0.81              |
| 26:S:435:LYS:HD3  | 27:T:198:ASP:OD2  | 1.80                     | 0.81              |
| 27:T:112:ASN:HB2  | 27:T:177:PHE:HZ   | 1.45                     | 0.81              |
| 29:V:71:MET:HE1   | 29:V:83:VAL:CG1   | 2.09                     | 0.81              |
| 33:Z:509:LEU:HB2  | 33:Z:530:LEU:HD21 | 1.62                     | 0.81              |
| 1:1:1:THR:HG22    | 1:1:129:SER:H     | 1.45                     | 0.81              |
| 1:1:57:ASP:C      | 8:A:106:TYR:HE1   | 1.88                     | 0.81              |
| 7:7:192:ILE:HG12  | 7:7:198:LEU:HD13  | 1.60                     | 0.81              |
| 17:J:167:PRO:CD   | 17:J:174:PHE:HZ   | 1.92                     | 0.81              |
| 24:Q:151:TYR:OH   | 24:Q:187:LYS:HG2  | 1.79                     | 0.81              |
| 6:6:91:LYS:CB     | 6:6:96:TYR:CE1    | 2.63                     | 0.81              |
| 17:J:224:GLY:C    | 17:J:225:GLU:CA   | 2.53                     | 0.81              |
| 20:M:282:GLU:OE2  | 20:M:328:ASN:ND2  | 2.14                     | 0.81              |
| 21:N:67:LYS:HG2   | 21:N:97:PHE:CD1   | 2.15                     | 0.81              |
| 23:P:274:GLY:O    | 23:P:277:GLN:HG2  | 1.79                     | 0.81              |
| 33:Z:550:PHE:HZ   | 33:Z:566:LEU:HB3  | 1.41                     | 0.81              |
| 33:Z:562:TRP:CZ2  | 33:Z:566:LEU:HD11 | 2.16                     | 0.81              |
| 8:A:220:LYS:HD3   | 8:A:242:GLU:HB2   | 0.84                     | 0.81              |
| 10:C:194:LEU:HD12 | 10:C:242:THR:HG21 | 1.62                     | 0.81              |
| 11:D:159:TRP:CZ2  | 12:E:59:LEU:HD13  | 2.14                     | 0.81              |
| 15:H:389:PHE:CE1  | 15:H:419:LEU:HD22 | 2.16                     | 0.81              |
| 22:O:72:LYS:O     | 30:W:18:ASN:CB    | 2.29                     | 0.81              |
| 22:O:356:ARG:NH1  | 28:U:234:ASN:HB2  | 1.94                     | 0.81              |
| 8:A:19:PHE:HA     | 8:A:25:LEU:HD21   | 1.63                     | 0.81              |
| 15:H:69:VAL:HG11  | 16:I:133:LEU:HD21 | 1.62                     | 0.81              |
| 16:I:175:LYS:O    | 17:J:282:PHE:CZ   | 2.33                     | 0.81              |
| 22:O:157:LEU:HD22 | 22:O:171:PHE:CD1  | 2.16                     | 0.81              |
| 27:T:89:TYR:CE1   | 27:T:102:LYS:HD3  | 2.15                     | 0.81              |
| 31:X:75:TRP:CH2   | 31:X:125:MET:CE   | 2.41                     | 0.81              |
| 1:1:8:PHE:CE1     | 1:1:13:ILE:HG13   | 2.16                     | 0.81              |
| 9:B:44:VAL:HG22   | 9:B:213:ILE:HG22  | 1.60                     | 0.81              |
| 14:G:106:ILE:HG12 | 14:G:114:ARG:NH2  | 1.94                     | 0.81              |
| 16:I:103:PRO:HB3  | 17:J:120:TYR:CZ   | 2.15                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:K:224:LYS:NZ   | 18:K:236:ARG:HH22 | 1.78                     | 0.81              |
| 24:Q:61:LEU:CG    | 24:Q:65:TYR:CZ    | 2.64                     | 0.81              |
| 25:R:209:ARG:CG   | 25:R:213:TYR:HE2  | 1.92                     | 0.81              |
| 33:Z:51:LEU:HB3   | 33:Z:91:PHE:HZ    | 1.44                     | 0.81              |
| 33:Z:182:SER:O    | 33:Z:183:LYS:HB2  | 1.79                     | 0.81              |
| 10:C:161:LYS:HD2  | 11:D:56:ASP:CB    | 2.08                     | 0.81              |
| 18:K:132:LYS:HB2  | 18:K:135:MET:HG3  | 1.63                     | 0.81              |
| 19:L:88:TYR:CE1   | 20:M:62:ILE:HG12  | 2.16                     | 0.81              |
| 25:R:399:GLN:O    | 25:R:403:LEU:HG   | 1.81                     | 0.81              |
| 14:G:173:ALA:HB1  | 19:L:420:ARG:NH2  | 1.91                     | 0.81              |
| 21:N:549:TYR:OH   | 21:N:738:GLN:NE2  | 2.12                     | 0.81              |
| 26:S:461:PHE:CE1  | 28:U:278:ILE:CB   | 2.64                     | 0.81              |
| 6:6:73:LYS:HD2    | 12:E:108:ASN:HD21 | 1.45                     | 0.80              |
| 12:E:20:ARG:HD3   | 20:M:432:PHE:HZ   | 1.44                     | 0.80              |
| 13:F:84:LEU:CD2   | 13:F:132:LEU:HD11 | 2.07                     | 0.80              |
| 17:J:116:ARG:HB3  | 17:J:118:ASP:OD1  | 1.82                     | 0.80              |
| 22:O:250:TRP:HZ2  | 22:O:271:LYS:CG   | 1.95                     | 0.80              |
| 8:A:54:ILE:CG2    | 8:A:210:MET:HE1   | 2.11                     | 0.80              |
| 8:A:128:TYR:CZ    | 8:A:134:MET:CE    | 2.63                     | 0.80              |
| 9:B:43:VAL:HG11   | 9:B:137:ALA:HB1   | 1.63                     | 0.80              |
| 13:F:179:PHE:CE2  | 13:F:192:ALA:HB1  | 2.16                     | 0.80              |
| 19:L:178:ILE:HD13 | 19:L:230:LEU:CD2  | 2.11                     | 0.80              |
| 23:P:154:ASP:OD1  | 23:P:190:LYS:NZ   | 2.14                     | 0.80              |
| 29:V:107:TRP:HZ3  | 29:V:109:HIS:CG   | 1.97                     | 0.80              |
| 33:Z:290:GLU:CG   | 33:Z:293:MET:HE3  | 2.09                     | 0.80              |
| 33:Z:574:TYR:OH   | 33:Z:584:VAL:HG21 | 1.80                     | 0.80              |
| 3:3:129:VAL:CG2   | 3:3:138:PHE:CD1   | 2.62                     | 0.80              |
| 23:P:202:LYS:HE2  | 23:P:206:LYS:HZ1  | 1.44                     | 0.80              |
| 15:H:156:VAL:HG22 | 15:H:181:TYR:HH   | 1.46                     | 0.80              |
| 15:H:392:HIS:CE1  | 15:H:420:ARG:HG3  | 2.16                     | 0.80              |
| 29:V:53:MET:HE2   | 29:V:65:VAL:HG11  | 1.63                     | 0.80              |
| 33:Z:158:ALA:HB2  | 33:Z:207:ILE:HD13 | 1.63                     | 0.80              |
| 7:7:118:PHE:CZ    | 7:7:120:ARG:HD2   | 2.15                     | 0.80              |
| 10:C:66:LEU:CD1   | 10:C:212:GLU:HG2  | 2.11                     | 0.80              |
| 17:J:156:GLN:HE21 | 17:J:160:ILE:HB   | 1.45                     | 0.80              |
| 19:L:362:LYS:HA   | 19:L:376:PHE:CZ   | 2.16                     | 0.80              |
| 25:R:158:LEU:CD1  | 25:R:197:MET:HE1  | 2.11                     | 0.80              |
| 14:G:173:ALA:HB2  | 19:L:420:ARG:HH21 | 1.43                     | 0.80              |
| 15:H:172:MET:C    | 16:I:129:TYR:HE2  | 1.88                     | 0.80              |
| 15:H:254:THR:OG1  | 15:H:377:PHE:CE1  | 2.35                     | 0.80              |
| 19:L:117:TYR:CE1  | 19:L:131:VAL:HG11 | 2.17                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:L:178:ILE:HD13 | 19:L:230:LEU:HD22 | 1.61                     | 0.80              |
| 23:P:79:LEU:CD1   | 23:P:100:VAL:HG21 | 2.11                     | 0.80              |
| 25:R:105:LYS:CE   | 25:R:109:LYS:NZ   | 2.44                     | 0.80              |
| 33:Z:338:HIS:HD2  | 33:Z:339:PHE:CE2  | 2.00                     | 0.80              |
| 33:Z:863:THR:OG1  | 33:Z:911:LYS:NZ   | 2.14                     | 0.80              |
| 1:I:57:ASP:O      | 8:A:106:TYR:CE1   | 2.34                     | 0.80              |
| 14:G:108:ILE:CG2  | 14:G:148:TYR:CE1  | 2.64                     | 0.80              |
| 18:K:126:LEU:HD22 | 18:K:149:ILE:CD1  | 2.12                     | 0.80              |
| 21:N:502:PHE:CZ   | 21:N:538:LYS:HB3  | 2.17                     | 0.80              |
| 24:Q:99:THR:HG22  | 24:Q:103:LYS:HE3  | 1.62                     | 0.80              |
| 29:V:186:GLN:O    | 29:V:190:HIS:CD2  | 2.35                     | 0.80              |
| 33:Z:763:HIS:O    | 33:Z:766:HIS:ND1  | 2.15                     | 0.80              |
| 6:6:48:PHE:CE2    | 6:6:50:ALA:HB3    | 2.17                     | 0.80              |
| 18:K:280:LYS:HZ2  | 18:K:296:LEU:HD23 | 1.44                     | 0.80              |
| 21:N:549:TYR:CD2  | 21:N:586:ALA:HB2  | 2.17                     | 0.80              |
| 23:P:431:HIS:ND1  | 28:U:156:HIS:HB2  | 1.97                     | 0.80              |
| 24:Q:51:ARG:NH1   | 24:Q:55:GLU:OE2   | 2.13                     | 0.80              |
| 24:Q:146:TYR:CE1  | 24:Q:151:TYR:HE1  | 2.00                     | 0.80              |
| 24:Q:415:LEU:HD13 | 28:U:282:VAL:HG11 | 1.61                     | 0.80              |
| 13:F:137:TYR:CZ   | 13:F:218:LYS:HA   | 2.16                     | 0.80              |
| 15:H:102:CYS:CB   | 15:H:105:ILE:CD1  | 2.59                     | 0.80              |
| 15:H:147:ILE:HD12 | 15:H:181:TYR:HB3  | 1.64                     | 0.80              |
| 16:I:317:ASP:HB3  | 16:I:343:ARG:HH21 | 1.47                     | 0.80              |
| 19:L:117:TYR:CE1  | 19:L:131:VAL:CG1  | 2.64                     | 0.80              |
| 21:N:362:TRP:CH2  | 29:V:23:THR:CG2   | 2.65                     | 0.80              |
| 26:S:315:LYS:NZ   | 26:S:345:TYR:CE1  | 2.50                     | 0.80              |
| 33:Z:866:VAL:HB   | 33:Z:873:LEU:HG   | 1.63                     | 0.80              |
| 1:I:137:TYR:OH    | 1:I:157:HIS:CD2   | 2.35                     | 0.80              |
| 12:E:15:PHE:CZ    | 13:F:126:ARG:NH2  | 2.49                     | 0.80              |
| 22:O:373:TRP:CZ2  | 28:U:200:LEU:HD21 | 2.16                     | 0.80              |
| 24:Q:232:TYR:HB2  | 24:Q:272:LEU:HD21 | 1.61                     | 0.80              |
| 24:Q:348:CYS:HB3  | 24:Q:386:PHE:CE1  | 2.17                     | 0.80              |
| 2:2:8:PHE:CE2     | 2:2:10:ASN:C      | 2.60                     | 0.79              |
| 11:D:70:HIS:HE1   | 11:D:97:ARG:HH22  | 1.30                     | 0.79              |
| 15:H:102:CYS:HB3  | 15:H:105:ILE:HD11 | 1.62                     | 0.79              |
| 22:O:185:PHE:CE2  | 22:O:223:LEU:HD13 | 2.16                     | 0.79              |
| 31:X:75:TRP:NE1   | 31:X:125:MET:HB2  | 1.97                     | 0.79              |
| 33:Z:481:PRO:O    | 33:Z:482:ASP:CG   | 2.25                     | 0.79              |
| 33:Z:833:GLN:NE2  | 33:Z:837:TYR:OH   | 2.16                     | 0.79              |
| 5:5:81:LYS:HD3    | 5:5:121:ARG:HE    | 1.45                     | 0.79              |
| 15:H:396:MET:HE2  | 15:H:438:ALA:HB1  | 1.16                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:L:145:ARG:HH21 | 19:L:163:THR:CA   | 1.95                     | 0.79              |
| 20:M:196:ALA:HB2  | 20:M:345:ARG:NE   | 1.96                     | 0.79              |
| 29:V:107:TRP:CH2  | 29:V:109:HIS:CD2  | 2.70                     | 0.79              |
| 6:6:58:ARG:HD3    | 6:6:87:LEU:HD22   | 1.63                     | 0.79              |
| 21:N:406:TYR:CE1  | 21:N:448:LEU:HB3  | 2.17                     | 0.79              |
| 23:P:119:ILE:HG21 | 23:P:143:LEU:HD22 | 1.65                     | 0.79              |
| 6:6:66:TYR:HE2    | 6:6:73:LYS:O      | 1.65                     | 0.79              |
| 9:B:174:PHE:HB3   | 9:B:178:ARG:NH1   | 1.97                     | 0.79              |
| 19:L:88:TYR:CE1   | 20:M:62:ILE:CG1   | 2.65                     | 0.79              |
| 20:M:59:LEU:O     | 20:M:63:LYS:HG3   | 1.83                     | 0.79              |
| 20:M:394:VAL:HA   | 20:M:423:GLN:HE22 | 1.46                     | 0.79              |
| 24:Q:249:LEU:O    | 24:Q:250:THR:CG2  | 2.29                     | 0.79              |
| 2:2:160:GLN:HE21  | 2:2:164:TRP:HE1   | 1.31                     | 0.79              |
| 11:D:11:PHE:CE2   | 12:E:26:TYR:CB    | 2.65                     | 0.79              |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:HA   | 1.65                     | 0.79              |
| 21:N:315:ASN:HA   | 21:N:318:LYS:HZ3  | 1.46                     | 0.79              |
| 22:O:190:TYR:HD1  | 22:O:227:ILE:CD1  | 1.95                     | 0.79              |
| 25:R:70:TYR:CE2   | 25:R:76:GLN:HA    | 2.17                     | 0.79              |
| 33:Z:394:TYR:CD2  | 33:Z:396:ASN:ND2  | 2.45                     | 0.79              |
| 21:N:398:ARG:HD2  | 21:N:438:ASP:CB   | 2.08                     | 0.79              |
| 27:T:89:TYR:CD1   | 27:T:102:LYS:CD   | 2.63                     | 0.79              |
| 29:V:53:MET:HE2   | 29:V:65:VAL:HG21  | 1.64                     | 0.79              |
| 30:W:141:ILE:HG21 | 30:W:154:LEU:HD13 | 1.64                     | 0.79              |
| 14:G:64:VAL:HG12  | 14:G:66:ILE:H     | 1.45                     | 0.79              |
| 15:H:217:GLN:NE2  | 15:H:248:LEU:HD13 | 1.98                     | 0.79              |
| 26:S:360:PHE:O    | 26:S:364:ILE:HG12 | 1.83                     | 0.79              |
| 17:J:167:PRO:N    | 17:J:174:PHE:HZ   | 1.81                     | 0.79              |
| 20:M:218:ALA:HB3  | 20:M:324:LEU:CD2  | 2.13                     | 0.79              |
| 24:Q:74:LEU:HD23  | 24:Q:104:PHE:CE1  | 2.17                     | 0.79              |
| 24:Q:74:LEU:HD23  | 24:Q:104:PHE:CD1  | 2.17                     | 0.79              |
| 33:Z:553:ARG:NH1  | 33:Z:595:MET:HE3  | 1.98                     | 0.79              |
| 14:G:183:PRO:O    | 14:G:184:GLU:HG2  | 1.82                     | 0.79              |
| 16:I:174:ASP:OD2  | 16:I:177:PRO:HB3  | 1.83                     | 0.79              |
| 16:I:384:LYS:NZ   | 16:I:420:LYS:NZ   | 2.11                     | 0.79              |
| 25:R:63:TYR:OH    | 25:R:93:LYS:O     | 2.01                     | 0.79              |
| 25:R:410:LEU:HD21 | 28:U:285:ILE:HG21 | 1.65                     | 0.79              |
| 30:W:186:ALA:HB1  | 30:W:191:ILE:CG2  | 2.13                     | 0.79              |
| 3:3:37:TYR:CZ     | 3:3:59:ARG:HB2    | 2.18                     | 0.78              |
| 4:4:45:PHE:CE2    | 4:4:101:VAL:HG11  | 2.18                     | 0.78              |
| 12:E:15:PHE:CD1   | 12:E:21:LEU:HD12  | 2.16                     | 0.78              |
| 12:E:20:ARG:CD    | 20:M:432:PHE:HZ   | 1.95                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:104:LEU:HD21 | 16:I:149:LEU:O    | 1.83                     | 0.78              |
| 33:Z:518:LEU:HD11 | 33:Z:562:TRP:CE3  | 2.19                     | 0.78              |
| 10:C:3:SER:HB3    | 11:D:6:ARG:CZ     | 2.13                     | 0.78              |
| 11:D:97:ARG:HH12  | 11:D:103:PRO:HG3  | 1.45                     | 0.78              |
| 15:H:147:ILE:HG13 | 15:H:183:ILE:CG1  | 2.13                     | 0.78              |
| 26:S:343:LEU:HD11 | 26:S:347:HIS:HE1  | 1.45                     | 0.78              |
| 27:T:139:ASP:OD2  | 27:T:142:LEU:HG   | 1.83                     | 0.78              |
| 10:C:3:SER:CB     | 11:D:6:ARG:NH2    | 2.45                     | 0.78              |
| 12:E:207:VAL:HA   | 15:H:409:ARG:HH12 | 1.47                     | 0.78              |
| 15:H:97:LEU:HB3   | 15:H:173:ARG:HG3  | 1.64                     | 0.78              |
| 20:M:203:ARG:HD3  | 20:M:206:LYS:HD2  | 1.65                     | 0.78              |
| 25:R:334:ARG:NH1  | 25:R:363:PHE:CZ   | 2.49                     | 0.78              |
| 2:2:82:MET:HE3    | 2:2:86:HIS:HE1    | 1.48                     | 0.78              |
| 18:K:98:GLN:HE22  | 18:K:136:SER:HB2  | 1.47                     | 0.78              |
| 21:N:315:ASN:O    | 21:N:318:LYS:HG2  | 1.84                     | 0.78              |
| 21:N:328:PHE:HZ   | 21:N:693:GLY:HA2  | 1.47                     | 0.78              |
| 24:Q:36:SER:O     | 24:Q:46:VAL:CG2   | 2.31                     | 0.78              |
| 33:Z:224:LEU:HD13 | 33:Z:233:LEU:CD2  | 2.08                     | 0.78              |
| 25:R:411:LEU:CD2  | 26:S:464:ARG:NH1  | 2.43                     | 0.78              |
| 30:W:133:LYS:CE   | 30:W:163:ASN:HD21 | 1.97                     | 0.78              |
| 33:Z:474:LEU:CD2  | 33:Z:493:LEU:HD23 | 2.12                     | 0.78              |
| 3:3:60:TYR:CE2    | 10:C:96:GLN:CB    | 2.66                     | 0.78              |
| 7:7:33:ARG:NH2    | 7:7:46:SER:HA     | 1.96                     | 0.78              |
| 23:P:440:HIS:CE1  | 28:U:209:GLU:HB3  | 2.18                     | 0.78              |
| 29:V:57:PHE:HZ    | 29:V:135:ARG:NH1  | 1.81                     | 0.78              |
| 33:Z:119:LEU:HD13 | 33:Z:137:TYR:CZ   | 2.19                     | 0.78              |
| 2:2:160:GLN:HE21  | 2:2:164:TRP:CD1   | 2.02                     | 0.78              |
| 8:A:164:VAL:CB    | 9:B:61:LEU:HD21   | 2.13                     | 0.78              |
| 13:F:3:ARG:HH21   | 15:H:359:ASN:HD21 | 1.31                     | 0.78              |
| 20:M:119:VAL:CG1  | 20:M:155:ILE:HD11 | 2.12                     | 0.78              |
| 20:M:197:ILE:HB   | 20:M:322:LYS:CD   | 2.13                     | 0.78              |
| 22:O:233:LEU:HD22 | 22:O:238:ILE:CD1  | 2.11                     | 0.78              |
| 23:P:131:PHE:CE2  | 23:P:167:THR:CG2  | 2.59                     | 0.78              |
| 31:X:104:LYS:HE3  | 31:X:108:ASN:ND2  | 1.99                     | 0.78              |
| 1:1:30:VAL:HG23   | 1:1:172:VAL:HG21  | 1.65                     | 0.78              |
| 19:L:389:ALA:CB   | 20:M:339:ARG:HE   | 1.97                     | 0.78              |
| 27:T:70:ILE:HD11  | 27:T:78:PHE:CE1   | 2.18                     | 0.78              |
| 33:Z:169:VAL:HG11 | 33:Z:183:LYS:HG2  | 1.65                     | 0.78              |
| 2:2:8:PHE:CE1     | 2:2:11:GLY:C      | 2.62                     | 0.78              |
| 18:K:280:LYS:HZ1  | 18:K:296:LEU:HD23 | 1.49                     | 0.78              |
| 25:R:219:LEU:O    | 25:R:325:HIS:CE1  | 2.36                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:301:TYR:HE1  | 25:R:305:PHE:HZ   | 1.29                     | 0.78              |
| 33:Z:407:VAL:HG12 | 33:Z:415:MET:HE1  | 1.66                     | 0.78              |
| 6:6:10:ASP:OD2    | 6:6:165:TYR:OH    | 2.01                     | 0.78              |
| 15:H:183:ILE:HG22 | 15:H:183:ILE:O    | 1.81                     | 0.78              |
| 17:J:146:THR:HG23 | 17:J:148:ASP:H    | 1.48                     | 0.78              |
| 19:L:290:ARG:HH12 | 19:L:293:GLU:HB3  | 1.48                     | 0.78              |
| 25:R:209:ARG:HE   | 25:R:243:LEU:CD2  | 1.96                     | 0.78              |
| 27:T:8:THR:HG23   | 27:T:61:ILE:HG12  | 1.65                     | 0.78              |
| 1:1:8:PHE:HE2     | 1:1:10:ASP:HB2    | 1.49                     | 0.77              |
| 17:J:305:LEU:CD2  | 17:J:313:LYS:HE3  | 2.07                     | 0.77              |
| 23:P:271:SER:C    | 23:P:344:ARG:HD2  | 2.09                     | 0.77              |
| 26:S:464:ARG:HB3  | 28:U:281:LEU:HD22 | 1.65                     | 0.77              |
| 7:7:7:GLN:HG3     | 7:7:101:PRO:HD2   | 1.64                     | 0.77              |
| 9:B:70:ASP:OD1    | 9:B:71:ILE:HG13   | 1.83                     | 0.77              |
| 16:I:314:ASP:OD1  | 16:I:340:ARG:NE   | 2.16                     | 0.77              |
| 26:S:461:PHE:HE1  | 28:U:278:ILE:CB   | 1.96                     | 0.77              |
| 29:V:57:PHE:HZ    | 29:V:135:ARG:CZ   | 1.96                     | 0.77              |
| 8:A:128:TYR:CE2   | 8:A:134:MET:HE2   | 2.20                     | 0.77              |
| 13:F:144:LEU:O    | 13:F:155:GLU:HG3  | 1.84                     | 0.77              |
| 13:F:157:TYR:CD2  | 14:G:57:LEU:O     | 2.38                     | 0.77              |
| 23:P:413:ASN:OD1  | 29:V:245:VAL:HG13 | 1.83                     | 0.77              |
| 25:R:209:ARG:O    | 25:R:213:TYR:CD2  | 2.36                     | 0.77              |
| 26:S:461:PHE:CZ   | 28:U:278:ILE:HB   | 2.19                     | 0.77              |
| 27:T:186:ARG:NH1  | 27:T:220:PHE:CE2  | 2.53                     | 0.77              |
| 11:D:159:TRP:CZ3  | 12:E:59:LEU:HD13  | 2.18                     | 0.77              |
| 18:K:212:TYR:CZ   | 18:K:320:ARG:HA   | 2.18                     | 0.77              |
| 18:K:280:LYS:NZ   | 18:K:296:LEU:CD2  | 2.47                     | 0.77              |
| 19:L:401:PHE:CE1  | 19:L:404:ARG:NH1  | 2.52                     | 0.77              |
| 25:R:315:VAL:O    | 25:R:319:CYS:SG   | 2.40                     | 0.77              |
| 26:S:464:ARG:CB   | 28:U:281:LEU:HD22 | 2.14                     | 0.77              |
| 33:Z:865:ASP:OD2  | 33:Z:909:ARG:CZ   | 2.32                     | 0.77              |
| 16:I:320:GLY:HA2  | 16:I:323:LYS:CE   | 2.13                     | 0.77              |
| 13:F:101:ARG:NH1  | 13:F:103:LEU:HD12 | 2.00                     | 0.77              |
| 27:T:256:LYS:HE3  | 29:V:298:ALA:O    | 1.85                     | 0.77              |
| 33:Z:829:GLN:HG2  | 33:Z:832:ARG:NH2  | 2.00                     | 0.77              |
| 13:F:65:LYS:HE2   | 13:F:222:PHE:HD2  | 1.49                     | 0.77              |
| 16:I:264:CYS:SG   | 16:I:305:THR:HG23 | 2.24                     | 0.77              |
| 25:R:170:VAL:CG1  | 25:R:194:VAL:HG21 | 2.14                     | 0.77              |
| 31:X:27:ILE:HB    | 31:X:59:ARG:HH22  | 1.50                     | 0.77              |
| 31:X:91:PHE:N     | 31:X:96:ARG:HG2   | 1.97                     | 0.77              |
| 33:Z:562:TRP:CE2  | 33:Z:566:LEU:HD21 | 2.19                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:66:TYR:CD2    | 1:1:73:PRO:HB3    | 2.20                     | 0.77              |
| 16:I:395:MET:HG3  | 16:I:420:LYS:HD3  | 1.65                     | 0.77              |
| 21:N:362:TRP:CH2  | 29:V:23:THR:HG21  | 2.20                     | 0.77              |
| 33:Z:126:TYR:CD2  | 33:Z:128:GLU:HB2  | 2.19                     | 0.77              |
| 13:F:158:GLY:O    | 14:G:57:LEU:HD13  | 1.85                     | 0.77              |
| 21:N:145:LEU:HD22 | 21:N:173:LYS:HZ1  | 1.50                     | 0.77              |
| 21:N:222:TYR:N    | 21:N:894:ARG:NH2  | 2.32                     | 0.77              |
| 25:R:246:TYR:OH   | 25:R:275:GLU:OE2  | 2.02                     | 0.77              |
| 30:W:7:VAL:HG23   | 30:W:98:LEU:CD2   | 2.15                     | 0.77              |
| 33:Z:812:ILE:CG1  | 33:Z:834:LEU:HD22 | 2.14                     | 0.77              |
| 33:Z:924:LYS:NZ   | 33:Z:993:GLU:HG3  | 2.00                     | 0.77              |
| 15:H:358:PRO:HB2  | 15:H:374:LYS:HZ2  | 1.50                     | 0.77              |
| 19:L:227:GLY:HA2  | 19:L:230:LEU:HD12 | 1.66                     | 0.77              |
| 20:M:303:ARG:NH1  | 20:M:307:GLU:HB2  | 1.99                     | 0.77              |
| 26:S:218:LEU:HG   | 26:S:256:LYS:HZ2  | 1.50                     | 0.77              |
| 15:H:436:LYS:CE   | 33:Z:365:SER:HB2  | 2.09                     | 0.76              |
| 16:I:148:LEU:CD2  | 16:I:160:LEU:HD22 | 2.16                     | 0.76              |
| 33:Z:382:ALA:HB1  | 33:Z:849:ARG:HG2  | 1.67                     | 0.76              |
| 33:Z:392:LEU:HD13 | 33:Z:424:SER:O    | 1.84                     | 0.76              |
| 3:3:52:THR:CB     | 4:4:84:ARG:NH2    | 2.48                     | 0.76              |
| 6:6:39:ASP:O      | 6:6:40:ASN:HB2    | 1.83                     | 0.76              |
| 7:7:174:ARG:NE    | 7:7:207:GLU:O     | 2.17                     | 0.76              |
| 19:L:357:ARG:O    | 19:L:361:PHE:CD2  | 2.38                     | 0.76              |
| 26:S:151:GLU:OE2  | 26:S:153:GLU:HB3  | 1.84                     | 0.76              |
| 28:U:277:TYR:OH   | 29:V:295:VAL:CG1  | 2.32                     | 0.76              |
| 28:U:283:ARG:NH1  | 29:V:291:ASN:HD22 | 1.82                     | 0.76              |
| 2:2:42:TRP:CD1    | 2:2:178:MET:SD    | 2.78                     | 0.76              |
| 10:C:33:GLY:HA2   | 10:C:51:LYS:HE3   | 1.67                     | 0.76              |
| 19:L:283:VAL:HG22 | 19:L:286:ILE:HD11 | 1.68                     | 0.76              |
| 22:O:15:ARG:CZ    | 22:O:73:ILE:CD1   | 2.55                     | 0.76              |
| 23:P:130:ILE:HG22 | 23:P:136:ARG:HH22 | 1.50                     | 0.76              |
| 28:U:67:PHE:HE2   | 30:W:100:HIS:ND1  | 1.82                     | 0.76              |
| 29:V:57:PHE:CE2   | 29:V:59:ASP:O     | 2.39                     | 0.76              |
| 21:N:158:LEU:HD12 | 21:N:202:PHE:HE2  | 1.49                     | 0.76              |
| 21:N:315:ASN:CA   | 21:N:318:LYS:HZ3  | 1.97                     | 0.76              |
| 23:P:94:GLN:OE1   | 23:P:136:ARG:HG2  | 1.86                     | 0.76              |
| 23:P:167:THR:HB   | 23:P:168:TYR:CD1  | 2.21                     | 0.76              |
| 24:Q:141:LEU:HG   | 24:Q:145:HIS:CD2  | 2.20                     | 0.76              |
| 25:R:202:GLY:HA2  | 25:R:207:ARG:HH21 | 1.51                     | 0.76              |
| 31:X:75:TRP:CD2   | 31:X:125:MET:HB3  | 2.20                     | 0.76              |
| 5:5:158:LYS:HE3   | 5:5:196:LEU:HD11  | 1.68                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:205:PHE:CZ    | 8:A:209:HIS:NE2   | 2.53                     | 0.76              |
| 14:G:108:ILE:HG22 | 14:G:148:TYR:CE1  | 2.21                     | 0.76              |
| 14:G:111:PHE:HD1  | 14:G:114:ARG:HH22 | 0.81                     | 0.76              |
| 20:M:384:ASP:H    | 20:M:386:PHE:HE1  | 1.34                     | 0.76              |
| 24:Q:61:LEU:CD2   | 24:Q:65:TYR:OH    | 2.32                     | 0.76              |
| 29:V:57:PHE:CZ    | 29:V:135:ARG:NH1  | 2.54                     | 0.76              |
| 31:X:75:TRP:CE3   | 31:X:125:MET:HE3  | 2.20                     | 0.76              |
| 33:Z:188:ALA:HB3  | 33:Z:201:LEU:HD11 | 1.65                     | 0.76              |
| 33:Z:363:ASP:O    | 33:Z:366:LYS:NZ   | 2.17                     | 0.76              |
| 1:1:-4:VAL:HG12   | 1:1:49:ALA:HB3    | 1.66                     | 0.76              |
| 4:4:102:LEU:HD22  | 4:4:117:GLN:HG2   | 1.67                     | 0.76              |
| 8:A:31:ALA:HA     | 14:G:14:PHE:CZ    | 2.19                     | 0.76              |
| 8:A:220:LYS:CG    | 8:A:242:GLU:HB2   | 2.15                     | 0.76              |
| 10:C:144:TYR:HB2  | 10:C:147:GLN:HE21 | 1.49                     | 0.76              |
| 14:G:108:ILE:CG2  | 14:G:148:TYR:CD1  | 2.69                     | 0.76              |
| 17:J:214:SER:HB3  | 17:J:217:GLU:OE1  | 1.86                     | 0.76              |
| 19:L:107:GLU:OE2  | 19:L:145:ARG:NH2  | 2.19                     | 0.76              |
| 19:L:401:PHE:CD1  | 19:L:404:ARG:CZ   | 2.69                     | 0.76              |
| 22:O:219:ILE:HG23 | 22:O:274:ILE:HD13 | 1.68                     | 0.76              |
| 33:Z:348:LEU:HD23 | 33:Z:353:VAL:HB   | 1.66                     | 0.76              |
| 18:K:141:ARG:NH1  | 19:L:153:LEU:HD11 | 2.00                     | 0.76              |
| 25:R:408:ASP:CG   | 26:S:464:ARG:HH22 | 1.93                     | 0.76              |
| 30:W:133:LYS:HE3  | 30:W:163:ASN:HD21 | 1.48                     | 0.76              |
| 33:Z:106:TRP:HB2  | 33:Z:112:LYS:NZ   | 2.00                     | 0.76              |
| 33:Z:443:ASP:HB3  | 33:Z:447:VAL:HB   | 1.66                     | 0.76              |
| 33:Z:975:SER:O    | 33:Z:977:ILE:HG23 | 1.86                     | 0.76              |
| 1:1:94:THR:HG23   | 1:1:115:LEU:HD22  | 1.66                     | 0.76              |
| 3:3:140:MET:HE3   | 3:3:144:LEU:HD11  | 1.66                     | 0.76              |
| 7:7:145:PRO:CB    | 7:7:148:ARG:HH21  | 1.99                     | 0.76              |
| 10:C:46:LEU:HD11  | 10:C:138:ALA:HB3  | 1.67                     | 0.76              |
| 11:D:19:GLN:NE2   | 11:D:121:THR:HA   | 2.01                     | 0.76              |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:CA   | 2.16                     | 0.76              |
| 21:N:490:LEU:HD21 | 21:N:526:TYR:CD2  | 2.21                     | 0.76              |
| 22:O:72:LYS:O     | 30:W:18:ASN:CG    | 2.28                     | 0.76              |
| 2:2:7:LYS:O       | 2:2:146:LEU:HD23  | 1.86                     | 0.76              |
| 7:7:33:ARG:NH2    | 7:7:46:SER:CA     | 2.49                     | 0.76              |
| 25:R:411:LEU:HD22 | 26:S:464:ARG:HH11 | 1.50                     | 0.76              |
| 33:Z:89:LEU:HD13  | 33:Z:125:THR:HB   | 1.67                     | 0.76              |
| 33:Z:363:ASP:O    | 33:Z:366:LYS:CE   | 2.34                     | 0.76              |
| 33:Z:509:LEU:CD1  | 33:Z:530:LEU:HD23 | 2.16                     | 0.76              |
| 33:Z:776:VAL:HG13 | 33:Z:777:PRO:HD3  | 1.65                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:813:PHE:CE1  | 33:Z:847:ILE:HG23 | 2.21                     | 0.76              |
| 2:2:104:ASP:HB3   | 2:2:105:PRO:HD2   | 1.68                     | 0.75              |
| 9:B:190:HIS:NE2   | 24:Q:94:VAL:HG21  | 2.01                     | 0.75              |
| 22:O:228:TYR:CD2  | 22:O:229:ASN:N    | 2.49                     | 0.75              |
| 24:Q:232:TYR:HB2  | 24:Q:272:LEU:CD2  | 2.15                     | 0.75              |
| 26:S:163:VAL:HA   | 26:S:167:LEU:HD23 | 1.66                     | 0.75              |
| 26:S:184:TRP:CH2  | 26:S:217:PHE:HE2  | 2.02                     | 0.75              |
| 27:T:86:LYS:HE2   | 27:T:128:TYR:CD2  | 2.21                     | 0.75              |
| 27:T:226:TRP:CZ3  | 27:T:235:PHE:HE2  | 2.04                     | 0.75              |
| 33:Z:763:HIS:CA   | 33:Z:766:HIS:CE1  | 2.69                     | 0.75              |
| 2:2:59:ILE:HD12   | 2:2:82:MET:HB3    | 1.67                     | 0.75              |
| 6:6:10:ASP:OD1    | 6:6:11:PHE:HD1    | 1.69                     | 0.75              |
| 12:E:98:THR:CG2   | 12:E:102:TYR:CE2  | 2.69                     | 0.75              |
| 16:I:75:PHE:CD2   | 16:I:76:VAL:HG23  | 2.20                     | 0.75              |
| 16:I:200:LEU:HB3  | 33:Z:931:GLN:HG2  | 1.68                     | 0.75              |
| 16:I:395:MET:HE2  | 16:I:420:LYS:HZ1  | 1.47                     | 0.75              |
| 17:J:247:MET:HE2  | 17:J:272:MET:HG3  | 1.68                     | 0.75              |
| 18:K:159:SER:OG   | 18:K:244:HIS:NE2  | 2.08                     | 0.75              |
| 19:L:290:ARG:HH11 | 19:L:293:GLU:C    | 1.94                     | 0.75              |
| 24:Q:38:SER:OG    | 24:Q:88:PHE:CE1   | 2.39                     | 0.75              |
| 24:Q:263:LYS:HE2  | 24:Q:295:GLY:HA3  | 1.67                     | 0.75              |
| 33:Z:74:SER:CB    | 33:Z:79:THR:CG2   | 2.64                     | 0.75              |
| 25:R:130:GLN:NE2  | 25:R:134:TRP:HE1  | 1.84                     | 0.75              |
| 27:T:221:ALA:CB   | 27:T:228:ILE:HD11 | 2.17                     | 0.75              |
| 33:Z:443:ASP:HB3  | 33:Z:447:VAL:CG1  | 2.13                     | 0.75              |
| 5:5:145:LYS:HE3   | 5:5:147:ASP:HB2   | 1.68                     | 0.75              |
| 9:B:67:LEU:HD11   | 9:B:73:ALA:HB2    | 1.69                     | 0.75              |
| 13:F:105:VAL:CG2  | 13:F:145:LEU:CB   | 2.63                     | 0.75              |
| 23:P:308:LEU:HD22 | 23:P:369:LEU:CD2  | 2.15                     | 0.75              |
| 33:Z:428:TRP:CZ3  | 33:Z:461:GLY:CA   | 2.63                     | 0.75              |
| 33:Z:428:TRP:CE3  | 33:Z:461:GLY:HA3  | 2.20                     | 0.75              |
| 33:Z:463:HIS:NE2  | 33:Z:497:PHE:HD1  | 1.82                     | 0.75              |
| 7:7:88:LEU:HD21   | 7:7:106:ILE:CD1   | 2.16                     | 0.75              |
| 10:C:4:ARG:CG     | 11:D:6:ARG:HD2    | 2.16                     | 0.75              |
| 10:C:207:THR:HG23 | 10:C:210:ARG:HH21 | 1.51                     | 0.75              |
| 18:K:159:SER:HB3  | 18:K:244:HIS:HE2  | 1.52                     | 0.75              |
| 22:O:190:TYR:CD1  | 22:O:227:ILE:HD11 | 2.18                     | 0.75              |
| 23:P:95:TYR:HD2   | 23:P:96:MET:HE3   | 1.50                     | 0.75              |
| 24:Q:146:TYR:CE1  | 24:Q:184:VAL:CA   | 2.63                     | 0.75              |
| 29:V:127:LYS:HE3  | 29:V:194:ARG:NE   | 2.01                     | 0.75              |
| 33:Z:900:LEU:HD22 | 33:Z:903:MET:HE2  | 1.68                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:81:MET:SD     | 8:A:143:PHE:CE1   | 2.79                     | 0.75              |
| 16:I:245:LEU:HG   | 16:I:247:ILE:HD11 | 1.67                     | 0.75              |
| 21:N:424:LYS:HA   | 21:N:427:ILE:HD12 | 1.68                     | 0.75              |
| 24:Q:146:TYR:CE1  | 24:Q:151:TYR:CE1  | 2.75                     | 0.75              |
| 9:B:139:HIS:CD2   | 9:B:234:ARG:HD3   | 2.22                     | 0.75              |
| 18:K:126:LEU:HD22 | 18:K:149:ILE:HD11 | 1.66                     | 0.75              |
| 18:K:242:PHE:C    | 18:K:243:VAL:CA   | 2.59                     | 0.75              |
| 21:N:163:LEU:HB3  | 21:N:209:LYS:NZ   | 2.02                     | 0.75              |
| 22:O:116:ASN:HB3  | 22:O:127:LEU:CD1  | 2.14                     | 0.75              |
| 33:Z:863:THR:CB   | 33:Z:911:LYS:HZ2  | 1.98                     | 0.75              |
| 6:6:85:GLN:HG3    | 6:6:122:TYR:HD1   | 1.51                     | 0.75              |
| 10:C:46:LEU:HD11  | 10:C:138:ALA:CB   | 2.16                     | 0.75              |
| 16:I:340:ARG:NH1  | 16:I:343:ARG:HG2  | 2.01                     | 0.75              |
| 18:K:205:PRO:HD2  | 18:K:207:ARG:NH2  | 2.01                     | 0.75              |
| 23:P:184:MET:HB3  | 23:P:223:LEU:HD13 | 1.67                     | 0.75              |
| 24:Q:389:VAL:HG13 | 24:Q:400:TYR:HB2  | 1.66                     | 0.75              |
| 25:R:378:ASN:HB3  | 25:R:391:ASN:OD1  | 1.86                     | 0.75              |
| 33:Z:338:HIS:HD2  | 33:Z:339:PHE:CZ   | 2.05                     | 0.75              |
| 1:1:190:PRO:HA    | 1:1:193:TYR:CE2   | 2.22                     | 0.75              |
| 3:3:155:PHE:HD1   | 3:3:180:ILE:HD11  | 1.52                     | 0.75              |
| 7:7:103:TRP:O     | 7:7:103:TRP:CD1   | 2.39                     | 0.75              |
| 19:L:219:LEU:HD23 | 19:L:346:LYS:HG3  | 1.68                     | 0.75              |
| 21:N:654:GLN:NE2  | 21:N:697:PHE:HD2  | 1.85                     | 0.75              |
| 21:N:909:GLU:HB3  | 21:N:911:LYS:NZ   | 2.01                     | 0.75              |
| 29:V:135:ARG:HA   | 29:V:157:ARG:NH2  | 2.02                     | 0.75              |
| 30:W:35:PHE:CE2   | 30:W:182:TYR:CD2  | 2.75                     | 0.75              |
| 33:Z:493:LEU:HG   | 33:Z:497:PHE:CE2  | 2.22                     | 0.75              |
| 33:Z:574:TYR:OH   | 33:Z:584:VAL:CG1  | 2.35                     | 0.75              |
| 33:Z:823:ASN:CB   | 33:Z:856:HIS:CE1  | 2.65                     | 0.75              |
| 16:I:310:LEU:CD1  | 16:I:338:LEU:HA   | 2.17                     | 0.74              |
| 21:N:16:ASN:O     | 21:N:17:GLN:HG2   | 1.87                     | 0.74              |
| 24:Q:50:ARG:NH2   | 24:Q:53:GLU:HB3   | 2.02                     | 0.74              |
| 26:S:378:GLN:HB3  | 26:S:382:ARG:NH1  | 2.02                     | 0.74              |
| 33:Z:748:LEU:CD2  | 33:Z:783:VAL:HA   | 2.16                     | 0.74              |
| 7:7:193:ASP:CB    | 7:7:196:THR:OG1   | 2.35                     | 0.74              |
| 8:A:83:VAL:HG22   | 8:A:141:LEU:CD2   | 2.17                     | 0.74              |
| 11:D:53:LYS:HG3   | 11:D:55:GLN:HG2   | 1.67                     | 0.74              |
| 14:G:7:TYR:CE1    | 14:G:13:VAL:HG23  | 2.20                     | 0.74              |
| 14:G:168:ARG:HE   | 14:G:172:LYS:HZ1  | 1.34                     | 0.74              |
| 14:G:173:ALA:HA   | 19:L:420:ARG:CZ   | 2.16                     | 0.74              |
| 15:H:59:ILE:HD13  | 16:I:92:GLU:OE2   | 1.87                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:281:ILE:CG2  | 16:I:284:ILE:HD11 | 2.16                     | 0.74              |
| 19:L:336:ALA:C    | 19:L:342:ARG:NH1  | 2.45                     | 0.74              |
| 22:O:30:GLU:CG    | 22:O:58:ARG:NH1   | 2.50                     | 0.74              |
| 30:W:21:PHE:CE1   | 30:W:144:PHE:CE2  | 2.74                     | 0.74              |
| 33:Z:443:ASP:HB3  | 33:Z:447:VAL:HG11 | 1.67                     | 0.74              |
| 9:B:159:TRP:CZ3   | 10:C:57:LEU:HB2   | 2.22                     | 0.74              |
| 15:H:284:VAL:CB   | 20:M:254:MET:CB   | 2.55                     | 0.74              |
| 19:L:290:ARG:NH1  | 19:L:293:GLU:CA   | 2.50                     | 0.74              |
| 19:L:357:ARG:O    | 19:L:361:PHE:HD2  | 1.71                     | 0.74              |
| 20:M:81:ASN:HD21  | 20:M:143:ASN:H    | 1.35                     | 0.74              |
| 24:Q:289:GLU:HB2  | 24:Q:291:TYR:CD1  | 2.23                     | 0.74              |
| 33:Z:154:ILE:CG2  | 33:Z:211:PHE:CE1  | 2.70                     | 0.74              |
| 1:1:-2:LEU:CD1    | 1:1:1:THR:H       | 2.01                     | 0.74              |
| 6:6:48:PHE:HE2    | 6:6:50:ALA:HB3    | 1.52                     | 0.74              |
| 6:6:58:ARG:HH12   | 6:6:91:LYS:HD2    | 1.52                     | 0.74              |
| 8:A:220:LYS:HG3   | 8:A:242:GLU:OE1   | 1.87                     | 0.74              |
| 13:F:91:GLN:NE2   | 13:F:111:LEU:HD23 | 2.03                     | 0.74              |
| 15:H:284:VAL:CB   | 20:M:254:MET:N    | 2.48                     | 0.74              |
| 17:J:212:ARG:NH1  | 17:J:246:PHE:HE2  | 1.83                     | 0.74              |
| 23:P:141:LYS:HB2  | 23:P:179:PHE:CE1  | 2.20                     | 0.74              |
| 25:R:353:MET:HA   | 25:R:357:PHE:HD2  | 1.52                     | 0.74              |
| 29:V:53:MET:HE2   | 29:V:65:VAL:CG1   | 2.18                     | 0.74              |
| 3:3:52:THR:HG21   | 4:4:84:ARG:CZ     | 2.17                     | 0.74              |
| 22:O:71:ASP:O     | 30:W:18:ASN:HB2   | 1.86                     | 0.74              |
| 26:S:256:LYS:O    | 26:S:259:TYR:CE1  | 2.39                     | 0.74              |
| 26:S:343:LEU:CD1  | 26:S:347:HIS:CE1  | 2.70                     | 0.74              |
| 33:Z:604:GLY:O    | 33:Z:608:TYR:HD2  | 1.70                     | 0.74              |
| 5:5:40:PHE:HB3    | 5:5:73:ARG:HH21   | 1.46                     | 0.74              |
| 14:G:61:GLN:HA    | 14:G:64:VAL:HG23  | 1.69                     | 0.74              |
| 16:I:103:PRO:HB3  | 17:J:120:TYR:CE2  | 2.22                     | 0.74              |
| 17:J:337:LEU:CD2  | 17:J:377:VAL:HB   | 2.16                     | 0.74              |
| 21:N:386:MET:O    | 21:N:390:LEU:HG   | 1.87                     | 0.74              |
| 24:Q:50:ARG:HH21  | 24:Q:53:GLU:CB    | 2.00                     | 0.74              |
| 24:Q:50:ARG:HH21  | 24:Q:53:GLU:HB3   | 1.51                     | 0.74              |
| 33:Z:748:LEU:HD22 | 33:Z:783:VAL:O    | 1.88                     | 0.74              |
| 23:P:344:ARG:NH2  | 23:P:347:GLU:OE1  | 2.20                     | 0.74              |
| 24:Q:353:PRO:O    | 24:Q:354:PHE:HD1  | 1.71                     | 0.74              |
| 22:O:15:ARG:HH12  | 22:O:73:ILE:HG13  | 1.52                     | 0.74              |
| 22:O:266:PHE:CZ   | 22:O:280:LEU:HD22 | 2.18                     | 0.74              |
| 22:O:373:TRP:CH2  | 28:U:200:LEU:HD21 | 2.22                     | 0.74              |
| 27:T:157:TYR:OH   | 27:T:188:GLU:CG   | 2.30                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:X:12:ALA:HB3   | 31:X:33:ILE:HG23  | 1.70                     | 0.74              |
| 8:A:232:LYS:HD2   | 8:A:234:PHE:HE1   | 1.52                     | 0.74              |
| 17:J:219:VAL:HG11 | 18:K:284:ALA:HA   | 1.68                     | 0.74              |
| 24:Q:11:ALA:HB2   | 24:Q:26:VAL:CG1   | 2.16                     | 0.74              |
| 33:Z:135:LEU:O    | 33:Z:139:LEU:HG   | 1.88                     | 0.74              |
| 7:7:154:GLU:HA    | 7:7:157:ILE:HD12  | 1.68                     | 0.74              |
| 15:H:156:VAL:HG13 | 15:H:181:TYR:HE1  | 1.53                     | 0.74              |
| 16:I:148:LEU:HD21 | 16:I:160:LEU:HD22 | 1.70                     | 0.74              |
| 16:I:310:LEU:CD1  | 16:I:337:ALA:O    | 2.36                     | 0.74              |
| 18:K:186:GLU:HA   | 18:K:190:LEU:HD12 | 1.70                     | 0.74              |
| 19:L:290:ARG:CD   | 19:L:293:GLU:HA   | 2.18                     | 0.74              |
| 21:N:762:ARG:HG3  | 21:N:890:PHE:HE2  | 1.52                     | 0.74              |
| 23:P:353:ILE:HG23 | 23:P:357:TYR:CD2  | 2.23                     | 0.74              |
| 29:V:131:GLN:NE2  | 29:V:194:ARG:NH2  | 2.32                     | 0.74              |
| 33:Z:272:TYR:HE2  | 33:Z:284:LEU:HD11 | 1.53                     | 0.74              |
| 3:3:155:PHE:CD1   | 3:3:180:ILE:HD11  | 2.23                     | 0.73              |
| 9:B:119:GLN:OE1   | 10:C:82:ALA:HB1   | 1.87                     | 0.73              |
| 9:B:139:HIS:ND1   | 9:B:145:PHE:CD1   | 2.56                     | 0.73              |
| 17:J:241:ALA:CB   | 17:J:288:ILE:HD11 | 2.17                     | 0.73              |
| 24:Q:104:PHE:CD2  | 24:Q:114:GLN:OE1  | 2.41                     | 0.73              |
| 33:Z:829:GLN:HG2  | 33:Z:832:ARG:HH22 | 1.53                     | 0.73              |
| 21:N:424:LYS:HZ2  | 21:N:461:GLU:HB3  | 1.52                     | 0.73              |
| 23:P:131:PHE:N    | 23:P:136:ARG:NH1  | 2.28                     | 0.73              |
| 24:Q:74:LEU:CD2   | 24:Q:104:PHE:CD1  | 2.71                     | 0.73              |
| 26:S:315:LYS:CD   | 26:S:345:TYR:CZ   | 2.63                     | 0.73              |
| 31:X:75:TRP:CE2   | 31:X:125:MET:HB3  | 2.21                     | 0.73              |
| 33:Z:190:THR:HG21 | 33:Z:195:PHE:HB2  | 1.70                     | 0.73              |
| 1:1:30:VAL:HG22   | 1:1:174:ARG:HH21  | 1.53                     | 0.73              |
| 4:4:81:SER:HA     | 4:4:124:LYS:NZ    | 2.03                     | 0.73              |
| 15:H:147:ILE:HB   | 15:H:183:ILE:HD11 | 1.70                     | 0.73              |
| 17:J:27:ILE:HD13  | 18:K:50:LYS:HD3   | 1.69                     | 0.73              |
| 18:K:307:ASP:OD1  | 18:K:312:VAL:O    | 2.05                     | 0.73              |
| 22:O:23:HIS:ND1   | 22:O:24:PRO:HD2   | 2.02                     | 0.73              |
| 24:Q:250:THR:HG23 | 24:Q:251:THR:N    | 2.03                     | 0.73              |
| 29:V:131:GLN:HE22 | 29:V:194:ARG:NH2  | 1.85                     | 0.73              |
| 33:Z:562:TRP:NE1  | 33:Z:566:LEU:HG   | 2.03                     | 0.73              |
| 9:B:139:HIS:ND1   | 9:B:145:PHE:CE1   | 2.56                     | 0.73              |
| 19:L:159:LEU:CD1  | 19:L:160:PRO:O    | 2.37                     | 0.73              |
| 33:Z:221:VAL:HG11 | 33:Z:248:TYR:HD2  | 1.54                     | 0.73              |
| 8:A:64:LEU:HD13   | 14:G:157:TRP:CD1  | 2.22                     | 0.73              |
| 15:H:351:VAL:CG1  | 15:H:353:PHE:CZ   | 2.71                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:O:233:LEU:CD2  | 22:O:238:ILE:HD11 | 2.16                     | 0.73              |
| 22:O:266:PHE:CZ   | 22:O:280:LEU:HD21 | 2.22                     | 0.73              |
| 24:Q:141:LEU:CD1  | 24:Q:145:HIS:NE2  | 2.51                     | 0.73              |
| 25:R:239:THR:HG22 | 25:R:246:TYR:HB2  | 1.69                     | 0.73              |
| 25:R:366:ASN:O    | 25:R:370:LYS:HG3  | 1.88                     | 0.73              |
| 30:W:87:MET:HE1   | 30:W:114:VAL:HG22 | 1.71                     | 0.73              |
| 33:Z:64:TYR:CZ    | 33:Z:115:LEU:HD21 | 2.23                     | 0.73              |
| 33:Z:557:GLU:OE1  | 33:Z:562:TRP:CZ3  | 2.40                     | 0.73              |
| 33:Z:776:VAL:CG1  | 33:Z:777:PRO:CD   | 2.63                     | 0.73              |
| 17:J:162:GLU:HA   | 17:J:166:LEU:HD12 | 1.70                     | 0.73              |
| 18:K:346:ARG:HG2  | 18:K:349:ARG:HH22 | 1.53                     | 0.73              |
| 19:L:362:LYS:HA   | 19:L:376:PHE:CE2  | 2.24                     | 0.73              |
| 24:Q:61:LEU:HD11  | 24:Q:65:TYR:CE1   | 2.23                     | 0.73              |
| 25:R:378:ASN:ND2  | 25:R:393:PRO:HA   | 2.03                     | 0.73              |
| 33:Z:165:TYR:OH   | 33:Z:188:ALA:CB   | 2.36                     | 0.73              |
| 33:Z:497:PHE:CD2  | 33:Z:505:VAL:CG1  | 2.71                     | 0.73              |
| 33:Z:812:ILE:HG12 | 33:Z:834:LEU:CD2  | 2.18                     | 0.73              |
| 5:5:8:PHE:CZ      | 5:5:13:ILE:CD1    | 2.71                     | 0.73              |
| 16:I:171:MET:HB3  | 16:I:245:LEU:HD11 | 1.71                     | 0.73              |
| 16:I:229:LYS:NZ   | 16:I:283:GLU:OE2  | 2.21                     | 0.73              |
| 21:N:75:TYR:O     | 21:N:79:VAL:HG23  | 1.88                     | 0.73              |
| 25:R:55:LYS:NZ    | 25:R:91:TRP:CE2   | 2.57                     | 0.73              |
| 26:S:286:TYR:CE1  | 26:S:323:LEU:CB   | 2.70                     | 0.73              |
| 10:C:144:TYR:HB2  | 10:C:147:GLN:NE2  | 2.03                     | 0.73              |
| 16:I:253:ILE:CD1  | 16:I:287:ILE:CG2  | 2.64                     | 0.73              |
| 16:I:428:VAL:HG12 | 16:I:428:VAL:O    | 1.87                     | 0.73              |
| 20:M:59:LEU:HG    | 20:M:63:LYS:HE3   | 1.69                     | 0.73              |
| 21:N:536:ILE:CD1  | 21:N:555:ILE:HG12 | 2.19                     | 0.73              |
| 23:P:130:ILE:O    | 23:P:136:ARG:NH1  | 2.22                     | 0.73              |
| 23:P:203:ILE:HG12 | 23:P:220:TYR:HH   | 1.52                     | 0.73              |
| 26:S:428:ARG:HA   | 27:T:195:LEU:HD22 | 1.69                     | 0.73              |
| 27:T:112:ASN:HB2  | 27:T:177:PHE:CZ   | 2.23                     | 0.73              |
| 29:V:53:MET:CE    | 29:V:65:VAL:HG21  | 2.19                     | 0.73              |
| 33:Z:312:TYR:CE1  | 33:Z:348:LEU:HD22 | 2.23                     | 0.73              |
| 33:Z:761:PHE:CD2  | 33:Z:780:MET:CE   | 2.70                     | 0.73              |
| 17:J:167:PRO:HD3  | 17:J:174:PHE:HZ   | 1.50                     | 0.73              |
| 25:R:252:TYR:HE1  | 25:R:319:CYS:SG   | 2.11                     | 0.73              |
| 26:S:461:PHE:CE2  | 28:U:277:TYR:HB2  | 2.24                     | 0.73              |
| 28:U:277:TYR:HE1  | 29:V:295:VAL:HG11 | 0.95                     | 0.73              |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:O    | 1.85                     | 0.73              |
| 11:D:120:TYR:CD1  | 11:D:126:VAL:HG21 | 2.24                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:295:PHE:CZ   | 15:H:336:LEU:HD12 | 2.23                     | 0.73              |
| 21:N:282:TYR:CE2  | 21:N:286:LEU:HB3  | 2.24                     | 0.73              |
| 21:N:460:ILE:HG22 | 21:N:494:LYS:HE3  | 1.70                     | 0.73              |
| 21:N:596:LEU:CD2  | 21:N:717:LEU:CD1  | 2.57                     | 0.73              |
| 22:O:72:LYS:O     | 30:W:18:ASN:HB2   | 1.89                     | 0.73              |
| 6:6:-5:TYR:CE1    | 6:6:97:TYR:CB     | 2.72                     | 0.72              |
| 8:A:64:LEU:HD12   | 14:G:158:GLY:O    | 1.88                     | 0.72              |
| 8:A:154:ILE:HD11  | 8:A:169:THR:HG22  | 1.68                     | 0.72              |
| 12:E:207:VAL:HA   | 15:H:409:ARG:NH1  | 2.04                     | 0.72              |
| 15:H:49:LEU:HD22  | 33:Z:758:LEU:O    | 1.89                     | 0.72              |
| 19:L:336:ALA:O    | 19:L:342:ARG:HD2  | 1.89                     | 0.72              |
| 21:N:300:ASN:HD22 | 21:N:920:VAL:HG21 | 1.54                     | 0.72              |
| 21:N:579:SER:HA   | 21:N:584:ARG:HH21 | 1.52                     | 0.72              |
| 21:N:615:ALA:CB   | 21:N:651:PHE:CZ   | 2.72                     | 0.72              |
| 23:P:212:LYS:HD3  | 23:P:247:THR:HG23 | 1.70                     | 0.72              |
| 25:R:55:LYS:NZ    | 25:R:91:TRP:CZ2   | 2.57                     | 0.72              |
| 26:S:184:TRP:CH2  | 26:S:217:PHE:CE2  | 2.78                     | 0.72              |
| 26:S:286:TYR:HE1  | 26:S:323:LEU:HD13 | 1.53                     | 0.72              |
| 28:U:293:GLU:HG2  | 29:V:277:LYS:CE   | 2.18                     | 0.72              |
| 29:V:53:MET:HE3   | 29:V:65:VAL:HG11  | 1.71                     | 0.72              |
| 33:Z:550:PHE:CE1  | 33:Z:566:LEU:CB   | 2.71                     | 0.72              |
| 8:A:232:LYS:HD2   | 8:A:234:PHE:CE1   | 2.24                     | 0.72              |
| 21:N:36:TRP:HZ3   | 26:S:252:ASP:HB3  | 1.53                     | 0.72              |
| 26:S:461:PHE:CE1  | 28:U:278:ILE:CA   | 2.72                     | 0.72              |
| 30:W:172:LEU:HD11 | 30:W:190:ILE:HB   | 1.70                     | 0.72              |
| 17:J:221:LYS:HD3  | 18:K:288:SER:HA   | 1.69                     | 0.72              |
| 19:L:386:PHE:HE1  | 19:L:422:VAL:HG12 | 1.54                     | 0.72              |
| 21:N:162:ARG:NH1  | 21:N:165:ILE:HD11 | 2.04                     | 0.72              |
| 25:R:214:TYR:CD2  | 25:R:230:LEU:HD12 | 2.23                     | 0.72              |
| 31:X:9:LYS:HG2    | 31:X:34:GLU:HG2   | 1.69                     | 0.72              |
| 33:Z:912:PHE:HE2  | 33:Z:980:VAL:HG23 | 1.55                     | 0.72              |
| 1:1:114:PRO:HG2   | 1:1:118:SER:HB2   | 1.71                     | 0.72              |
| 3:3:68:LYS:HG2    | 10:C:92:ARG:NH1   | 2.05                     | 0.72              |
| 4:4:38:SER:HB3    | 4:4:39:PRO:HD2    | 1.72                     | 0.72              |
| 8:A:252:ASP:CG    | 23:P:85:LYS:HZ1   | 1.61                     | 0.72              |
| 14:G:98:PHE:CE2   | 14:G:106:ILE:HA   | 2.25                     | 0.72              |
| 22:O:253:GLN:HB2  | 22:O:269:LEU:CD1  | 2.19                     | 0.72              |
| 25:R:266:LEU:HD21 | 25:R:293:THR:CG2  | 2.19                     | 0.72              |
| 26:S:315:LYS:HD3  | 26:S:345:TYR:OH   | 1.89                     | 0.72              |
| 1:1:175:MET:CE    | 1:1:188:PHE:HE1   | 2.01                     | 0.72              |
| 9:B:66:LEU:HD11   | 9:B:235:PHE:CD2   | 2.24                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:204:HIS:HB3  | 16:I:207:LEU:CD1  | 2.20                     | 0.72              |
| 16:I:246:ARG:HD2  | 17:J:278:GLN:NE2  | 2.05                     | 0.72              |
| 22:O:250:TRP:CZ2  | 22:O:271:LYS:CG   | 2.71                     | 0.72              |
| 31:X:104:LYS:HE3  | 31:X:108:ASN:HD21 | 1.54                     | 0.72              |
| 33:Z:463:HIS:HA   | 33:Z:466:GLU:OE2  | 1.89                     | 0.72              |
| 33:Z:612:GLY:HA3  | 33:Z:746:ILE:CG2  | 2.20                     | 0.72              |
| 16:I:395:MET:HE2  | 16:I:420:LYS:HE2  | 1.69                     | 0.72              |
| 19:L:196:VAL:HG23 | 19:L:197:ILE:HG13 | 1.71                     | 0.72              |
| 22:O:359:SER:HB3  | 22:O:363:ILE:HG13 | 1.70                     | 0.72              |
| 24:Q:322:GLU:HG3  | 24:Q:326:MET:HE3  | 1.69                     | 0.72              |
| 1:I:19:ARG:CZ     | 1:I:171:GLY:N     | 2.50                     | 0.72              |
| 15:H:221:LEU:HD21 | 15:H:263:VAL:HB   | 1.70                     | 0.72              |
| 20:M:264:ARG:HA   | 20:M:311:GLN:HE22 | 1.53                     | 0.72              |
| 22:O:384:MET:HE2  | 28:U:189:ARG:C    | 2.15                     | 0.72              |
| 25:R:241:ILE:CG2  | 25:R:242:GLU:HG3  | 2.18                     | 0.72              |
| 27:T:103:SER:CB   | 27:T:141:LEU:HD12 | 2.20                     | 0.72              |
| 33:Z:612:GLY:CA   | 33:Z:746:ILE:HG23 | 2.20                     | 0.72              |
| 4:4:103:ILE:HD12  | 4:4:118:ILE:HD12  | 1.72                     | 0.72              |
| 17:J:212:ARG:NH2  | 17:J:248:ASP:OD1  | 2.22                     | 0.72              |
| 20:M:50:ARG:O     | 20:M:54:GLU:HG3   | 1.89                     | 0.72              |
| 21:N:406:TYR:HD1  | 21:N:448:LEU:CB   | 2.03                     | 0.72              |
| 22:O:99:LEU:HD11  | 22:O:132:GLU:HG3  | 1.71                     | 0.72              |
| 33:Z:497:PHE:HB2  | 33:Z:533:VAL:HG22 | 1.72                     | 0.72              |
| 2:2:160:GLN:NE2   | 2:2:164:TRP:HE1   | 1.83                     | 0.72              |
| 5:5:135:PHE:HB2   | 5:5:167:ARG:HH22  | 1.54                     | 0.72              |
| 7:7:119:LEU:HG    | 7:7:134:LEU:HD12  | 1.72                     | 0.72              |
| 15:H:299:ARG:NH2  | 15:H:344:ASP:HA   | 2.05                     | 0.72              |
| 23:P:342:GLN:HE21 | 23:P:346:ILE:CD1  | 2.01                     | 0.72              |
| 28:U:67:PHE:CD2   | 30:W:100:HIS:CE1  | 2.78                     | 0.72              |
| 30:W:94:ALA:O     | 30:W:98:LEU:HG    | 1.89                     | 0.72              |
| 33:Z:92:LEU:O     | 33:Z:95:THR:OG1   | 2.05                     | 0.72              |
| 10:C:14:SER:HB2   | 10:C:15:PRO:HD2   | 1.72                     | 0.72              |
| 13:F:7:ASP:CA     | 13:F:21:GLN:NE2   | 2.50                     | 0.72              |
| 21:N:75:TYR:OH    | 26:S:223:LEU:CD1  | 2.38                     | 0.72              |
| 23:P:234:TYR:OH   | 23:P:340:ASP:OD2  | 2.06                     | 0.72              |
| 33:Z:612:GLY:HA3  | 33:Z:746:ILE:HG21 | 1.72                     | 0.72              |
| 33:Z:857:LEU:HD21 | 33:Z:908:ILE:HD11 | 1.72                     | 0.72              |
| 1:I:8:LYS:NZ      | 2:2:117:GLY:CA    | 2.52                     | 0.71              |
| 1:I:57:ASP:C      | 8:A:106:TYR:CE1   | 2.68                     | 0.71              |
| 19:L:95:ILE:CG2   | 20:M:68:LYS:HZ2   | 2.03                     | 0.71              |
| 19:L:392:ARG:HH21 | 20:M:213:ARG:HG3  | 1.55                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:245:TYR:O    | 27:T:246:GLU:CB   | 2.38                     | 0.71              |
| 33:Z:371:SER:O    | 33:Z:372:ALA:CB   | 2.38                     | 0.71              |
| 21:N:642:ASP:HB2  | 21:N:643:PRO:HD3  | 1.73                     | 0.71              |
| 21:N:712:ASN:OD1  | 21:N:873:ARG:HG2  | 1.90                     | 0.71              |
| 24:Q:273:ASN:ND2  | 24:Q:306:TYR:OH   | 2.22                     | 0.71              |
| 5:5:34:VAL:CG1    | 5:5:42:LEU:HD22   | 2.20                     | 0.71              |
| 13:F:12:THR:CG2   | 13:F:19:LEU:HD11  | 2.19                     | 0.71              |
| 18:K:135:MET:CG   | 18:K:259:ARG:HH22 | 2.02                     | 0.71              |
| 18:K:224:LYS:CE   | 18:K:236:ARG:HH22 | 1.99                     | 0.71              |
| 19:L:104:LEU:HD23 | 20:M:127:VAL:HG12 | 1.71                     | 0.71              |
| 20:M:75:LEU:HA    | 20:M:77:TYR:CD1   | 2.21                     | 0.71              |
| 21:N:318:LYS:HA   | 29:V:180:LEU:CG   | 2.20                     | 0.71              |
| 23:P:271:SER:O    | 23:P:344:ARG:HD2  | 1.91                     | 0.71              |
| 25:R:62:TYR:CZ    | 25:R:180:PHE:HB3  | 2.25                     | 0.71              |
| 28:U:67:PHE:CE2   | 30:W:100:HIS:ND1  | 2.59                     | 0.71              |
| 28:U:275:VAL:O    | 28:U:278:ILE:CG2  | 2.32                     | 0.71              |
| 29:V:57:PHE:CZ    | 29:V:135:ARG:CZ   | 2.73                     | 0.71              |
| 33:Z:557:GLU:OE1  | 33:Z:562:TRP:CE3  | 2.43                     | 0.71              |
| 1:1:10:ASP:O      | 1:1:102:TYR:CE1   | 2.44                     | 0.71              |
| 17:J:212:ARG:NH1  | 17:J:246:PHE:CD2  | 2.58                     | 0.71              |
| 27:T:247:ASP:OD1  | 27:T:248:GLU:N    | 2.23                     | 0.71              |
| 30:W:9:VAL:HG22   | 30:W:52:ILE:CG1   | 2.19                     | 0.71              |
| 7:7:145:PRO:HB3   | 7:7:148:ARG:HH21  | 1.55                     | 0.71              |
| 16:I:126:PRO:CB   | 16:I:154:MET:HE3  | 2.19                     | 0.71              |
| 33:Z:574:TYR:CE1  | 33:Z:584:VAL:HG21 | 2.24                     | 0.71              |
| 33:Z:795:THR:HG22 | 33:Z:799:PHE:CE2  | 2.24                     | 0.71              |
| 33:Z:915:ALA:HB1  | 33:Z:983:LEU:HD12 | 1.73                     | 0.71              |
| 33:Z:924:LYS:CE   | 33:Z:993:GLU:HG3  | 2.20                     | 0.71              |
| 16:I:230:THR:HG22 | 16:I:234:LYS:HE3  | 1.73                     | 0.71              |
| 19:L:336:ALA:CA   | 19:L:342:ARG:NH1  | 2.54                     | 0.71              |
| 20:M:160:PRO:HB2  | 20:M:166:ARG:HH22 | 1.56                     | 0.71              |
| 21:N:770:LYS:HE3  | 21:N:917:ILE:HD13 | 1.72                     | 0.71              |
| 24:Q:309:ARG:HE   | 24:Q:345:SER:CB   | 2.02                     | 0.71              |
| 27:T:119:THR:HG23 | 27:T:123:HIS:HE1  | 1.56                     | 0.71              |
| 29:V:53:MET:HE2   | 29:V:65:VAL:CG2   | 2.19                     | 0.71              |
| 33:Z:303:ASP:O    | 33:Z:307:HIS:CD2  | 2.43                     | 0.71              |
| 33:Z:493:LEU:CG   | 33:Z:497:PHE:CE2  | 2.74                     | 0.71              |
| 1:1:57:ASP:O      | 8:A:106:TYR:HE1   | 1.73                     | 0.71              |
| 1:1:116:GLY:HA3   | 7:7:-4:ILE:HD11   | 1.73                     | 0.71              |
| 1:1:177:VAL:HG12  | 1:1:179:THR:HG23  | 1.71                     | 0.71              |
| 2:2:36:ARG:CZ     | 2:2:38:SER:HA     | 2.20                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:6:196:LEU:HD22  | 6:6:205:LYS:HG2   | 1.73                     | 0.71              |
| 7:7:187:PHE:CE2   | 7:7:204:LEU:HB2   | 2.25                     | 0.71              |
| 10:C:33:GLY:HA2   | 10:C:51:LYS:CE    | 2.20                     | 0.71              |
| 10:C:136:ILE:HD11 | 10:C:165:VAL:HG22 | 1.73                     | 0.71              |
| 16:I:205:PRO:HA   | 16:I:208:TYR:CE2  | 2.26                     | 0.71              |
| 20:M:82:VAL:HG22  | 20:M:119:VAL:HG12 | 1.71                     | 0.71              |
| 21:N:529:GLN:HE22 | 21:N:559:TYR:HA   | 1.53                     | 0.71              |
| 26:S:461:PHE:HE2  | 28:U:274:MET:HA   | 1.55                     | 0.71              |
| 33:Z:139:LEU:HD11 | 33:Z:194:GLU:O    | 1.90                     | 0.71              |
| 33:Z:612:GLY:CA   | 33:Z:746:ILE:CG2  | 2.68                     | 0.71              |
| 19:L:114:GLU:HB3  | 19:L:137:ARG:HD3  | 1.70                     | 0.71              |
| 24:Q:275:ILE:CD1  | 24:Q:306:TYR:HD2  | 2.03                     | 0.71              |
| 4:4:13:ILE:HD11   | 4:4:153:THR:HG23  | 1.71                     | 0.71              |
| 21:N:549:TYR:CE2  | 21:N:586:ALA:HB2  | 2.26                     | 0.71              |
| 27:T:183:SER:HA   | 27:T:186:ARG:NE   | 2.06                     | 0.71              |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:HE2  | 1.50                     | 0.71              |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:CD2  | 2.21                     | 0.71              |
| 1:1:124:TYR:OH    | 1:1:139:ASP:OD1   | 2.04                     | 0.71              |
| 18:K:212:TYR:CE1  | 18:K:320:ARG:C    | 2.69                     | 0.71              |
| 25:R:31:PHE:CG    | 25:R:320:LYS:HG2  | 2.26                     | 0.71              |
| 25:R:353:MET:HA   | 25:R:357:PHE:CD2  | 2.26                     | 0.71              |
| 33:Z:387:ASN:ND2  | 33:Z:400:ILE:HD11 | 2.05                     | 0.71              |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:CB   | 2.21                     | 0.71              |
| 4:4:32:ASP:HB3    | 4:4:35:ARG:HH12   | 1.56                     | 0.70              |
| 9:B:231:LYS:HD3   | 9:B:234:ARG:HH22  | 1.56                     | 0.70              |
| 17:J:219:VAL:HB   | 18:K:281:ARG:CD   | 2.20                     | 0.70              |
| 18:K:242:PHE:N    | 18:K:243:VAL:N    | 2.39                     | 0.70              |
| 20:M:148:VAL:CG2  | 20:M:155:ILE:HG12 | 2.21                     | 0.70              |
| 21:N:539:MET:HE2  | 21:N:551:GLY:CA   | 2.21                     | 0.70              |
| 22:O:377:VAL:HG11 | 28:U:200:LEU:CD1  | 2.20                     | 0.70              |
| 24:Q:94:VAL:HG22  | 24:Q:130:ARG:HH11 | 1.56                     | 0.70              |
| 26:S:330:LEU:HD13 | 26:S:346:TYR:CD1  | 2.26                     | 0.70              |
| 13:F:18:ARG:HH12  | 13:F:23:GLU:HB2   | 1.56                     | 0.70              |
| 18:K:135:MET:HG2  | 18:K:259:ARG:NH2  | 2.05                     | 0.70              |
| 28:U:67:PHE:HZ    | 30:W:97:THR:HG23  | 1.54                     | 0.70              |
| 30:W:31:ASP:O     | 30:W:35:PHE:CD1   | 2.40                     | 0.70              |
| 33:Z:549:ASN:ND2  | 33:Z:562:TRP:HH2  | 1.89                     | 0.70              |
| 33:Z:929:VAL:O    | 33:Z:955:VAL:CG2  | 2.39                     | 0.70              |
| 2:2:124:TYR:OH    | 2:2:139:GLU:HB2   | 1.91                     | 0.70              |
| 11:D:8:LEU:O      | 11:D:18:PHE:CZ    | 2.43                     | 0.70              |
| 12:E:163:THR:HG22 | 13:F:78:ALA:HB3   | 1.71                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:29:LYS:HD2   | 25:R:49:PHE:CD2   | 2.26                     | 0.70              |
| 33:Z:748:LEU:HD11 | 33:Z:783:VAL:HA   | 1.71                     | 0.70              |
| 7:7:93:TYR:HE1    | 7:7:96:ARG:NH2    | 1.82                     | 0.70              |
| 18:K:193:VAL:HG12 | 18:K:194:GLN:HG2  | 1.72                     | 0.70              |
| 19:L:145:ARG:NH2  | 19:L:163:THR:C    | 2.49                     | 0.70              |
| 21:N:183:VAL:HG11 | 21:N:221:ASP:OD2  | 1.90                     | 0.70              |
| 21:N:315:ASN:CA   | 21:N:318:LYS:NZ   | 2.53                     | 0.70              |
| 31:X:57:VAL:H     | 31:X:59:ARG:NH1   | 1.88                     | 0.70              |
| 1:1:175:MET:CE    | 1:1:188:PHE:CE1   | 2.74                     | 0.70              |
| 3:3:44:ILE:HG22   | 3:3:51:VAL:HG22   | 1.74                     | 0.70              |
| 3:3:177:VAL:HG12  | 3:3:190:TYR:CD1   | 2.26                     | 0.70              |
| 4:4:48:GLU:OE1    | 4:4:51:ASP:OD2    | 2.09                     | 0.70              |
| 7:7:70:ASN:HD22   | 13:F:107:ARG:NH2  | 1.89                     | 0.70              |
| 17:J:377:VAL:CG1  | 17:J:382:PHE:CE2  | 2.75                     | 0.70              |
| 21:N:14:ARG:NH2   | 21:N:42:GLU:OE2   | 2.25                     | 0.70              |
| 12:E:219:LEU:HD12 | 12:E:236:THR:HG22 | 1.71                     | 0.70              |
| 17:J:199:ALA:HB1  | 17:J:210:PHE:HE1  | 1.57                     | 0.70              |
| 33:Z:103:TYR:OH   | 33:Z:140:LEU:HD12 | 1.92                     | 0.70              |
| 33:Z:205:LEU:CG   | 33:Z:236:PHE:CE1  | 2.58                     | 0.70              |
| 33:Z:299:ASP:OD1  | 33:Z:341:TYR:OH   | 2.10                     | 0.70              |
| 1:1:57:ASP:HB3    | 8:A:106:TYR:HE1   | 1.49                     | 0.70              |
| 11:D:10:ILE:N     | 11:D:18:PHE:HE2   | 1.86                     | 0.70              |
| 13:F:64:ILE:HD12  | 13:F:72:LEU:HD11  | 1.73                     | 0.70              |
| 16:I:204:HIS:CG   | 16:I:207:LEU:HD13 | 2.18                     | 0.70              |
| 21:N:94:LYS:HE2   | 21:N:143:LYS:NZ   | 2.06                     | 0.70              |
| 22:O:15:ARG:O     | 30:W:20:ASP:HA    | 1.91                     | 0.70              |
| 23:P:272:PRO:O    | 23:P:273:TYR:CG   | 2.45                     | 0.70              |
| 26:S:211:ARG:NH2  | 26:S:241:PHE:CE1  | 2.60                     | 0.70              |
| 3:3:79:THR:HG23   | 3:3:115:PHE:CZ    | 2.27                     | 0.70              |
| 7:7:187:PHE:CZ    | 7:7:204:LEU:CB    | 2.74                     | 0.70              |
| 13:F:65:LYS:HB2   | 13:F:222:PHE:HE2  | 1.55                     | 0.70              |
| 14:G:200:TYR:HE1  | 14:G:246:ILE:CG2  | 2.05                     | 0.70              |
| 16:I:128:TYR:CD2  | 16:I:154:MET:HG3  | 2.27                     | 0.70              |
| 19:L:386:PHE:CE1  | 19:L:422:VAL:HG12 | 2.27                     | 0.70              |
| 22:O:325:GLU:OE1  | 23:P:364:ARG:NH1  | 2.25                     | 0.70              |
| 26:S:211:ARG:O    | 26:S:215:MET:HG3  | 1.91                     | 0.70              |
| 31:X:79:LYS:CE    | 31:X:98:PHE:CD2   | 2.74                     | 0.70              |
| 33:Z:56:LEU:HD23  | 33:Z:68:LEU:HD23  | 1.72                     | 0.70              |
| 33:Z:761:PHE:CD2  | 33:Z:780:MET:HE2  | 2.27                     | 0.70              |
| 1:1:14:LEU:HD11   | 1:1:100:ALA:CB    | 2.21                     | 0.70              |
| 4:4:174:ASP:OD1   | 4:4:176:LYS:NZ    | 2.24                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:224:GLU:HG3  | 10:C:225:VAL:HG23 | 1.74                     | 0.70              |
| 19:L:145:ARG:HH21 | 19:L:163:THR:HA   | 1.56                     | 0.70              |
| 21:N:96:GLN:O     | 21:N:100:THR:HG23 | 1.91                     | 0.70              |
| 21:N:539:MET:CE   | 21:N:551:GLY:HA2  | 2.22                     | 0.70              |
| 3:3:18:LEU:HD11   | 3:3:177:VAL:HG13  | 1.72                     | 0.70              |
| 4:4:77:GLN:HG2    | 4:4:116:TYR:OH    | 1.92                     | 0.70              |
| 8:A:162:TYR:CZ    | 8:A:164:VAL:HG11  | 2.27                     | 0.70              |
| 15:H:101:ARG:NH2  | 15:H:150:LYS:CD   | 2.55                     | 0.70              |
| 17:J:26:LYS:HE2   | 18:K:51:LEU:CD2   | 2.21                     | 0.70              |
| 17:J:378:THR:O    | 17:J:382:PHE:CD2  | 2.45                     | 0.70              |
| 18:K:224:LYS:CE   | 18:K:236:ARG:HH21 | 2.04                     | 0.70              |
| 21:N:13:LEU:HD22  | 21:N:49:LEU:HD11  | 1.74                     | 0.70              |
| 21:N:98:VAL:O     | 21:N:102:VAL:HG23 | 1.92                     | 0.70              |
| 21:N:450:ILE:HG21 | 21:N:466:LEU:HD21 | 1.72                     | 0.70              |
| 24:Q:82:THR:O     | 24:Q:86:MET:HG2   | 1.92                     | 0.70              |
| 27:T:7:LEU:HD12   | 27:T:33:GLU:HG3   | 1.71                     | 0.70              |
| 27:T:183:SER:HA   | 27:T:186:ARG:HE   | 1.56                     | 0.70              |
| 27:T:221:ALA:HB1  | 27:T:228:ILE:HD11 | 1.74                     | 0.70              |
| 1:1:2:LEU:HB2     | 1:1:33:LYS:HE3    | 1.72                     | 0.69              |
| 2:2:50:ALA:HB3    | 3:3:118:ILE:HG21  | 1.71                     | 0.69              |
| 26:S:211:ARG:NE   | 26:S:240:ASP:OD2  | 2.25                     | 0.69              |
| 32:Y:82:ASP:HB3   | 32:Y:86:ARG:NH1   | 2.07                     | 0.69              |
| 33:Z:242:PHE:HB2  | 33:Z:275:GLN:HG3  | 1.73                     | 0.69              |
| 14:G:108:ILE:HG21 | 14:G:148:TYR:CD1  | 2.27                     | 0.69              |
| 23:P:203:ILE:HG12 | 23:P:220:TYR:CZ   | 2.26                     | 0.69              |
| 25:R:363:PHE:HE1  | 32:Y:78:LYS:CD    | 1.92                     | 0.69              |
| 33:Z:301:THR:CG2  | 33:Z:307:HIS:CE1  | 2.73                     | 0.69              |
| 1:1:8:PHE:HE1     | 1:1:13:ILE:HG13   | 1.55                     | 0.69              |
| 1:1:32:ASP:O      | 1:1:45:ARG:NH2    | 2.25                     | 0.69              |
| 1:1:70:TYR:HD1    | 14:G:110:ALA:CB   | 2.05                     | 0.69              |
| 6:6:-5:TYR:CD1    | 6:6:97:TYR:CD2    | 2.81                     | 0.69              |
| 15:H:285:GLY:C    | 15:H:287:GLY:N    | 2.50                     | 0.69              |
| 18:K:212:TYR:HE1  | 18:K:320:ARG:C    | 2.00                     | 0.69              |
| 25:R:304:TYR:OH   | 25:R:333:MET:HE2  | 1.92                     | 0.69              |
| 26:S:211:ARG:HD2  | 26:S:240:ASP:OD2  | 1.91                     | 0.69              |
| 30:W:4:GLU:HG2    | 30:W:107:HIS:HB2  | 1.73                     | 0.69              |
| 1:1:2:LEU:HD12    | 1:1:1:THR:N       | 2.06                     | 0.69              |
| 7:7:7:LYS:HE3     | 7:7:119:LEU:HB3   | 1.74                     | 0.69              |
| 15:H:308:PHE:CE1  | 15:H:351:VAL:HG13 | 2.28                     | 0.69              |
| 17:J:224:GLY:C    | 17:J:225:GLU:C    | 2.60                     | 0.69              |
| 21:N:390:LEU:HD23 | 21:N:404:SER:HB3  | 1.74                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:585:ARG:NH2  | 21:N:623:PHE:CD2  | 2.60                     | 0.69              |
| 23:P:95:TYR:CD2   | 23:P:96:MET:HE2   | 2.28                     | 0.69              |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:CD1  | 1.96                     | 0.69              |
| 27:T:103:SER:HB2  | 27:T:141:LEU:HD12 | 1.72                     | 0.69              |
| 33:Z:442:VAL:CG1  | 33:Z:443:ASP:N    | 2.20                     | 0.69              |
| 33:Z:748:LEU:HD23 | 33:Z:783:VAL:CG1  | 2.13                     | 0.69              |
| 5:5:8:PHE:CE1     | 5:5:13:ILE:CG1    | 2.72                     | 0.69              |
| 10:C:44:ILE:HD11  | 10:C:146:TYR:HB3  | 1.74                     | 0.69              |
| 18:K:139:LEU:HD23 | 18:K:146:LEU:HA   | 1.74                     | 0.69              |
| 18:K:244:HIS:CG   | 19:L:256:ILE:HG23 | 2.28                     | 0.69              |
| 21:N:406:TYR:CD1  | 21:N:448:LEU:CB   | 2.74                     | 0.69              |
| 23:P:72:TRP:CH2   | 23:P:103:TYR:HB2  | 2.26                     | 0.69              |
| 25:R:194:VAL:HA   | 25:R:197:MET:SD   | 2.33                     | 0.69              |
| 25:R:239:THR:HG22 | 25:R:246:TYR:CB   | 2.23                     | 0.69              |
| 1:1:70:TYR:CD1    | 14:G:110:ALA:HB1  | 2.28                     | 0.69              |
| 1:1:98:ILE:HD11   | 1:1:127:ALA:CB    | 2.22                     | 0.69              |
| 15:H:365:LEU:HD22 | 15:H:370:ARG:NH2  | 2.08                     | 0.69              |
| 20:M:236:ALA:CB   | 20:M:277:ILE:HD12 | 2.22                     | 0.69              |
| 20:M:303:ARG:HH12 | 20:M:307:GLU:HB2  | 1.56                     | 0.69              |
| 22:O:79:VAL:HB    | 22:O:128:LEU:HD23 | 1.74                     | 0.69              |
| 22:O:83:LEU:HD12  | 22:O:128:LEU:HD23 | 1.73                     | 0.69              |
| 30:W:21:PHE:CE1   | 30:W:144:PHE:HE2  | 2.11                     | 0.69              |
| 7:7:187:PHE:CE2   | 7:7:204:LEU:CB    | 2.75                     | 0.69              |
| 15:H:244:LYS:HB2  | 15:H:346:ARG:HG2  | 1.73                     | 0.69              |
| 23:P:395:ARG:HD2  | 24:Q:357:VAL:HG12 | 1.74                     | 0.69              |
| 23:P:425:HIS:HA   | 28:U:228:LYS:HZ1  | 1.58                     | 0.69              |
| 26:S:343:LEU:O    | 26:S:347:HIS:ND1  | 2.20                     | 0.69              |
| 28:U:203:LYS:HE2  | 28:U:229:LEU:HD23 | 1.74                     | 0.69              |
| 31:X:15:CYS:HB2   | 31:X:100:TRP:HB2  | 1.73                     | 0.69              |
| 2:2:50:ALA:HB2    | 3:3:118:ILE:CG2   | 2.09                     | 0.69              |
| 8:A:252:ASP:OD1   | 23:P:85:LYS:NZ    | 0.54                     | 0.69              |
| 10:C:107:PRO:HB3  | 10:C:143:ARG:NH2  | 2.08                     | 0.69              |
| 15:H:379:LEU:HD22 | 15:H:415:THR:HG22 | 1.74                     | 0.69              |
| 16:I:174:ASP:CG   | 16:I:177:PRO:HB3  | 2.18                     | 0.69              |
| 16:I:205:PRO:HA   | 16:I:208:TYR:CD2  | 2.27                     | 0.69              |
| 16:I:222:TYR:CZ   | 16:I:349:LEU:CB   | 2.72                     | 0.69              |
| 16:I:340:ARG:NH1  | 16:I:343:ARG:CG   | 2.55                     | 0.69              |
| 21:N:145:LEU:CD2  | 21:N:173:LYS:HZ1  | 2.05                     | 0.69              |
| 21:N:221:ASP:CB   | 21:N:894:ARG:HH22 | 2.06                     | 0.69              |
| 21:N:615:ALA:CB   | 21:N:651:PHE:HZ   | 2.05                     | 0.69              |
| 25:R:58:GLU:OE2   | 25:R:109:LYS:HD2  | 1.92                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:161:TRP:HE3  | 27:T:162:ASP:OD1  | 1.76                     | 0.69              |
| 27:T:263:ALA:HA   | 27:T:266:TYR:CE2  | 2.27                     | 0.69              |
| 29:V:261:LEU:HD21 | 29:V:284:ALA:HB2  | 1.74                     | 0.69              |
| 30:W:7:VAL:HG23   | 30:W:98:LEU:HD23  | 1.73                     | 0.69              |
| 1:1:8:PHE:CE2     | 1:1:10:ASP:HB2    | 2.28                     | 0.69              |
| 3:3:28:SER:HB2    | 4:4:127:LEU:HD21  | 1.74                     | 0.69              |
| 4:4:38:SER:HB3    | 4:4:73:GLU:OE2    | 1.93                     | 0.69              |
| 8:A:56:GLN:HE22   | 8:A:214:LEU:HD13  | 1.54                     | 0.69              |
| 14:G:111:PHE:CE2  | 14:G:115:LEU:HD11 | 2.28                     | 0.69              |
| 17:J:167:PRO:CB   | 17:J:174:PHE:CZ   | 2.75                     | 0.69              |
| 18:K:123:LEU:HG   | 18:K:146:LEU:O    | 1.92                     | 0.69              |
| 19:L:170:MET:HG2  | 19:L:266:MET:HE2  | 1.74                     | 0.69              |
| 21:N:329:HIS:HB3  | 29:V:182:LYS:CE   | 2.10                     | 0.69              |
| 30:W:20:ASP:CG    | 30:W:25:ARG:HH21  | 2.01                     | 0.69              |
| 33:Z:509:LEU:HD12 | 33:Z:530:LEU:HD23 | 1.73                     | 0.69              |
| 16:I:220:ILE:HG13 | 16:I:344:ILE:HG21 | 1.75                     | 0.69              |
| 17:J:163:VAL:HG21 | 17:J:314:ILE:HD11 | 1.75                     | 0.69              |
| 19:L:361:PHE:CZ   | 19:L:391:ILE:CD1  | 2.72                     | 0.69              |
| 25:R:209:ARG:CG   | 25:R:213:TYR:CE2  | 2.70                     | 0.69              |
| 27:T:211:PHE:CZ   | 27:T:220:PHE:CZ   | 2.81                     | 0.69              |
| 33:Z:497:PHE:CE2  | 33:Z:505:VAL:CG1  | 2.76                     | 0.69              |
| 3:3:37:TYR:HH     | 3:3:59:ARG:HB2    | 1.57                     | 0.68              |
| 5:5:7:ARG:NE      | 5:5:110:PRO:HG2   | 2.09                     | 0.68              |
| 11:D:19:GLN:HE22  | 11:D:121:THR:HA   | 1.56                     | 0.68              |
| 18:K:346:ARG:HG2  | 18:K:349:ARG:HH21 | 1.57                     | 0.68              |
| 19:L:263:ILE:HG23 | 19:L:267:PHE:CE1  | 2.29                     | 0.68              |
| 21:N:179:THR:HG21 | 21:N:219:ASN:ND2  | 2.08                     | 0.68              |
| 21:N:221:ASP:HA   | 21:N:894:ARG:NH2  | 2.05                     | 0.68              |
| 21:N:599:TYR:CD1  | 21:N:634:LEU:HD22 | 2.28                     | 0.68              |
| 26:S:294:ILE:HG12 | 26:S:317:HIS:HE1  | 1.56                     | 0.68              |
| 33:Z:138:ARG:NE   | 33:Z:157:LEU:CG   | 2.45                     | 0.68              |
| 33:Z:188:ALA:CB   | 33:Z:201:LEU:HD11 | 2.23                     | 0.68              |
| 8:A:164:VAL:HG12  | 9:B:61:LEU:HD22   | 1.75                     | 0.68              |
| 11:D:39:LYS:HD2   | 11:D:186:ALA:HB2  | 1.74                     | 0.68              |
| 12:E:50:VAL:HG22  | 12:E:67:ILE:HD11  | 1.75                     | 0.68              |
| 14:G:108:ILE:HG21 | 14:G:148:TYR:CE1  | 2.27                     | 0.68              |
| 15:H:147:ILE:HG13 | 15:H:183:ILE:HG13 | 1.75                     | 0.68              |
| 16:I:126:PRO:HB3  | 16:I:128:TYR:CZ   | 2.24                     | 0.68              |
| 33:Z:924:LYS:HE2  | 33:Z:993:GLU:HG3  | 1.75                     | 0.68              |
| 6:6:58:ARG:NH1    | 6:6:91:LYS:HD2    | 2.08                     | 0.68              |
| 8:A:205:PHE:HZ    | 8:A:209:HIS:HE1   | 1.38                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:18:ARG:HH21  | 11:D:29:ARG:HH22  | 1.40                     | 0.68              |
| 16:I:204:HIS:HB3  | 16:I:207:LEU:HD12 | 1.73                     | 0.68              |
| 26:S:256:LYS:O    | 26:S:259:TYR:HE1  | 1.75                     | 0.68              |
| 26:S:397:LEU:CD2  | 26:S:402:ILE:HG21 | 2.22                     | 0.68              |
| 33:Z:187:SER:HA   | 33:Z:198:GLU:HG2  | 1.75                     | 0.68              |
| 33:Z:306:MET:HE3  | 33:Z:310:LEU:CD2  | 2.21                     | 0.68              |
| 1:1:51:ASP:OD1    | 1:1:93:LEU:HD22   | 1.94                     | 0.68              |
| 4:4:81:SER:CA     | 4:4:124:LYS:HZ3   | 2.03                     | 0.68              |
| 19:L:282:GLU:OE2  | 20:M:306:LEU:HD13 | 1.94                     | 0.68              |
| 21:N:293:LEU:HD23 | 21:N:379:LEU:HD13 | 1.75                     | 0.68              |
| 26:S:461:PHE:CE1  | 28:U:278:ILE:N    | 2.61                     | 0.68              |
| 33:Z:165:TYR:HE1  | 33:Z:190:THR:OG1  | 1.73                     | 0.68              |
| 33:Z:552:GLU:HB3  | 33:Z:554:THR:HG23 | 1.74                     | 0.68              |
| 33:Z:763:HIS:ND1  | 33:Z:766:HIS:HE1  | 1.89                     | 0.68              |
| 10:C:198:SER:HA   | 10:C:206:LEU:HD22 | 1.75                     | 0.68              |
| 13:F:70:MET:SD    | 13:F:135:ILE:O    | 2.52                     | 0.68              |
| 17:J:340:GLY:CA   | 25:R:238:PHE:HE1  | 2.06                     | 0.68              |
| 19:L:88:TYR:HD1   | 20:M:62:ILE:CD1   | 2.02                     | 0.68              |
| 21:N:145:LEU:HB3  | 21:N:173:LYS:HZ1  | 1.59                     | 0.68              |
| 22:O:26:PHE:HZ    | 22:O:64:ASN:HD22  | 1.41                     | 0.68              |
| 22:O:30:GLU:HG2   | 22:O:58:ARG:NH1   | 2.08                     | 0.68              |
| 25:R:79:LEU:O     | 25:R:93:LYS:HD3   | 1.93                     | 0.68              |
| 26:S:343:LEU:HB3  | 26:S:344:PRO:HD3  | 1.76                     | 0.68              |
| 29:V:134:SER:O    | 29:V:157:ARG:NH2  | 2.27                     | 0.68              |
| 16:I:362:LEU:CD2  | 16:I:377:LEU:HD22 | 2.23                     | 0.68              |
| 17:J:378:THR:O    | 17:J:382:PHE:HD2  | 1.76                     | 0.68              |
| 22:O:30:GLU:HB3   | 22:O:58:ARG:HH12  | 1.59                     | 0.68              |
| 22:O:310:PHE:CE2  | 22:O:346:GLU:HA   | 2.29                     | 0.68              |
| 16:I:103:PRO:HD3  | 17:J:120:TYR:CE1  | 2.29                     | 0.68              |
| 26:S:425:ARG:HH11 | 27:T:155:GLY:HA2  | 1.59                     | 0.68              |
| 28:U:13:LEU:HD11  | 29:V:36:LYS:HG3   | 1.76                     | 0.68              |
| 28:U:70:HIS:NE2   | 28:U:109:LEU:HD22 | 2.09                     | 0.68              |
| 33:Z:483:THR:CG2  | 33:Z:521:GLU:HG3  | 2.23                     | 0.68              |
| 33:Z:812:ILE:CD1  | 33:Z:834:LEU:HD22 | 2.22                     | 0.68              |
| 18:K:224:LYS:HE2  | 18:K:236:ARG:HH21 | 1.56                     | 0.68              |
| 19:L:88:TYR:CD1   | 20:M:62:ILE:CB    | 2.75                     | 0.68              |
| 20:M:253:GLN:HG3  | 20:M:258:GLU:HB2  | 1.76                     | 0.68              |
| 21:N:31:VAL:HG23  | 21:N:35:LEU:HD12  | 1.74                     | 0.68              |
| 24:Q:50:ARG:NH2   | 24:Q:53:GLU:CB    | 2.56                     | 0.68              |
| 24:Q:409:TYR:HA   | 25:R:403:LEU:CD2  | 2.07                     | 0.68              |
| 25:R:286:LEU:HD12 | 25:R:289:ILE:HD13 | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:126:LEU:CD2  | 27:T:136:LEU:HD21 | 2.19                     | 0.68              |
| 31:X:62:ASP:OD1   | 31:X:63:PRO:O     | 2.11                     | 0.68              |
| 33:Z:554:THR:O    | 33:Z:558:LEU:HG   | 1.93                     | 0.68              |
| 1:1:14:LEU:CD2    | 1:1:100:ALA:CB    | 2.32                     | 0.68              |
| 6:6:68:PHE:CZ     | 13:F:66:CYS:C     | 2.72                     | 0.68              |
| 18:K:342:SER:O    | 18:K:343:LEU:HB2  | 1.93                     | 0.68              |
| 19:L:125:PRO:HB2  | 19:L:127:TYR:CZ   | 2.28                     | 0.68              |
| 21:N:221:ASP:CA   | 21:N:894:ARG:NH2  | 2.49                     | 0.68              |
| 23:P:130:ILE:CG2  | 23:P:136:ARG:HH22 | 2.07                     | 0.68              |
| 23:P:323:ASN:OD1  | 23:P:324:GLU:HG2  | 1.93                     | 0.68              |
| 24:Q:61:LEU:CD1   | 24:Q:65:TYR:CE1   | 2.77                     | 0.68              |
| 24:Q:294:ARG:NH2  | 24:Q:324:GLU:HB2  | 2.08                     | 0.68              |
| 27:T:229:VAL:HB   | 27:T:234:TYR:HE1  | 1.58                     | 0.68              |
| 33:Z:103:TYR:HE1  | 33:Z:116:ALA:HB2  | 1.58                     | 0.68              |
| 12:E:109:VAL:HG12 | 12:E:156:PHE:CD1  | 2.29                     | 0.68              |
| 16:I:164:ALA:O    | 16:I:165:ASP:HB2  | 1.93                     | 0.68              |
| 17:J:363:THR:HA   | 18:K:203:ILE:CD1  | 2.24                     | 0.68              |
| 21:N:245:LEU:HD21 | 21:N:254:SER:HA   | 1.75                     | 0.68              |
| 21:N:749:LEU:CD2  | 21:N:753:PHE:CZ   | 2.77                     | 0.68              |
| 24:Q:382:LEU:CB   | 25:R:263:ARG:NH1  | 2.57                     | 0.68              |
| 26:S:181:ALA:HB2  | 26:S:232:MET:SD   | 2.34                     | 0.68              |
| 33:Z:972:SER:O    | 33:Z:984:LYS:HE2  | 1.93                     | 0.68              |
| 9:B:75:TYR:CG     | 9:B:82:TYR:CD1    | 2.82                     | 0.67              |
| 15:H:284:VAL:HG12 | 20:M:253:GLN:C    | 2.19                     | 0.67              |
| 17:J:167:PRO:CA   | 17:J:174:PHE:CE2  | 2.76                     | 0.67              |
| 21:N:67:LYS:HG2   | 21:N:97:PHE:CE1   | 2.29                     | 0.67              |
| 24:Q:94:VAL:HG13  | 24:Q:133:LEU:HD11 | 1.74                     | 0.67              |
| 25:R:193:ALA:O    | 25:R:197:MET:HG3  | 1.93                     | 0.67              |
| 25:R:211:LYS:NZ   | 25:R:234:SER:HA   | 2.09                     | 0.67              |
| 27:T:109:TYR:CE2  | 27:T:113:LEU:HD11 | 2.28                     | 0.67              |
| 29:V:154:ASP:HB3  | 29:V:156:PHE:CZ   | 2.28                     | 0.67              |
| 33:Z:188:ALA:N    | 33:Z:201:LEU:HD11 | 1.93                     | 0.67              |
| 33:Z:205:LEU:CD2  | 33:Z:236:PHE:CE1  | 2.76                     | 0.67              |
| 33:Z:900:LEU:CD2  | 33:Z:903:MET:HE2  | 2.24                     | 0.67              |
| 8:A:56:GLN:NE2    | 8:A:214:LEU:CD1   | 2.57                     | 0.67              |
| 14:G:200:TYR:OH   | 14:G:248:GLY:N    | 2.28                     | 0.67              |
| 15:H:244:LYS:HE2  | 15:H:340:LEU:HD22 | 1.76                     | 0.67              |
| 21:N:657:MET:HG2  | 21:N:682:PHE:HE1  | 1.60                     | 0.67              |
| 25:R:266:LEU:CA   | 25:R:270:VAL:CG2  | 2.68                     | 0.67              |
| 29:V:153:ILE:HG23 | 29:V:201:ILE:HD13 | 1.76                     | 0.67              |
| 33:Z:368:VAL:HG12 | 33:Z:369:PHE:O    | 1.94                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:E:98:THR:HG22  | 12:E:102:TYR:CE2  | 2.29                     | 0.67              |
| 14:G:168:ARG:NE   | 14:G:172:LYS:NZ   | 2.40                     | 0.67              |
| 27:T:253:GLU:O    | 27:T:254:ASP:HB2  | 1.94                     | 0.67              |
| 30:W:152:GLU:HG2  | 30:W:155:ASP:H    | 1.58                     | 0.67              |
| 33:Z:490:ILE:HD11 | 33:Z:512:ILE:HD13 | 1.75                     | 0.67              |
| 8:A:205:PHE:CE1   | 8:A:209:HIS:NE2   | 2.63                     | 0.67              |
| 18:K:242:PHE:C    | 18:K:244:HIS:H    | 2.02                     | 0.67              |
| 19:L:247:PRO:HB3  | 20:M:303:ARG:HH21 | 1.59                     | 0.67              |
| 20:M:303:ARG:NH1  | 20:M:307:GLU:OE1  | 2.27                     | 0.67              |
| 23:P:170:SER:O    | 23:P:173:MET:HE3  | 1.93                     | 0.67              |
| 26:S:330:LEU:HB3  | 26:S:346:TYR:CE1  | 2.29                     | 0.67              |
| 33:Z:81:SER:O     | 33:Z:82:MET:HB2   | 1.95                     | 0.67              |
| 1:1:75:THR:HG22   | 1:1:111:TYR:CD1   | 2.29                     | 0.67              |
| 8:A:162:TYR:OH    | 8:A:164:VAL:HG11  | 1.94                     | 0.67              |
| 15:H:306:ILE:HG21 | 15:H:308:PHE:CZ   | 2.29                     | 0.67              |
| 21:N:282:TYR:CE2  | 21:N:286:LEU:CB   | 2.78                     | 0.67              |
| 21:N:325:PHE:CE1  | 29:V:167:ASN:OD1  | 2.47                     | 0.67              |
| 22:O:41:LEU:HD21  | 22:O:62:TYR:HB2   | 1.75                     | 0.67              |
| 22:O:366:MET:HG2  | 28:U:233:PHE:HE2  | 1.59                     | 0.67              |
| 25:R:54:ILE:HG21  | 25:R:63:TYR:HB2   | 1.75                     | 0.67              |
| 29:V:188:LEU:C    | 29:V:188:LEU:HD13 | 2.20                     | 0.67              |
| 3:3:20:LEU:HD12   | 3:3:31:PHE:CD1    | 2.30                     | 0.67              |
| 6:6:66:TYR:HE2    | 6:6:73:LYS:C      | 2.02                     | 0.67              |
| 8:A:167:LYS:HE3   | 9:B:57:MET:HG2    | 1.76                     | 0.67              |
| 12:E:109:VAL:CG1  | 12:E:156:PHE:CD1  | 2.78                     | 0.67              |
| 20:M:362:GLN:O    | 20:M:366:ARG:HG3  | 1.93                     | 0.67              |
| 21:N:588:VAL:HG13 | 21:N:621:THR:HG22 | 1.73                     | 0.67              |
| 24:Q:11:ALA:HA    | 24:Q:14:LEU:HD12  | 1.75                     | 0.67              |
| 25:R:91:TRP:CH2   | 25:R:97:GLU:OE1   | 2.48                     | 0.67              |
| 26:S:184:TRP:CZ2  | 26:S:217:PHE:CD2  | 2.82                     | 0.67              |
| 26:S:211:ARG:CD   | 26:S:240:ASP:OD2  | 2.42                     | 0.67              |
| 28:U:20:ASP:OD2   | 28:U:24:ARG:NE    | 2.19                     | 0.67              |
| 4:4:145:HIS:HD2   | 4:4:146:HIS:CE1   | 2.11                     | 0.67              |
| 19:L:157:ARG:NH2  | 20:M:128:PHE:CE2  | 2.63                     | 0.67              |
| 21:N:117:TYR:OH   | 21:N:202:PHE:N    | 2.28                     | 0.67              |
| 21:N:221:ASP:C    | 21:N:894:ARG:HH22 | 2.03                     | 0.67              |
| 22:O:228:TYR:CA   | 22:O:290:LYS:HZ1  | 2.07                     | 0.67              |
| 23:P:306:ASN:OD1  | 23:P:352:VAL:HG21 | 1.94                     | 0.67              |
| 24:Q:382:LEU:HB3  | 25:R:263:ARG:HH11 | 1.58                     | 0.67              |
| 25:R:410:LEU:HD23 | 28:U:285:ILE:HD13 | 1.75                     | 0.67              |
| 33:Z:205:LEU:HG   | 33:Z:236:PHE:CZ   | 2.28                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:317:GLN:HG3  | 33:Z:317:GLN:O    | 1.94                     | 0.67              |
| 6:6:3:ILE:HG23    | 6:6:46:ASN:HD22   | 1.59                     | 0.67              |
| 7:7:6:MET:HG2     | 7:7:169:ILE:HD11  | 1.77                     | 0.67              |
| 13:F:74:LEU:HD22  | 13:F:81:ALA:CB    | 2.24                     | 0.67              |
| 13:F:91:GLN:CD    | 13:F:111:LEU:HD23 | 2.19                     | 0.67              |
| 20:M:385:GLU:O    | 20:M:385:GLU:CD   | 2.38                     | 0.67              |
| 21:N:47:GLU:OE2   | 21:N:69:TYR:OH    | 2.12                     | 0.67              |
| 27:T:47:GLN:O     | 27:T:48:ASN:OD1   | 2.12                     | 0.67              |
| 31:X:38:ASN:HB3   | 31:X:41:GLU:HA    | 1.75                     | 0.67              |
| 31:X:38:ASN:OD1   | 31:X:43:LEU:HD12  | 1.95                     | 0.67              |
| 33:Z:168:GLN:OE1  | 33:Z:195:PHE:CZ   | 2.47                     | 0.67              |
| 33:Z:182:SER:O    | 33:Z:183:LYS:CB   | 2.41                     | 0.67              |
| 9:B:211:LEU:HD22  | 9:B:238:LEU:HD12  | 1.76                     | 0.67              |
| 16:I:310:LEU:HB2  | 16:I:338:LEU:HD13 | 1.76                     | 0.67              |
| 17:J:224:GLY:CA   | 17:J:225:GLU:N    | 2.57                     | 0.67              |
| 17:J:252:SER:HB2  | 17:J:259:GLU:HG2  | 1.77                     | 0.67              |
| 19:L:145:ARG:NE   | 19:L:162:GLU:HG3  | 2.08                     | 0.67              |
| 22:O:250:TRP:C    | 22:O:269:LEU:HD11 | 2.12                     | 0.67              |
| 29:V:145:GLN:HG2  | 29:V:148:LYS:CE   | 2.22                     | 0.67              |
| 33:Z:964:GLU:HG2  | 33:Z:965:LEU:HG   | 1.76                     | 0.67              |
| 10:C:171:ALA:HA   | 16:I:425:LYS:HD2  | 1.77                     | 0.67              |
| 14:G:196:ALA:HA   | 14:G:213:LEU:HD11 | 1.77                     | 0.67              |
| 15:H:192:ASP:HB2  | 15:H:193:PRO:HD2  | 1.76                     | 0.67              |
| 22:O:269:LEU:HD23 | 22:O:269:LEU:O    | 1.95                     | 0.67              |
| 24:Q:409:TYR:CA   | 25:R:403:LEU:HD21 | 2.07                     | 0.67              |
| 26:S:399:TYR:HB3  | 26:S:402:ILE:CD1  | 2.25                     | 0.67              |
| 33:Z:338:HIS:CD2  | 33:Z:339:PHE:CE2  | 2.83                     | 0.67              |
| 33:Z:886:VAL:HA   | 33:Z:893:PHE:HE2  | 1.58                     | 0.67              |
| 3:3:140:MET:HE3   | 3:3:144:LEU:CD1   | 2.24                     | 0.66              |
| 8:A:148:GLU:CD    | 8:A:230:LYS:HE2   | 2.20                     | 0.66              |
| 11:D:208:LYS:HE2  | 11:D:226:SER:CB   | 2.25                     | 0.66              |
| 17:J:340:GLY:HA3  | 25:R:238:PHE:CE1  | 2.29                     | 0.66              |
| 22:O:82:LEU:HD21  | 22:O:98:TYR:OH    | 1.94                     | 0.66              |
| 24:Q:289:GLU:CD   | 24:Q:291:TYR:HE1  | 2.03                     | 0.66              |
| 28:U:283:ARG:HD3  | 29:V:287:THR:HG22 | 1.76                     | 0.66              |
| 16:I:230:THR:CG2  | 16:I:234:LYS:HE3  | 2.25                     | 0.66              |
| 21:N:222:TYR:H    | 21:N:894:ARG:NH2  | 1.89                     | 0.66              |
| 10:C:66:LEU:HD11  | 10:C:212:GLU:HG2  | 1.77                     | 0.66              |
| 11:D:18:PHE:CD1   | 11:D:19:GLN:N     | 2.63                     | 0.66              |
| 21:N:365:PHE:CE2  | 21:N:402:GLY:C    | 2.74                     | 0.66              |
| 33:Z:850:LEU:HD21 | 33:Z:854:LEU:HD11 | 1.78                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:141:ASN:HB2   | 1:1:154:PHE:HE1   | 1.61                     | 0.66              |
| 2:2:36:ARG:NH2    | 2:2:39:PRO:HD3    | 2.11                     | 0.66              |
| 18:K:168:ASP:OD1  | 19:L:315:PHE:HE1  | 1.79                     | 0.66              |
| 18:K:258:PHE:HZ   | 18:K:299:LEU:HD12 | 1.61                     | 0.66              |
| 19:L:290:ARG:HD2  | 19:L:293:GLU:CA   | 2.22                     | 0.66              |
| 21:N:717:LEU:HD21 | 21:N:733:LEU:CD1  | 2.24                     | 0.66              |
| 24:Q:387:TYR:HB3  | 24:Q:400:TYR:HD2  | 1.59                     | 0.66              |
| 25:R:137:LEU:HD22 | 25:R:141:TYR:CZ   | 2.30                     | 0.66              |
| 27:T:249:MET:O    | 27:T:250:MET:HB2  | 1.94                     | 0.66              |
| 33:Z:53:VAL:HG11  | 33:Z:95:THR:CG2   | 2.24                     | 0.66              |
| 33:Z:463:HIS:CE1  | 33:Z:497:PHE:CE1  | 2.83                     | 0.66              |
| 33:Z:481:PRO:O    | 33:Z:482:ASP:CB   | 2.43                     | 0.66              |
| 33:Z:509:LEU:CB   | 33:Z:530:LEU:HD21 | 2.25                     | 0.66              |
| 20:M:203:ARG:NH1  | 20:M:206:LYS:HZ2  | 1.94                     | 0.66              |
| 21:N:221:ASP:C    | 21:N:894:ARG:NH2  | 2.54                     | 0.66              |
| 21:N:362:TRP:CZ2  | 29:V:23:THR:CG2   | 2.77                     | 0.66              |
| 21:N:654:GLN:NE2  | 21:N:697:PHE:CD2  | 2.64                     | 0.66              |
| 23:P:267:PHE:HE1  | 23:P:329:PHE:CD2  | 2.06                     | 0.66              |
| 25:R:54:ILE:O     | 25:R:54:ILE:HG22  | 1.94                     | 0.66              |
| 2:2:65:LEU:HD13   | 9:B:94:HIS:ND1    | 2.10                     | 0.66              |
| 3:3:7:THR:HG23    | 3:3:112:ILE:CD1   | 2.26                     | 0.66              |
| 6:6:196:LEU:HD23  | 6:6:205:LYS:HG2   | 1.77                     | 0.66              |
| 15:H:365:LEU:CD2  | 15:H:370:ARG:NH2  | 2.59                     | 0.66              |
| 20:M:196:ALA:CB   | 20:M:345:ARG:HE   | 2.05                     | 0.66              |
| 20:M:197:ILE:HB   | 20:M:322:LYS:CE   | 2.24                     | 0.66              |
| 23:P:342:GLN:NE2  | 23:P:346:ILE:HD11 | 2.09                     | 0.66              |
| 25:R:239:THR:CG2  | 25:R:246:TYR:HB2  | 2.26                     | 0.66              |
| 27:T:245:TYR:HD2  | 27:T:246:GLU:H    | 1.40                     | 0.66              |
| 12:E:165:TYR:CB   | 12:E:167:TYR:CZ   | 2.78                     | 0.66              |
| 17:J:199:ALA:HB1  | 17:J:210:PHE:CE1  | 2.30                     | 0.66              |
| 18:K:388:GLN:HB2  | 19:L:340:PRO:HG2  | 1.77                     | 0.66              |
| 23:P:130:ILE:O    | 23:P:130:ILE:HG23 | 1.95                     | 0.66              |
| 24:Q:94:VAL:HG22  | 24:Q:130:ARG:NH1  | 2.10                     | 0.66              |
| 24:Q:385:ILE:HG22 | 24:Q:386:PHE:CD1  | 2.31                     | 0.66              |
| 26:S:365:THR:O    | 26:S:368:LYS:HG3  | 1.95                     | 0.66              |
| 31:X:79:LYS:CE    | 31:X:98:PHE:HE2   | 1.96                     | 0.66              |
| 9:B:48:GLU:HG3    | 9:B:200:VAL:HG11  | 1.78                     | 0.66              |
| 9:B:57:MET:O      | 9:B:61:LEU:HG     | 1.96                     | 0.66              |
| 11:D:193:LYS:HG3  | 11:D:197:ARG:CZ   | 2.26                     | 0.66              |
| 18:K:227:ALA:HB2  | 18:K:268:ILE:HD12 | 1.78                     | 0.66              |
| 23:P:79:LEU:HD11  | 23:P:100:VAL:HG21 | 1.76                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:168:ILE:CG2  | 15:H:172:MET:HA   | 2.26                     | 0.66              |
| 15:H:174:VAL:CG1  | 15:H:183:ILE:CG2  | 2.72                     | 0.66              |
| 21:N:599:TYR:CE1  | 21:N:634:LEU:HD13 | 2.28                     | 0.66              |
| 22:O:280:LEU:HD23 | 22:O:280:LEU:C    | 2.20                     | 0.66              |
| 25:R:237:THR:HG22 | 25:R:275:GLU:OE1  | 1.96                     | 0.66              |
| 33:Z:102:ILE:HG23 | 33:Z:115:LEU:HD13 | 1.77                     | 0.66              |
| 4:4:45:PHE:CE2    | 4:4:101:VAL:CG1   | 2.79                     | 0.66              |
| 7:7:192:ILE:HG12  | 7:7:198:LEU:CD1   | 2.26                     | 0.66              |
| 13:F:117:GLN:HG3  | 13:F:121:GLN:HE21 | 1.61                     | 0.66              |
| 15:H:101:ARG:HH21 | 15:H:150:LYS:CE   | 2.09                     | 0.66              |
| 19:L:263:ILE:HG23 | 19:L:267:PHE:HE1  | 1.59                     | 0.66              |
| 24:Q:4:PRO:HB3    | 24:Q:50:ARG:HH11  | 1.61                     | 0.66              |
| 24:Q:61:LEU:HD11  | 24:Q:65:TYR:CZ    | 2.30                     | 0.66              |
| 27:T:119:THR:CG2  | 27:T:123:HIS:CE1  | 2.78                     | 0.66              |
| 4:4:34:THR:CG2    | 4:4:181:LYS:NZ    | 2.59                     | 0.65              |
| 17:J:59:LYS:HE2   | 17:J:63:ARG:NH1   | 2.11                     | 0.65              |
| 17:J:305:LEU:HB3  | 17:J:313:LYS:CE   | 2.26                     | 0.65              |
| 21:N:539:MET:HE2  | 21:N:551:GLY:HA2  | 1.78                     | 0.65              |
| 22:O:48:PHE:CE1   | 22:O:80:LYS:NZ    | 2.60                     | 0.65              |
| 27:T:211:PHE:HZ   | 27:T:220:PHE:CZ   | 2.13                     | 0.65              |
| 28:U:67:PHE:HD2   | 30:W:100:HIS:CE1  | 2.13                     | 0.65              |
| 33:Z:313:ILE:HG21 | 33:Z:977:ILE:HD11 | 1.78                     | 0.65              |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:HG   | 1.77                     | 0.65              |
| 15:H:223:GLU:HB3  | 20:M:400:MET:CE   | 2.26                     | 0.65              |
| 17:J:167:PRO:CA   | 17:J:174:PHE:CE1  | 2.77                     | 0.65              |
| 23:P:332:GLU:HB2  | 23:P:337:HIS:HE1  | 1.58                     | 0.65              |
| 29:V:53:MET:HG3   | 29:V:108:TYR:HD1  | 1.61                     | 0.65              |
| 31:X:38:ASN:ND2   | 31:X:42:GLU:H     | 1.93                     | 0.65              |
| 33:Z:776:VAL:HG13 | 33:Z:777:PRO:CD   | 2.25                     | 0.65              |
| 33:Z:813:PHE:CD1  | 33:Z:847:ILE:HG23 | 2.32                     | 0.65              |
| 1:1:30:VAL:HG23   | 1:1:172:VAL:HG22  | 1.76                     | 0.65              |
| 11:D:11:PHE:HA    | 11:D:17:ILE:CD1   | 2.26                     | 0.65              |
| 20:M:72:ASN:HB3   | 20:M:156:LEU:CD2  | 2.26                     | 0.65              |
| 22:O:250:TRP:HZ2  | 22:O:271:LYS:HG3  | 1.60                     | 0.65              |
| 25:R:137:LEU:HD22 | 25:R:141:TYR:OH   | 1.96                     | 0.65              |
| 25:R:338:TYR:CZ   | 25:R:368:LEU:HD13 | 2.31                     | 0.65              |
| 26:S:188:TYR:CE2  | 26:S:239:ARG:NH1  | 2.64                     | 0.65              |
| 1:1:61:TYR:CE1    | 8:A:103:GLU:HA    | 2.30                     | 0.65              |
| 5:5:100:MET:SD    | 5:5:127:PHE:CB    | 2.84                     | 0.65              |
| 15:H:50:LYS:HZ3   | 33:Z:791:LYS:HA   | 1.60                     | 0.65              |
| 15:H:379:LEU:HD13 | 15:H:413:ASN:OD1  | 1.95                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:K:159:SER:CB   | 18:K:244:HIS:NE2  | 2.54                     | 0.65              |
| 21:N:315:ASN:CB   | 21:N:318:LYS:NZ   | 2.59                     | 0.65              |
| 24:Q:311:LEU:HD22 | 24:Q:343:LEU:HD12 | 1.75                     | 0.65              |
| 25:R:316:LEU:HD22 | 25:R:322:LEU:HB3  | 1.78                     | 0.65              |
| 29:V:78:VAL:O     | 29:V:121:VAL:HG22 | 1.97                     | 0.65              |
| 33:Z:278:LEU:HD13 | 33:Z:297:VAL:CG1  | 2.27                     | 0.65              |
| 33:Z:574:TYR:HE2  | 33:Z:584:VAL:HG11 | 0.90                     | 0.65              |
| 2:2:124:TYR:CZ    | 2:2:139:GLU:HB3   | 2.31                     | 0.65              |
| 15:H:97:LEU:CB    | 15:H:173:ARG:HG3  | 2.27                     | 0.65              |
| 15:H:147:ILE:CB   | 15:H:183:ILE:HD11 | 2.27                     | 0.65              |
| 18:K:253:MET:O    | 18:K:257:VAL:HG23 | 1.96                     | 0.65              |
| 21:N:536:ILE:CD1  | 21:N:555:ILE:CG1  | 2.73                     | 0.65              |
| 21:N:909:GLU:HB3  | 21:N:911:LYS:HZ1  | 1.59                     | 0.65              |
| 24:Q:61:LEU:HG    | 24:Q:65:TYR:CE2   | 2.30                     | 0.65              |
| 25:R:70:TYR:CZ    | 25:R:76:GLN:HA    | 2.32                     | 0.65              |
| 28:U:92:TRP:CZ2   | 28:U:120:LEU:HG   | 2.32                     | 0.65              |
| 31:X:75:TRP:CE2   | 31:X:125:MET:HB2  | 2.24                     | 0.65              |
| 33:Z:401:VAL:HG22 | 33:Z:439:TYR:CE2  | 2.31                     | 0.65              |
| 2:2:210:THR:HG23  | 3:3:160:GLN:HE21  | 1.61                     | 0.65              |
| 21:N:330:THR:CG2  | 21:N:739:PHE:HE1  | 2.01                     | 0.65              |
| 22:O:373:TRP:CH2  | 28:U:200:LEU:CD2  | 2.79                     | 0.65              |
| 31:X:48:PHE:CZ    | 31:X:68:LEU:HD22  | 2.30                     | 0.65              |
| 33:Z:884:THR:O    | 33:Z:888:LEU:HD11 | 1.96                     | 0.65              |
| 3:3:52:THR:HG1    | 4:4:84:ARG:NH2    | 1.94                     | 0.65              |
| 19:L:114:GLU:O    | 19:L:137:ARG:NE   | 2.30                     | 0.65              |
| 22:O:40:GLN:HB2   | 22:O:58:ARG:NE    | 2.11                     | 0.65              |
| 23:P:353:ILE:HG23 | 23:P:357:TYR:HD2  | 1.62                     | 0.65              |
| 26:S:399:TYR:HB3  | 26:S:402:ILE:HD11 | 1.79                     | 0.65              |
| 30:W:19:GLY:O     | 30:W:20:ASP:OD1   | 2.15                     | 0.65              |
| 5:5:40:PHE:CB     | 5:5:73:ARG:NH2    | 2.60                     | 0.65              |
| 7:7:152:ASP:OD1   | 7:7:156:ASP:OD2   | 2.15                     | 0.65              |
| 9:B:189:ILE:HD11  | 9:B:213:ILE:HG21  | 1.79                     | 0.65              |
| 11:D:70:HIS:CE1   | 11:D:97:ARG:HH22  | 2.14                     | 0.65              |
| 11:D:92:GLU:OE2   | 11:D:108:TYR:CE2  | 2.45                     | 0.65              |
| 12:E:14:THR:CG2   | 12:E:22:PHE:HE2   | 2.10                     | 0.65              |
| 12:E:17:PRO:HA    | 13:F:24:TYR:CZ    | 2.31                     | 0.65              |
| 13:F:179:PHE:CZ   | 13:F:192:ALA:HB2  | 2.32                     | 0.65              |
| 16:I:204:HIS:CB   | 16:I:207:LEU:CD1  | 2.68                     | 0.65              |
| 18:K:224:LYS:HZ3  | 18:K:236:ARG:HH22 | 1.42                     | 0.65              |
| 19:L:88:TYR:CD1   | 20:M:62:ILE:CD1   | 2.78                     | 0.65              |
| 21:N:615:ALA:HB3  | 21:N:651:PHE:CZ   | 2.29                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:382:LEU:HD13 | 25:R:263:ARG:NH1  | 2.11                     | 0.65              |
| 25:R:410:LEU:CD2  | 28:U:285:ILE:HD13 | 2.26                     | 0.65              |
| 26:S:192:GLU:CG   | 26:S:239:ARG:HH12 | 2.02                     | 0.65              |
| 33:Z:608:TYR:CG   | 33:Z:616:LEU:HD11 | 2.32                     | 0.65              |
| 10:C:46:LEU:HD21  | 10:C:138:ALA:HB2  | 1.78                     | 0.65              |
| 13:F:49:LEU:HD22  | 13:F:201:LEU:HD21 | 1.79                     | 0.65              |
| 15:H:53:GLU:HB2   | 33:Z:765:MET:SD   | 2.36                     | 0.65              |
| 17:J:249:GLU:HG2  | 17:J:249:GLU:O    | 1.97                     | 0.65              |
| 19:L:365:THR:HG1  | 19:L:376:PHE:HE1  | 0.67                     | 0.65              |
| 21:N:268:GLN:NE2  | 21:N:457:SER:HA   | 2.12                     | 0.65              |
| 21:N:666:GLN:HG2  | 21:N:875:LEU:HD23 | 1.79                     | 0.65              |
| 24:Q:78:ILE:HB    | 24:Q:79:PRO:HD3   | 1.78                     | 0.65              |
| 25:R:378:ASN:HD22 | 25:R:393:PRO:HA   | 1.60                     | 0.65              |
| 28:U:65:VAL:HG12  | 30:W:96:LEU:CD1   | 2.26                     | 0.65              |
| 33:Z:53:VAL:CG2   | 33:Z:91:PHE:CE2   | 2.78                     | 0.65              |
| 33:Z:506:LEU:HB2  | 33:Z:534:PHE:HZ   | 1.62                     | 0.65              |
| 3:3:37:TYR:HE1    | 3:3:59:ARG:HG3    | 1.58                     | 0.65              |
| 9:B:49:LYS:HE2    | 9:B:210:GLU:HB2   | 1.77                     | 0.65              |
| 15:H:172:MET:HB2  | 16:I:129:TYR:CZ   | 2.27                     | 0.65              |
| 15:H:299:ARG:HH21 | 15:H:344:ASP:HA   | 1.61                     | 0.65              |
| 17:J:27:ILE:HG21  | 18:K:50:LYS:CE    | 2.27                     | 0.65              |
| 28:U:24:ARG:HD3   | 29:V:100:ARG:HG2  | 1.79                     | 0.65              |
| 33:Z:160:GLU:O    | 33:Z:164:VAL:HG23 | 1.97                     | 0.65              |
| 33:Z:415:MET:HB3  | 33:Z:446:GLU:HB3  | 1.78                     | 0.65              |
| 33:Z:515:SER:O    | 33:Z:516:THR:OG1  | 2.10                     | 0.65              |
| 9:B:184:GLU:HG2   | 9:B:186:GLU:H     | 1.62                     | 0.64              |
| 16:I:204:HIS:HD2  | 16:I:207:LEU:HD13 | 1.10                     | 0.64              |
| 17:J:39:GLU:OE2   | 17:J:42:ARG:NH2   | 2.29                     | 0.64              |
| 18:K:386:ILE:HD13 | 18:K:411:TYR:HD1  | 1.62                     | 0.64              |
| 21:N:282:TYR:HE2  | 21:N:286:LEU:HB3  | 1.60                     | 0.64              |
| 22:O:228:TYR:CA   | 22:O:290:LYS:NZ   | 2.57                     | 0.64              |
| 24:Q:311:LEU:HD11 | 24:Q:339:TYR:CE1  | 2.32                     | 0.64              |
| 26:S:210:LEU:HG   | 26:S:214:MET:HE2  | 1.79                     | 0.64              |
| 1:1:19:ARG:HH22   | 1:1:171:GLY:H     | 1.39                     | 0.64              |
| 2:2:8:PHE:HE2     | 2:2:10:ASN:HB3    | 1.62                     | 0.64              |
| 21:N:162:ARG:CZ   | 21:N:165:ILE:HD11 | 2.28                     | 0.64              |
| 23:P:154:ASP:CG   | 23:P:190:LYS:NZ   | 2.54                     | 0.64              |
| 26:S:461:PHE:CD2  | 28:U:277:TYR:CB   | 2.77                     | 0.64              |
| 33:Z:553:ARG:HH12 | 33:Z:595:MET:CE   | 2.10                     | 0.64              |
| 33:Z:813:PHE:CD2  | 33:Z:888:LEU:HD22 | 2.33                     | 0.64              |
| 6:6:116:PHE:CE2   | 6:6:122:TYR:HB3   | 2.32                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:M:170:MET:SD   | 20:M:244:LEU:HB3  | 2.37                     | 0.64              |
| 21:N:596:LEU:HD22 | 21:N:717:LEU:HD13 | 1.73                     | 0.64              |
| 33:Z:383:SER:HB3  | 33:Z:849:ARG:HH12 | 1.62                     | 0.64              |
| 33:Z:744:ALA:HA   | 33:Z:783:VAL:CG2  | 2.27                     | 0.64              |
| 5:5:8:PHE:CZ      | 5:5:13:ILE:HG12   | 2.33                     | 0.64              |
| 8:A:92:ASN:HB2    | 14:G:120:GLN:OE1  | 1.98                     | 0.64              |
| 8:A:252:ASP:CB    | 23:P:85:LYS:HE3   | 2.25                     | 0.64              |
| 10:C:15:PRO:HA    | 11:D:22:TYR:CE1   | 2.33                     | 0.64              |
| 16:I:210:GLU:OE2  | 33:Z:822:THR:HB   | 1.97                     | 0.64              |
| 17:J:27:ILE:HG21  | 18:K:50:LYS:HD3   | 1.79                     | 0.64              |
| 21:N:324:LYS:HG3  | 21:N:325:PHE:HD2  | 1.62                     | 0.64              |
| 24:Q:226:HIS:HA   | 24:Q:229:ASP:OD1  | 1.98                     | 0.64              |
| 24:Q:429:LYS:HB2  | 29:V:269:ARG:CZ   | 2.25                     | 0.64              |
| 27:T:139:ASP:HB3  | 27:T:142:LEU:HD12 | 1.80                     | 0.64              |
| 33:Z:408:TYR:CZ   | 33:Z:411:LYS:NZ   | 2.63                     | 0.64              |
| 1:1:103:ASP:HB2   | 1:1:106:ASN:OD1   | 1.98                     | 0.64              |
| 7:7:7:LYS:HG2     | 7:7:12:VAL:HG12   | 1.80                     | 0.64              |
| 15:H:172:MET:HG3  | 16:I:129:TYR:CD2  | 2.30                     | 0.64              |
| 19:L:164:ASP:OD1  | 20:M:118:VAL:HG11 | 1.96                     | 0.64              |
| 22:O:250:TRP:CD1  | 22:O:269:LEU:O    | 2.49                     | 0.64              |
| 23:P:167:THR:CB   | 23:P:168:TYR:CE1  | 2.81                     | 0.64              |
| 23:P:180:ILE:HG22 | 23:P:184:MET:HE3  | 1.79                     | 0.64              |
| 25:R:158:LEU:HD21 | 25:R:197:MET:HE3  | 1.80                     | 0.64              |
| 26:S:159:ASN:HB3  | 26:S:187:ILE:HD11 | 1.80                     | 0.64              |
| 29:V:159:ILE:O    | 29:V:160:ASP:OD1  | 2.16                     | 0.64              |
| 33:Z:439:TYR:O    | 33:Z:443:ASP:OD2  | 2.14                     | 0.64              |
| 9:B:139:HIS:CD2   | 9:B:234:ARG:CD    | 2.80                     | 0.64              |
| 10:C:98:TYR:CE1   | 10:C:104:GLU:HG3  | 2.33                     | 0.64              |
| 15:H:249:TYR:CZ   | 15:H:376:GLU:CA   | 2.81                     | 0.64              |
| 21:N:36:TRP:CZ3   | 26:S:252:ASP:HB3  | 2.33                     | 0.64              |
| 28:U:67:PHE:CZ    | 30:W:97:THR:CA    | 2.79                     | 0.64              |
| 29:V:153:ILE:HG21 | 29:V:203:TYR:OH   | 1.96                     | 0.64              |
| 33:Z:463:HIS:CE1  | 33:Z:497:PHE:HE1  | 2.16                     | 0.64              |
| 1:1:137:TYR:CE1   | 1:1:157:HIS:CD2   | 2.85                     | 0.64              |
| 2:2:99:ILE:CG1    | 2:2:127:LEU:HD12  | 2.28                     | 0.64              |
| 20:M:289:LYS:HD3  | 20:M:305:MET:CE   | 2.27                     | 0.64              |
| 24:Q:225:LEU:O    | 24:Q:229:ASP:OD1  | 2.16                     | 0.64              |
| 26:S:159:ASN:CB   | 26:S:187:ILE:HD11 | 2.27                     | 0.64              |
| 28:U:16:LEU:HD23  | 28:U:19:LEU:CD1   | 2.23                     | 0.64              |
| 33:Z:884:THR:OG1  | 33:Z:904:LEU:HD21 | 1.98                     | 0.64              |
| 10:C:160:TRP:CD2  | 10:C:163:ILE:HD13 | 2.33                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:D:48:ARG:HH12  | 11:D:57:THR:HB    | 1.62                     | 0.64              |
| 11:D:193:LYS:CE   | 11:D:197:ARG:NH2  | 2.61                     | 0.64              |
| 16:I:246:ARG:HD2  | 17:J:278:GLN:HE21 | 1.63                     | 0.64              |
| 17:J:224:GLY:C    | 17:J:226:GLY:N    | 2.56                     | 0.64              |
| 33:Z:106:TRP:CA   | 33:Z:112:LYS:HD3  | 2.23                     | 0.64              |
| 33:Z:306:MET:CE   | 33:Z:310:LEU:HD21 | 2.25                     | 0.64              |
| 33:Z:436:LEU:HD23 | 33:Z:455:ILE:HG12 | 1.80                     | 0.64              |
| 33:Z:744:ALA:HA   | 33:Z:783:VAL:HG22 | 1.80                     | 0.64              |
| 33:Z:957:LEU:HD13 | 33:Z:958:ASN:O    | 1.98                     | 0.64              |
| 13:F:65:LYS:HB2   | 13:F:222:PHE:CE2  | 2.32                     | 0.64              |
| 18:K:241:GLU:OE2  | 19:L:307:GLU:OE1  | 2.16                     | 0.64              |
| 20:M:222:GLY:O    | 20:M:228:LYS:NZ   | 2.24                     | 0.64              |
| 22:O:233:LEU:HD13 | 22:O:251:LEU:HD22 | 1.79                     | 0.64              |
| 33:Z:106:TRP:HB2  | 33:Z:112:LYS:HZ3  | 1.59                     | 0.64              |
| 33:Z:119:LEU:HB3  | 33:Z:137:TYR:CE2  | 2.33                     | 0.64              |
| 8:A:128:TYR:CE1   | 8:A:131:ARG:NH1   | 2.66                     | 0.64              |
| 17:J:167:PRO:HB3  | 17:J:174:PHE:HE2  | 1.55                     | 0.64              |
| 20:M:411:LYS:HE3  | 20:M:413:GLU:HB2  | 1.79                     | 0.64              |
| 21:N:214:LEU:HA   | 21:N:217:MET:HE2  | 1.80                     | 0.64              |
| 21:N:492:THR:HA   | 21:N:528:ARG:HH11 | 1.63                     | 0.64              |
| 23:P:164:GLN:HE22 | 23:P:180:ILE:HA   | 1.63                     | 0.64              |
| 3:3:109:LYS:HE3   | 3:3:125:LYS:NZ    | 2.13                     | 0.63              |
| 13:F:159:THR:CA   | 13:F:169:LYS:HZ3  | 2.07                     | 0.63              |
| 15:H:367:ARG:HH12 | 20:M:223:PRO:HB3  | 1.62                     | 0.63              |
| 20:M:116:ALA:HB1  | 20:M:128:PHE:HE1  | 1.61                     | 0.63              |
| 21:N:315:ASN:OD1  | 21:N:318:LYS:NZ   | 2.29                     | 0.63              |
| 21:N:749:LEU:HG   | 21:N:753:PHE:CE1  | 2.33                     | 0.63              |
| 27:T:40:LEU:O     | 27:T:88:TYR:OH    | 2.15                     | 0.63              |
| 30:W:172:LEU:HD22 | 30:W:188:SER:HB3  | 1.79                     | 0.63              |
| 33:Z:823:ASN:CG   | 33:Z:856:HIS:HD1  | 2.06                     | 0.63              |
| 33:Z:929:VAL:HG22 | 33:Z:957:LEU:HD23 | 1.80                     | 0.63              |
| 33:Z:985:LYS:HD2  | 33:Z:991:GLU:H    | 1.62                     | 0.63              |
| 4:4:43:MET:HE3    | 4:4:103:ILE:CD1   | 2.28                     | 0.63              |
| 21:N:387:ALA:HA   | 21:N:390:LEU:HD12 | 1.79                     | 0.63              |
| 21:N:770:LYS:CE   | 21:N:917:ILE:HD13 | 2.28                     | 0.63              |
| 30:W:44:ASN:HB2   | 30:W:47:ASN:ND2   | 2.09                     | 0.63              |
| 33:Z:158:ALA:HB2  | 33:Z:207:ILE:CD1  | 2.28                     | 0.63              |
| 33:Z:887:GLY:N    | 33:Z:893:PHE:CD2  | 2.67                     | 0.63              |
| 1:1:-2:LEU:HD21   | 1:1:46:SER:HA     | 1.80                     | 0.63              |
| 3:3:54:LEU:HD11   | 3:3:96:VAL:HG11   | 1.79                     | 0.63              |
| 8:A:128:TYR:CD2   | 8:A:134:MET:HE2   | 2.33                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:66:LEU:HG    | 10:C:212:GLU:CD   | 2.22                     | 0.63              |
| 18:K:67:TYR:OH    | 21:N:609:LEU:CD2  | 2.46                     | 0.63              |
| 21:N:117:TYR:OH   | 21:N:202:PHE:CA   | 2.46                     | 0.63              |
| 21:N:383:LYS:HD2  | 21:N:390:LEU:HD13 | 1.81                     | 0.63              |
| 22:O:250:TRP:CZ2  | 22:O:271:LYS:HB2  | 2.33                     | 0.63              |
| 25:R:209:ARG:CZ   | 25:R:243:LEU:CD1  | 2.76                     | 0.63              |
| 26:S:311:GLN:HE22 | 26:S:338:MET:H    | 1.46                     | 0.63              |
| 30:W:6:THR:HG21   | 30:W:40:LYS:NZ    | 2.12                     | 0.63              |
| 33:Z:130:GLY:O    | 33:Z:131:LYS:HG3  | 1.99                     | 0.63              |
| 33:Z:327:GLN:HE22 | 33:Z:346:LEU:CD1  | 2.11                     | 0.63              |
| 3:3:173:GLY:HA2   | 3:3:193:MET:HE2   | 1.81                     | 0.63              |
| 9:B:239:THR:HG22  | 9:B:241:GLN:N     | 2.13                     | 0.63              |
| 17:J:221:LYS:HD3  | 18:K:288:SER:CA   | 2.28                     | 0.63              |
| 19:L:145:ARG:HH21 | 19:L:163:THR:C    | 2.05                     | 0.63              |
| 21:N:355:TRP:CH2  | 21:N:356:LEU:HD21 | 2.34                     | 0.63              |
| 21:N:508:THR:HG22 | 21:N:510:HIS:H    | 1.64                     | 0.63              |
| 23:P:308:LEU:HD11 | 23:P:349:ASN:HB2  | 0.67                     | 0.63              |
| 25:R:354:ALA:HB2  | 25:R:364:LEU:HD23 | 1.80                     | 0.63              |
| 26:S:388:ILE:HG21 | 26:S:422:MET:HE3  | 1.80                     | 0.63              |
| 33:Z:846:PHE:HE2  | 33:Z:889:VAL:HG11 | 1.63                     | 0.63              |
| 5:5:8:PHE:HE1     | 5:5:12:ILE:C      | 2.07                     | 0.63              |
| 5:5:38:ASN:ND2    | 5:5:41:LEU:HD12   | 2.11                     | 0.63              |
| 21:N:615:ALA:HB1  | 21:N:651:PHE:CZ   | 2.33                     | 0.63              |
| 23:P:101:MET:HE1  | 23:P:119:ILE:HD11 | 1.79                     | 0.63              |
| 25:R:266:LEU:HG   | 25:R:270:VAL:HG23 | 1.80                     | 0.63              |
| 33:Z:761:PHE:CD2  | 33:Z:780:MET:HE1  | 2.34                     | 0.63              |
| 7:7:42:VAL:CG2    | 7:7:192:ILE:HD11  | 2.28                     | 0.63              |
| 8:A:18:ILE:HB     | 9:B:20:GLN:HE22   | 1.64                     | 0.63              |
| 10:C:198:SER:CA   | 10:C:206:LEU:HD22 | 2.28                     | 0.63              |
| 13:F:101:ARG:NH1  | 13:F:103:LEU:CA   | 2.48                     | 0.63              |
| 13:F:201:LEU:O    | 13:F:202:ARG:CG   | 2.46                     | 0.63              |
| 17:J:76:ILE:HD11  | 17:J:87:LYS:HB2   | 1.79                     | 0.63              |
| 21:N:386:MET:HB2  | 21:N:390:LEU:HD11 | 1.81                     | 0.63              |
| 21:N:390:LEU:CD2  | 21:N:404:SER:HB3  | 2.28                     | 0.63              |
| 22:O:383:LYS:HD2  | 27:T:257:THR:HG21 | 1.80                     | 0.63              |
| 26:S:378:GLN:HB3  | 26:S:382:ARG:HH12 | 1.61                     | 0.63              |
| 28:U:277:TYR:OH   | 29:V:295:VAL:HG13 | 1.93                     | 0.63              |
| 1:1:112:THR:CG2   | 7:7:27:ARG:HH21   | 2.11                     | 0.63              |
| 3:3:6:MET:HE1     | 3:3:158:ILE:HA    | 1.79                     | 0.63              |
| 10:C:34:THR:HG22  | 10:C:167:ALA:O    | 1.99                     | 0.63              |
| 16:I:104:LEU:CG   | 16:I:149:LEU:O    | 2.47                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:380:LEU:HB3  | 16:I:420:LYS:HE3  | 1.81                     | 0.63              |
| 17:J:87:LYS:HG3   | 17:J:93:LYS:HG2   | 1.81                     | 0.63              |
| 17:J:250:ILE:HG13 | 17:J:293:ALA:O    | 1.99                     | 0.63              |
| 20:M:264:ARG:HG2  | 20:M:311:GLN:NE2  | 2.13                     | 0.63              |
| 21:N:327:LEU:HD23 | 21:N:743:PHE:CD1  | 2.33                     | 0.63              |
| 23:P:119:ILE:CG2  | 23:P:143:LEU:HD22 | 2.28                     | 0.63              |
| 23:P:287:ASP:CB   | 23:P:297:GLU:OE1  | 2.47                     | 0.63              |
| 23:P:391:ALA:O    | 24:Q:354:PHE:CE1  | 2.51                     | 0.63              |
| 33:Z:71:LEU:HD23  | 33:Z:118:VAL:CG1  | 2.29                     | 0.63              |
| 33:Z:442:VAL:HG12 | 33:Z:443:ASP:H    | 0.56                     | 0.63              |
| 2:2:213:LEU:HD13  | 3:3:192:LYS:HD2   | 1.79                     | 0.63              |
| 8:A:128:TYR:CE2   | 8:A:134:MET:CE    | 2.82                     | 0.63              |
| 10:C:36:ILE:HG21  | 10:C:197:LEU:HD21 | 1.81                     | 0.63              |
| 13:F:206:LEU:CD2  | 13:F:211:LEU:HD11 | 2.27                     | 0.63              |
| 21:N:500:ASP:O    | 21:N:504:TYR:CD2  | 2.52                     | 0.63              |
| 21:N:536:ILE:HG21 | 21:N:555:ILE:HD11 | 1.80                     | 0.63              |
| 25:R:338:TYR:CZ   | 25:R:368:LEU:CD1  | 2.82                     | 0.63              |
| 33:Z:501:LYS:HG3  | 33:Z:534:PHE:CE2  | 2.34                     | 0.63              |
| 5:5:207:PHE:O     | 5:5:208:ASN:OD1   | 2.16                     | 0.63              |
| 6:6:7:ALA:HB2     | 6:6:113:VAL:HG23  | 1.80                     | 0.63              |
| 8:A:135:ARG:NH2   | 14:G:14:PHE:CD2   | 2.67                     | 0.63              |
| 13:F:207:THR:OG1  | 13:F:210:ASN:ND2  | 2.31                     | 0.63              |
| 16:I:104:LEU:HG   | 16:I:149:LEU:O    | 1.99                     | 0.63              |
| 19:L:289:ARG:HH11 | 19:L:334:ASP:HA   | 1.64                     | 0.63              |
| 21:N:771:PHE:CE2  | 21:N:773:MET:HG2  | 2.34                     | 0.63              |
| 24:Q:61:LEU:CD1   | 24:Q:65:TYR:CZ    | 2.82                     | 0.63              |
| 30:W:174:VAL:HG13 | 30:W:184:ASN:HB3  | 1.81                     | 0.63              |
| 33:Z:772:ILE:HA   | 33:Z:775:MET:HE3  | 1.81                     | 0.63              |
| 3:3:26:GLY:HA3    | 3:3:174:TRP:NE1   | 2.14                     | 0.62              |
| 14:G:108:ILE:N    | 14:G:109:PRO:HD2  | 2.14                     | 0.62              |
| 15:H:299:ARG:CZ   | 15:H:345:PRO:HD3  | 2.29                     | 0.62              |
| 18:K:72:GLN:O     | 18:K:76:LYS:HG3   | 1.98                     | 0.62              |
| 21:N:492:THR:C    | 21:N:528:ARG:NH1  | 2.57                     | 0.62              |
| 23:P:67:ALA:HA    | 23:P:75:LEU:HD22  | 1.81                     | 0.62              |
| 25:R:266:LEU:HG   | 25:R:270:VAL:CG2  | 2.29                     | 0.62              |
| 29:V:92:MET:HA    | 29:V:95:LEU:HD12  | 1.81                     | 0.62              |
| 11:D:120:TYR:HE2  | 11:D:129:PHE:CZ   | 2.16                     | 0.62              |
| 13:F:50:LYS:HE3   | 13:F:212:SER:CB   | 2.28                     | 0.62              |
| 13:F:159:THR:CA   | 13:F:169:LYS:NZ   | 2.49                     | 0.62              |
| 16:I:362:LEU:HD23 | 16:I:377:LEU:HD22 | 1.79                     | 0.62              |
| 20:M:173:ASP:OD2  | 20:M:233:ARG:NH2  | 2.31                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:162:ARG:NE   | 21:N:165:ILE:HG12 | 2.14                     | 0.62              |
| 23:P:412:LEU:HD22 | 28:U:272:GLU:OE1  | 1.98                     | 0.62              |
| 24:Q:311:LEU:CD2  | 24:Q:343:LEU:CD1  | 2.71                     | 0.62              |
| 27:T:108:LEU:HD23 | 27:T:174:PHE:CE1  | 2.34                     | 0.62              |
| 27:T:226:TRP:CZ3  | 27:T:235:PHE:CE2  | 2.87                     | 0.62              |
| 28:U:50:ASN:HD22  | 28:U:87:GLU:CD    | 2.08                     | 0.62              |
| 31:X:38:ASN:HD21  | 31:X:43:LEU:HG    | 1.64                     | 0.62              |
| 33:Z:75:ILE:CG2   | 33:Z:75:ILE:O     | 2.44                     | 0.62              |
| 33:Z:89:LEU:HD22  | 33:Z:125:THR:OG1  | 1.99                     | 0.62              |
| 1:1:94:THR:HG22   | 1:1:115:LEU:HD22  | 1.81                     | 0.62              |
| 3:3:41:PHE:CD1    | 3:3:181:ILE:HD13  | 2.35                     | 0.62              |
| 9:B:75:TYR:CD1    | 9:B:82:TYR:CE1    | 2.86                     | 0.62              |
| 11:D:18:PHE:CE1   | 11:D:19:GLN:HB3   | 2.35                     | 0.62              |
| 11:D:74:SER:OG    | 11:D:134:LEU:HB2  | 1.98                     | 0.62              |
| 11:D:217:PRO:O    | 11:D:218:ASP:HB2  | 1.98                     | 0.62              |
| 12:E:165:TYR:HB2  | 12:E:167:TYR:CZ   | 2.34                     | 0.62              |
| 13:F:84:LEU:HD11  | 13:F:112:LEU:HD22 | 1.80                     | 0.62              |
| 14:G:108:ILE:HG22 | 14:G:148:TYR:CD1  | 2.33                     | 0.62              |
| 15:H:49:LEU:HD13  | 33:Z:758:LEU:HB3  | 1.79                     | 0.62              |
| 17:J:39:GLU:CD    | 17:J:42:ARG:HH21  | 2.06                     | 0.62              |
| 19:L:263:ILE:O    | 19:L:267:PHE:CD1  | 2.48                     | 0.62              |
| 21:N:223:LEU:CD1  | 21:N:722:THR:HG22 | 2.29                     | 0.62              |
| 21:N:602:VAL:O    | 21:N:606:VAL:HG22 | 2.00                     | 0.62              |
| 25:R:259:PHE:CE1  | 25:R:332:GLU:HB2  | 2.34                     | 0.62              |
| 28:U:171:VAL:HG13 | 29:V:213:LEU:HD22 | 1.80                     | 0.62              |
| 3:3:37:TYR:CE1    | 3:3:59:ARG:CG     | 2.82                     | 0.62              |
| 3:3:79:THR:HG23   | 3:3:115:PHE:HZ    | 1.64                     | 0.62              |
| 16:I:263:LEU:HD21 | 17:J:224:GLY:H    | 1.64                     | 0.62              |
| 23:P:267:PHE:HZ   | 23:P:329:PHE:CD2  | 2.16                     | 0.62              |
| 23:P:302:LEU:CD1  | 23:P:314:VAL:HG11 | 2.29                     | 0.62              |
| 28:U:297:GLN:HE22 | 29:V:277:LYS:HG3  | 1.64                     | 0.62              |
| 33:Z:56:LEU:HD11  | 33:Z:71:LEU:HD22  | 1.81                     | 0.62              |
| 33:Z:763:HIS:CA   | 33:Z:766:HIS:ND1  | 2.62                     | 0.62              |
| 1:1:19:ARG:NH2    | 1:1:170:GLY:C     | 2.53                     | 0.62              |
| 16:I:278:ILE:HG21 | 16:I:325:ILE:HD12 | 1.82                     | 0.62              |
| 20:M:195:GLU:HA   | 20:M:199:LEU:CD1  | 2.30                     | 0.62              |
| 21:N:749:LEU:CG   | 21:N:753:PHE:CZ   | 2.82                     | 0.62              |
| 22:O:269:LEU:HD23 | 22:O:269:LEU:C    | 2.24                     | 0.62              |
| 24:Q:262:LEU:HD23 | 24:Q:296:ILE:HD13 | 1.81                     | 0.62              |
| 27:T:201:PRO:HD2  | 27:T:204:ASN:HD22 | 1.63                     | 0.62              |
| 28:U:5:HIS:HE1    | 28:U:158:PRO:HG3  | 1.65                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:U:104:LEU:O    | 28:U:108:GLU:HG3  | 1.99                     | 0.62              |
| 33:Z:278:LEU:HD13 | 33:Z:297:VAL:HG13 | 1.81                     | 0.62              |
| 4:4:106:TYR:CZ    | 4:4:185:LYS:HB3   | 2.34                     | 0.62              |
| 10:C:207:THR:HG23 | 10:C:210:ARG:NH2  | 2.13                     | 0.62              |
| 11:D:10:ILE:HD11  | 12:E:10:ARG:CD    | 2.24                     | 0.62              |
| 12:E:179:ALA:O    | 12:E:183:LEU:HG   | 1.98                     | 0.62              |
| 23:P:307:GLU:OE1  | 23:P:307:GLU:N    | 2.33                     | 0.62              |
| 26:S:218:LEU:HG   | 26:S:256:LYS:HZ3  | 1.64                     | 0.62              |
| 26:S:343:LEU:HD11 | 26:S:347:HIS:CE1  | 2.31                     | 0.62              |
| 28:U:35:GLY:HA3   | 28:U:93:TYR:CZ    | 2.35                     | 0.62              |
| 33:Z:233:LEU:C    | 33:Z:271:ILE:HD11 | 2.24                     | 0.62              |
| 33:Z:865:ASP:OD1  | 33:Z:909:ARG:NE   | 2.32                     | 0.62              |
| 15:H:249:TYR:OH   | 15:H:376:GLU:CB   | 2.47                     | 0.62              |
| 19:L:348:GLU:HG2  | 19:L:350:PRO:HD3  | 1.82                     | 0.62              |
| 22:O:325:GLU:HB3  | 23:P:364:ARG:HH22 | 1.65                     | 0.62              |
| 23:P:306:ASN:ND2  | 23:P:349:ASN:HA   | 2.14                     | 0.62              |
| 24:Q:191:LEU:O    | 24:Q:195:LYS:HG3  | 2.00                     | 0.62              |
| 24:Q:353:PRO:O    | 24:Q:354:PHE:CD1  | 2.52                     | 0.62              |
| 26:S:475:TYR:CE1  | 28:U:291:LEU:O    | 2.52                     | 0.62              |
| 3:3:140:MET:CE    | 3:3:144:LEU:HD11  | 2.28                     | 0.62              |
| 4:4:65:LEU:CG     | 4:4:69:ARG:HE     | 2.13                     | 0.62              |
| 10:C:160:TRP:CG   | 10:C:163:ILE:HD13 | 2.35                     | 0.62              |
| 13:F:157:TYR:OH   | 14:G:59:VAL:CG2   | 2.48                     | 0.62              |
| 14:G:10:SER:HA    | 14:G:126:ASN:OD1  | 1.99                     | 0.62              |
| 14:G:72:HIS:CD2   | 14:G:73:ILE:HG13  | 2.34                     | 0.62              |
| 15:H:285:GLY:O    | 15:H:288:ALA:N    | 2.32                     | 0.62              |
| 20:M:216:LYS:NZ   | 20:M:321:VAL:HB   | 2.15                     | 0.62              |
| 22:O:4:ASN:HB2    | 22:O:39:PHE:CZ    | 2.34                     | 0.62              |
| 24:Q:389:VAL:O    | 24:Q:397:LEU:HD12 | 1.99                     | 0.62              |
| 25:R:70:TYR:OH    | 25:R:76:GLN:N     | 2.32                     | 0.62              |
| 25:R:239:THR:HG22 | 25:R:246:TYR:H    | 1.64                     | 0.62              |
| 33:Z:327:GLN:HG2  | 33:Z:349:THR:CB   | 2.26                     | 0.62              |
| 33:Z:518:LEU:CD1  | 33:Z:562:TRP:CE3  | 2.82                     | 0.62              |
| 33:Z:740:VAL:HG11 | 33:Z:764:LEU:HD11 | 1.81                     | 0.62              |
| 4:4:65:LEU:HG     | 4:4:69:ARG:HE     | 1.65                     | 0.62              |
| 11:D:19:GLN:HE21  | 11:D:121:THR:HG23 | 1.63                     | 0.62              |
| 14:G:51:LYS:HE2   | 14:G:63:ASN:HB2   | 1.82                     | 0.62              |
| 15:H:326:ASP:HA   | 15:H:329:VAL:HG22 | 1.81                     | 0.62              |
| 19:L:74:LEU:HD11  | 20:M:47:GLU:HG3   | 1.80                     | 0.62              |
| 21:N:302:PHE:CZ   | 21:N:757:THR:HB   | 2.35                     | 0.62              |
| 23:P:272:PRO:C    | 23:P:273:TYR:CD1  | 2.77                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:P:303:PHE:O    | 23:P:306:ASN:ND2  | 2.33                     | 0.62              |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:HB2  | 1.82                     | 0.62              |
| 33:Z:774:ARG:HE   | 33:Z:806:GLU:HB3  | 1.64                     | 0.62              |
| 16:I:318:ASP:HB3  | 16:I:321:ASP:OD1  | 1.99                     | 0.62              |
| 17:J:167:PRO:HD3  | 17:J:174:PHE:CZ   | 2.32                     | 0.62              |
| 18:K:183:GLU:CG   | 18:K:338:ILE:HG12 | 2.30                     | 0.62              |
| 22:O:4:ASN:N      | 22:O:39:PHE:CE1   | 2.68                     | 0.62              |
| 24:Q:146:TYR:CD1  | 24:Q:184:VAL:HG22 | 2.35                     | 0.62              |
| 27:T:150:ARG:O    | 27:T:154:GLU:HG3  | 2.00                     | 0.62              |
| 31:X:38:ASN:ND2   | 31:X:43:LEU:H     | 1.98                     | 0.62              |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:HD23 | 1.82                     | 0.62              |
| 21:N:21:LYS:O     | 21:N:25:LEU:HG    | 1.99                     | 0.61              |
| 21:N:145:LEU:CB   | 21:N:173:LYS:HZ1  | 2.13                     | 0.61              |
| 21:N:424:LYS:HZ2  | 21:N:461:GLU:CB   | 2.09                     | 0.61              |
| 22:O:233:LEU:CD2  | 22:O:238:ILE:CD1  | 2.78                     | 0.61              |
| 26:S:315:LYS:NZ   | 26:S:345:TYR:CD1  | 2.60                     | 0.61              |
| 2:2:8:PHE:CE1     | 2:2:12:VAL:N      | 2.68                     | 0.61              |
| 2:2:124:TYR:CE2   | 2:2:139:GLU:HA    | 2.35                     | 0.61              |
| 15:H:306:ILE:CG2  | 15:H:308:PHE:CZ   | 2.83                     | 0.61              |
| 18:K:258:PHE:CZ   | 18:K:299:LEU:HD12 | 2.35                     | 0.61              |
| 19:L:170:MET:HE1  | 19:L:265:GLU:CB   | 2.29                     | 0.61              |
| 22:O:377:VAL:HG12 | 28:U:197:LEU:HD13 | 1.81                     | 0.61              |
| 26:S:461:PHE:CE2  | 28:U:274:MET:HA   | 2.36                     | 0.61              |
| 33:Z:436:LEU:HD21 | 33:Z:455:ILE:HG13 | 1.83                     | 0.61              |
| 9:B:160:LYS:HE2   | 10:C:55:THR:O     | 2.00                     | 0.61              |
| 10:C:66:LEU:HG    | 10:C:212:GLU:OE2  | 1.99                     | 0.61              |
| 13:F:101:ARG:HH22 | 13:F:103:LEU:CD1  | 2.13                     | 0.61              |
| 14:G:200:TYR:HE1  | 14:G:246:ILE:HG21 | 1.62                     | 0.61              |
| 16:I:310:LEU:HD13 | 16:I:338:LEU:CA   | 2.28                     | 0.61              |
| 19:L:298:ASP:OD1  | 19:L:301:ILE:HD12 | 2.00                     | 0.61              |
| 20:M:337:LEU:HD22 | 20:M:343:LEU:HD12 | 1.81                     | 0.61              |
| 22:O:159:LYS:HE2  | 22:O:160:LYS:HE3  | 1.82                     | 0.61              |
| 23:P:177:ILE:O    | 23:P:181:LEU:HG   | 2.00                     | 0.61              |
| 27:T:53:ASN:O     | 27:T:54:ASP:OD1   | 2.18                     | 0.61              |
| 30:W:25:ARG:HH11  | 30:W:144:PHE:HE2  | 0.63                     | 0.61              |
| 30:W:115:CYS:SG   | 30:W:144:PHE:HZ   | 2.23                     | 0.61              |
| 31:X:38:ASN:HD22  | 31:X:42:GLU:N     | 1.98                     | 0.61              |
| 6:6:61:ASN:O      | 6:6:65:TRP:CD1    | 2.53                     | 0.61              |
| 6:6:66:TYR:OH     | 6:6:73:LYS:CG     | 2.48                     | 0.61              |
| 14:G:61:GLN:HA    | 14:G:64:VAL:CG2   | 2.29                     | 0.61              |
| 16:I:380:LEU:HD13 | 16:I:420:LYS:HE3  | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:L:88:TYR:CD1   | 20:M:62:ILE:CG1   | 2.84                     | 0.61              |
| 22:O:159:LYS:HG2  | 22:O:160:LYS:HG3  | 1.80                     | 0.61              |
| 23:P:220:TYR:O    | 23:P:224:LEU:HG   | 1.99                     | 0.61              |
| 25:R:211:LYS:HZ3  | 25:R:234:SER:HA   | 1.65                     | 0.61              |
| 33:Z:71:LEU:O     | 33:Z:75:ILE:CG1   | 2.41                     | 0.61              |
| 33:Z:546:ILE:HG23 | 33:Z:550:PHE:CE2  | 2.32                     | 0.61              |
| 33:Z:900:LEU:HD22 | 33:Z:903:MET:HE1  | 1.81                     | 0.61              |
| 1:1:34:LEU:HD13   | 1:1:176:VAL:HG23  | 1.82                     | 0.61              |
| 3:3:96:VAL:O      | 3:3:117:LEU:HD23  | 1.99                     | 0.61              |
| 5:5:158:LYS:HG2   | 5:5:196:LEU:HD21  | 1.83                     | 0.61              |
| 5:5:179:HIS:HB2   | 5:5:188:HIS:CD2   | 2.35                     | 0.61              |
| 7:7:92:MET:HA     | 7:7:102:LEU:HD12  | 1.82                     | 0.61              |
| 8:A:135:ARG:NH2   | 14:G:14:PHE:HD2   | 1.98                     | 0.61              |
| 9:B:139:HIS:HD2   | 9:B:234:ARG:CD    | 2.14                     | 0.61              |
| 19:L:145:ARG:HE   | 19:L:162:GLU:CG   | 2.11                     | 0.61              |
| 21:N:685:VAL:HG13 | 21:N:691:GLN:HG3  | 1.81                     | 0.61              |
| 24:Q:331:THR:HG22 | 24:Q:335:PHE:CE2  | 2.36                     | 0.61              |
| 26:S:464:ARG:HB2  | 28:U:281:LEU:CD2  | 2.30                     | 0.61              |
| 30:W:186:ALA:O    | 30:W:192:LEU:HG   | 1.99                     | 0.61              |
| 3:3:6:MET:CE      | 3:3:158:ILE:HA    | 2.31                     | 0.61              |
| 5:5:135:PHE:HE2   | 5:5:163:ALA:CB    | 1.98                     | 0.61              |
| 6:6:-5:TYR:HE1    | 6:6:97:TYR:CB     | 2.12                     | 0.61              |
| 8:A:128:TYR:HE1   | 8:A:131:ARG:NH1   | 1.98                     | 0.61              |
| 18:K:280:LYS:HZ2  | 18:K:296:LEU:CD2  | 2.12                     | 0.61              |
| 21:N:145:LEU:HB3  | 21:N:173:LYS:NZ   | 2.16                     | 0.61              |
| 21:N:163:LEU:HB3  | 21:N:209:LYS:HZ1  | 1.66                     | 0.61              |
| 21:N:671:LEU:HD13 | 21:N:877:GLN:HG3  | 1.83                     | 0.61              |
| 33:Z:574:TYR:OH   | 33:Z:584:VAL:HG22 | 2.01                     | 0.61              |
| 33:Z:795:THR:CG2  | 33:Z:799:PHE:HE2  | 2.11                     | 0.61              |
| 3:3:1:GLY:HA2     | 3:3:17:ASP:OD2    | 2.01                     | 0.61              |
| 6:6:31:GLU:OE1    | 7:7:129:TYR:CB    | 2.48                     | 0.61              |
| 7:7:178:TYR:CE1   | 7:7:210:LYS:HD3   | 2.35                     | 0.61              |
| 8:A:29:GLU:OE2    | 18:K:425:ASP:HB2  | 1.99                     | 0.61              |
| 10:C:113:ARG:HD3  | 11:D:83:ARG:HD2   | 1.81                     | 0.61              |
| 13:F:3:ARG:HE     | 15:H:359:ASN:CG   | 2.08                     | 0.61              |
| 17:J:28:GLN:HG3   | 26:S:225:HIS:NE2  | 2.16                     | 0.61              |
| 18:K:67:TYR:OH    | 21:N:609:LEU:HD23 | 2.01                     | 0.61              |
| 23:P:392:LYS:HG2  | 24:Q:354:PHE:CG   | 2.36                     | 0.61              |
| 25:R:327:ASP:O    | 25:R:331:ARG:HG3  | 2.01                     | 0.61              |
| 26:S:315:LYS:CE   | 26:S:345:TYR:CE1  | 2.83                     | 0.61              |
| 29:V:145:GLN:OE1  | 29:V:148:LYS:NZ   | 2.27                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:6:PHE:CE1     | 5:5:13:ILE:HB     | 2.35                     | 0.61              |
| 6:6:-5:TYR:CE1    | 6:6:97:TYR:HB3    | 2.36                     | 0.61              |
| 12:E:17:PRO:HA    | 13:F:24:TYR:CD2   | 2.35                     | 0.61              |
| 12:E:165:TYR:CB   | 12:E:167:TYR:HH   | 2.14                     | 0.61              |
| 12:E:219:LEU:HB2  | 12:E:236:THR:HG22 | 1.82                     | 0.61              |
| 15:H:275:ILE:HG21 | 16:I:308:GLU:OE1  | 2.01                     | 0.61              |
| 17:J:161:LYS:HG3  | 17:J:165:GLU:OE1  | 2.01                     | 0.61              |
| 17:J:236:MET:O    | 17:J:240:HIS:CD2  | 2.54                     | 0.61              |
| 19:L:178:ILE:CD1  | 19:L:230:LEU:HD22 | 2.29                     | 0.61              |
| 21:N:330:THR:O    | 21:N:334:VAL:HG23 | 2.01                     | 0.61              |
| 22:O:115:ARG:HH21 | 30:W:80:GLN:HE21  | 1.47                     | 0.61              |
| 22:O:228:TYR:CG   | 22:O:229:ASN:N    | 2.63                     | 0.61              |
| 23:P:395:ARG:CD   | 24:Q:357:VAL:HG12 | 2.30                     | 0.61              |
| 25:R:54:ILE:O     | 25:R:54:ILE:CG2   | 2.49                     | 0.61              |
| 27:T:245:TYR:CD2  | 27:T:246:GLU:N    | 2.68                     | 0.61              |
| 30:W:7:VAL:HG23   | 30:W:98:LEU:HD21  | 1.83                     | 0.61              |
| 33:Z:763:HIS:C    | 33:Z:766:HIS:CE1  | 2.79                     | 0.61              |
| 3:3:7:THR:HG23    | 3:3:112:ILE:HD11  | 1.83                     | 0.61              |
| 14:G:168:ARG:HE   | 14:G:172:LYS:HZ2  | 1.42                     | 0.61              |
| 16:I:207:LEU:CD2  | 33:Z:930:GLY:CA   | 2.77                     | 0.61              |
| 17:J:382:PHE:O    | 17:J:386:VAL:HG23 | 2.01                     | 0.61              |
| 21:N:482:ALA:HB1  | 21:N:517:LEU:HD23 | 1.83                     | 0.61              |
| 23:P:210:ASN:HB3  | 23:P:211:PRO:HD2  | 1.82                     | 0.61              |
| 30:W:95:GLN:NE2   | 30:W:132:LEU:HA   | 2.16                     | 0.61              |
| 33:Z:75:ILE:HG21  | 33:Z:121:ILE:HD13 | 1.81                     | 0.61              |
| 33:Z:205:LEU:HD23 | 33:Z:236:PHE:HE1  | 1.66                     | 0.61              |
| 11:D:96:HIS:NE2   | 11:D:100:LEU:HD22 | 2.15                     | 0.61              |
| 16:I:208:TYR:CD1  | 16:I:209:GLU:N    | 2.69                     | 0.61              |
| 16:I:221:LEU:HD23 | 16:I:348:ILE:HB   | 1.83                     | 0.61              |
| 24:Q:165:PHE:CE1  | 24:Q:173:SER:OG   | 2.49                     | 0.61              |
| 29:V:135:ARG:CD   | 29:V:157:ARG:NH2  | 2.39                     | 0.61              |
| 33:Z:232:LYS:HB3  | 33:Z:236:PHE:CE2  | 2.36                     | 0.61              |
| 2:2:97:TYR:CZ     | 2:2:115:ALA:HB3   | 2.36                     | 0.60              |
| 4:4:44:SER:OG     | 4:4:102:LEU:HB2   | 2.01                     | 0.60              |
| 6:6:73:LYS:HD2    | 12:E:108:ASN:ND2  | 2.16                     | 0.60              |
| 8:A:53:VAL:HG11   | 8:A:82:VAL:HG21   | 1.83                     | 0.60              |
| 15:H:285:GLY:H    | 15:H:331:ARG:HH12 | 1.49                     | 0.60              |
| 21:N:593:PHE:CZ   | 21:N:734:VAL:CG2  | 2.80                     | 0.60              |
| 28:U:293:GLU:HG2  | 29:V:277:LYS:HZ2  | 1.65                     | 0.60              |
| 33:Z:763:HIS:ND1  | 33:Z:766:HIS:CE1  | 2.69                     | 0.60              |
| 33:Z:880:SER:HB2  | 33:Z:906:ALA:HB3  | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:129:VAL:HG22  | 3:3:138:PHE:HE1   | 1.54                     | 0.60              |
| 8:A:24:ARG:NH1    | 18:K:426:PHE:CE2  | 2.70                     | 0.60              |
| 12:E:153:TYR:OH   | 12:E:223:THR:HA   | 2.01                     | 0.60              |
| 13:F:72:LEU:HD22  | 13:F:132:LEU:HD13 | 1.83                     | 0.60              |
| 15:H:223:GLU:HB3  | 20:M:400:MET:HE1  | 1.81                     | 0.60              |
| 16:I:126:PRO:HB2  | 16:I:154:MET:HE3  | 1.82                     | 0.60              |
| 18:K:159:SER:HB3  | 18:K:244:HIS:NE2  | 2.15                     | 0.60              |
| 21:N:602:VAL:HB   | 21:N:603:PRO:HD3  | 1.83                     | 0.60              |
| 21:N:770:LYS:CE   | 21:N:917:ILE:HG21 | 2.28                     | 0.60              |
| 23:P:422:LEU:HD12 | 28:U:262:GLN:NE2  | 2.17                     | 0.60              |
| 30:W:186:ALA:CA   | 30:W:191:ILE:HG21 | 1.99                     | 0.60              |
| 33:Z:224:LEU:CD2  | 33:Z:236:PHE:HE2  | 2.14                     | 0.60              |
| 33:Z:546:ILE:CG2  | 33:Z:550:PHE:HE2  | 2.09                     | 0.60              |
| 5:5:81:LYS:HD3    | 5:5:121:ARG:NE    | 2.16                     | 0.60              |
| 6:6:34:VAL:HG12   | 6:6:196:LEU:HD12  | 1.82                     | 0.60              |
| 6:6:89:TYR:CE1    | 6:6:92:ARG:NE     | 2.69                     | 0.60              |
| 12:E:20:ARG:CD    | 20:M:432:PHE:CZ   | 2.77                     | 0.60              |
| 17:J:329:ARG:NH1  | 17:J:333:ARG:NH1  | 2.50                     | 0.60              |
| 17:J:340:GLY:HA3  | 25:R:238:PHE:HE1  | 1.65                     | 0.60              |
| 21:N:361:ASN:HB3  | 21:N:399:PHE:CE2  | 2.36                     | 0.60              |
| 21:N:596:LEU:HD21 | 21:N:627:ILE:HG22 | 1.83                     | 0.60              |
| 22:O:237:PRO:HB2  | 22:O:241:THR:HG23 | 1.83                     | 0.60              |
| 22:O:250:TRP:CB   | 22:O:269:LEU:CD2  | 2.73                     | 0.60              |
| 23:P:425:HIS:CA   | 28:U:228:LYS:HZ1  | 2.14                     | 0.60              |
| 25:R:50:VAL:HG13  | 25:R:54:ILE:HD11  | 1.81                     | 0.60              |
| 26:S:401:LYS:CE   | 26:S:444:GLU:OE2  | 2.36                     | 0.60              |
| 31:X:25:THR:OG1   | 31:X:82:LYS:NZ    | 2.28                     | 0.60              |
| 33:Z:250:VAL:CG2  | 33:Z:272:TYR:OH   | 2.48                     | 0.60              |
| 2:2:36:ARG:HB2    | 2:2:42:TRP:CZ3    | 2.37                     | 0.60              |
| 2:2:59:ILE:HG13   | 2:2:83:LEU:HD23   | 1.83                     | 0.60              |
| 4:4:55:PHE:HZ     | 4:4:83:VAL:HG13   | 1.65                     | 0.60              |
| 7:7:186:ASN:OD1   | 7:7:205:GLN:HG2   | 2.01                     | 0.60              |
| 14:G:183:PRO:C    | 14:G:184:GLU:HG2  | 2.25                     | 0.60              |
| 20:M:290:ARG:HD3  | 20:M:294:GLU:HB2  | 1.83                     | 0.60              |
| 22:O:102:LEU:C    | 22:O:103:LYS:HG2  | 2.27                     | 0.60              |
| 27:T:157:TYR:CZ   | 27:T:188:GLU:HG2  | 2.36                     | 0.60              |
| 33:Z:295:ARG:NE   | 33:Z:325:GLY:O    | 2.34                     | 0.60              |
| 33:Z:821:GLY:CA   | 33:Z:863:THR:HG22 | 2.20                     | 0.60              |
| 1:1:-2:LEU:HD12   | 1:1:-1:GLY:N      | 2.16                     | 0.60              |
| 1:1:193:TYR:CD1   | 1:1:193:TYR:C     | 2.79                     | 0.60              |
| 4:4:34:THR:CG2    | 4:4:181:LYS:HZ1   | 2.14                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:177:GLN:NE2  | 11:D:52:LEU:HB3   | 2.16                     | 0.60              |
| 16:I:200:LEU:CB   | 33:Z:931:GLN:HG2  | 2.29                     | 0.60              |
| 17:J:27:ILE:HG21  | 18:K:50:LYS:CD    | 2.32                     | 0.60              |
| 18:K:205:PRO:HD2  | 18:K:207:ARG:HH22 | 1.66                     | 0.60              |
| 18:K:423:LYS:HE3  | 18:K:424:PHE:HE2  | 1.64                     | 0.60              |
| 21:N:67:LYS:CG    | 21:N:97:PHE:CE1   | 2.85                     | 0.60              |
| 21:N:331:ALA:HB2  | 21:N:697:PHE:HD1  | 1.67                     | 0.60              |
| 22:O:15:ARG:CA    | 30:W:20:ASP:OD1   | 2.49                     | 0.60              |
| 26:S:425:ARG:NH1  | 27:T:155:GLY:N    | 2.49                     | 0.60              |
| 33:Z:64:TYR:CE2   | 33:Z:111:LEU:HB3  | 2.36                     | 0.60              |
| 2:2:124:TYR:CZ    | 2:2:139:GLU:HA    | 2.37                     | 0.60              |
| 9:B:39:ALA:C      | 9:B:40:THR:HG23   | 2.26                     | 0.60              |
| 13:F:160:ALA:N    | 13:F:169:LYS:HD3  | 2.16                     | 0.60              |
| 13:F:203:ASP:OD1  | 13:F:204:GLU:HG3  | 2.01                     | 0.60              |
| 15:H:295:PHE:HZ   | 15:H:336:LEU:HD12 | 1.62                     | 0.60              |
| 16:I:290:LYS:HE3  | 16:I:336:PRO:HD3  | 1.84                     | 0.60              |
| 17:J:219:VAL:CB   | 18:K:281:ARG:HD2  | 2.27                     | 0.60              |
| 23:P:308:LEU:CD2  | 23:P:369:LEU:HD23 | 2.20                     | 0.60              |
| 27:T:144:TYR:HB2  | 27:T:145:PRO:HD3  | 1.83                     | 0.60              |
| 28:U:92:TRP:CZ2   | 28:U:120:LEU:CG   | 2.84                     | 0.60              |
| 2:2:8:PHE:CE2     | 2:2:10:ASN:HB3    | 2.36                     | 0.60              |
| 9:B:174:PHE:HB3   | 9:B:178:ARG:CZ    | 2.31                     | 0.60              |
| 14:G:168:ARG:O    | 14:G:172:LYS:HG3  | 2.01                     | 0.60              |
| 16:I:263:LEU:HD21 | 17:J:224:GLY:N    | 2.16                     | 0.60              |
| 17:J:363:THR:HA   | 18:K:203:ILE:HD13 | 1.83                     | 0.60              |
| 25:R:266:LEU:C    | 25:R:266:LEU:HD23 | 2.27                     | 0.60              |
| 31:X:91:PHE:H     | 31:X:96:ARG:CG    | 2.03                     | 0.60              |
| 33:Z:931:GLN:HB2  | 33:Z:955:VAL:HG21 | 1.82                     | 0.60              |
| 1:1:57:ASP:HB3    | 8:A:106:TYR:CZ    | 2.35                     | 0.60              |
| 10:C:193:ALA:O    | 10:C:197:LEU:HG   | 2.00                     | 0.60              |
| 11:D:193:LYS:HE3  | 11:D:197:ARG:CZ   | 2.32                     | 0.60              |
| 17:J:328:LEU:HD23 | 17:J:343:LEU:HD22 | 1.82                     | 0.60              |
| 21:N:405:LEU:HD22 | 21:N:423:LEU:CD2  | 2.31                     | 0.60              |
| 24:Q:309:ARG:CZ   | 24:Q:345:SER:CB   | 2.54                     | 0.60              |
| 27:T:229:VAL:HG12 | 27:T:230:ASN:N    | 2.17                     | 0.60              |
| 28:U:16:LEU:HD12  | 29:V:35:LEU:CD1   | 2.32                     | 0.60              |
| 29:V:159:ILE:HB   | 29:V:194:ARG:H    | 1.66                     | 0.60              |
| 33:Z:99:LEU:O     | 33:Z:102:ILE:HG22 | 2.02                     | 0.60              |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:CG   | 2.31                     | 0.60              |
| 4:4:37:LEU:HD22   | 4:4:43:MET:SD     | 2.41                     | 0.60              |
| 4:4:103:ILE:CD1   | 4:4:118:ILE:HD12  | 2.32                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:129:TYR:CD1   | 4:4:143:LEU:HD13  | 2.37                     | 0.60              |
| 8:A:54:ILE:HG22   | 8:A:210:MET:CE    | 2.27                     | 0.60              |
| 8:A:232:LYS:CD    | 8:A:234:PHE:HE1   | 2.15                     | 0.60              |
| 13:F:105:VAL:CG2  | 13:F:145:LEU:CD1  | 2.65                     | 0.60              |
| 15:H:249:TYR:CE2  | 15:H:374:LYS:HG2  | 2.37                     | 0.60              |
| 15:H:451:ILE:O    | 15:H:455:LYS:HG3  | 2.01                     | 0.60              |
| 18:K:386:ILE:HA   | 18:K:414:GLN:NE2  | 2.12                     | 0.60              |
| 20:M:81:ASN:ND2   | 20:M:143:ASN:H    | 2.00                     | 0.60              |
| 21:N:329:HIS:CG   | 29:V:182:LYS:HZ2  | 2.18                     | 0.60              |
| 21:N:405:LEU:HD13 | 21:N:446:ALA:HB2  | 1.83                     | 0.60              |
| 21:N:601:THR:O    | 21:N:605:ILE:HG12 | 2.01                     | 0.60              |
| 24:Q:11:ALA:HB1   | 24:Q:27:TYR:CE1   | 2.37                     | 0.60              |
| 24:Q:88:PHE:CD2   | 24:Q:89:ALA:N     | 2.69                     | 0.60              |
| 24:Q:383:ASP:OD1  | 25:R:267:LYS:NZ   | 2.35                     | 0.60              |
| 25:R:258:LEU:HD12 | 25:R:288:SER:HB2  | 1.83                     | 0.60              |
| 33:Z:608:TYR:CD2  | 33:Z:616:LEU:HD11 | 2.36                     | 0.60              |
| 1:1:174:ARG:HH11  | 1:1:185:ARG:HH21  | 1.42                     | 0.60              |
| 5:5:135:PHE:HB2   | 5:5:167:ARG:CZ    | 2.32                     | 0.60              |
| 18:K:192:LEU:HD21 | 18:K:266:PRO:HB3  | 1.84                     | 0.60              |
| 18:K:258:PHE:CD2  | 18:K:302:GLN:HB3  | 2.37                     | 0.60              |
| 18:K:272:ASP:CB   | 19:L:306:MET:HE2  | 2.01                     | 0.60              |
| 21:N:109:TYR:HE1  | 21:N:129:ILE:HD12 | 1.67                     | 0.60              |
| 21:N:330:THR:CG2  | 21:N:739:PHE:CE1  | 2.76                     | 0.60              |
| 21:N:596:LEU:CD1  | 21:N:717:LEU:HD13 | 2.29                     | 0.60              |
| 24:Q:275:ILE:CD1  | 24:Q:306:TYR:CD2  | 2.74                     | 0.60              |
| 26:S:242:LEU:HD21 | 26:S:279:ILE:HG13 | 1.83                     | 0.60              |
| 27:T:126:LEU:HD22 | 27:T:136:LEU:HD22 | 1.80                     | 0.60              |
| 33:Z:518:LEU:HG   | 33:Z:524:ALA:HB3  | 1.84                     | 0.60              |
| 5:5:93:ALA:HB1    | 6:6:93:PHE:HE1    | 1.67                     | 0.59              |
| 13:F:5:ASN:HB3    | 14:G:9:LEU:HD11   | 1.84                     | 0.59              |
| 16:I:220:ILE:CD1  | 16:I:344:ILE:HG21 | 2.32                     | 0.59              |
| 21:N:376:LYS:HE2  | 21:N:750:SER:O    | 2.02                     | 0.59              |
| 22:O:131:SER:HB3  | 22:O:135:ARG:NH1  | 2.16                     | 0.59              |
| 25:R:222:ARG:HA   | 25:R:224:PHE:CE2  | 2.37                     | 0.59              |
| 25:R:338:TYR:CE2  | 25:R:368:LEU:HD13 | 2.36                     | 0.59              |
| 26:S:425:ARG:HH11 | 27:T:155:GLY:CA   | 2.15                     | 0.59              |
| 27:T:245:TYR:O    | 27:T:246:GLU:HB2  | 2.01                     | 0.59              |
| 28:U:57:GLU:HG2   | 30:W:96:LEU:HD22  | 1.84                     | 0.59              |
| 28:U:92:TRP:HZ2   | 28:U:120:LEU:CD1  | 1.93                     | 0.59              |
| 33:Z:64:TYR:CD2   | 33:Z:68:LEU:HD11  | 2.37                     | 0.59              |
| 8:A:30:TYR:C      | 14:G:14:PHE:CE1   | 2.80                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:F:201:LEU:HD22 | 13:F:204:GLU:HB2  | 1.84                     | 0.59              |
| 17:J:27:ILE:CG2   | 18:K:50:LYS:HE2   | 2.32                     | 0.59              |
| 17:J:59:LYS:HE2   | 17:J:63:ARG:HH12  | 1.67                     | 0.59              |
| 20:M:345:ARG:HG3  | 20:M:347:ILE:HG13 | 1.85                     | 0.59              |
| 21:N:306:ASN:O    | 21:N:308:ASN:ND2  | 2.36                     | 0.59              |
| 22:O:83:LEU:HD12  | 22:O:128:LEU:CD2  | 2.32                     | 0.59              |
| 23:P:241:LEU:HD11 | 23:P:260:VAL:HG13 | 1.84                     | 0.59              |
| 23:P:395:ARG:HD2  | 24:Q:357:VAL:CG1  | 2.31                     | 0.59              |
| 25:R:422:ARG:NH1  | 26:S:474:GLU:HG3  | 2.17                     | 0.59              |
| 30:W:21:PHE:HZ    | 30:W:144:PHE:HD2  | 1.39                     | 0.59              |
| 9:B:179:TRP:CD1   | 9:B:183:LEU:HD12  | 2.36                     | 0.59              |
| 11:D:53:LYS:NZ    | 11:D:209:ASN:OD1  | 2.32                     | 0.59              |
| 12:E:46:VAL:HG11  | 12:E:145:ALA:HB1  | 1.84                     | 0.59              |
| 13:F:145:LEU:HD23 | 13:F:146:GLU:C    | 2.26                     | 0.59              |
| 14:G:183:PRO:O    | 14:G:184:GLU:CG   | 2.49                     | 0.59              |
| 16:I:208:TYR:CD1  | 16:I:208:TYR:C    | 2.80                     | 0.59              |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:HG21 | 1.85                     | 0.59              |
| 17:J:211:ILE:HD12 | 17:J:243:SER:OG   | 2.02                     | 0.59              |
| 20:M:218:ALA:HB3  | 20:M:324:LEU:HD23 | 1.84                     | 0.59              |
| 23:P:137:ALA:HB1  | 23:P:179:PHE:CE2  | 2.38                     | 0.59              |
| 29:V:186:GLN:O    | 29:V:190:HIS:HD2  | 1.85                     | 0.59              |
| 33:Z:327:GLN:NE2  | 33:Z:346:LEU:HD12 | 2.16                     | 0.59              |
| 33:Z:383:SER:O    | 33:Z:386:VAL:HG12 | 2.03                     | 0.59              |
| 33:Z:931:GLN:HG3  | 33:Z:931:GLN:O    | 2.01                     | 0.59              |
| 1:1:143:ARG:O     | 1:1:146:MET:HE2   | 2.02                     | 0.59              |
| 5:5:38:ASN:HB2    | 5:5:39:PRO:HD2    | 1.84                     | 0.59              |
| 14:G:203:HIS:CE1  | 14:G:211:PHE:HD1  | 2.21                     | 0.59              |
| 19:L:149:ASP:OD2  | 19:L:152:THR:N    | 2.24                     | 0.59              |
| 19:L:290:ARG:HH11 | 19:L:293:GLU:CA   | 2.13                     | 0.59              |
| 21:N:83:LEU:HD22  | 21:N:132:LYS:HB3  | 1.85                     | 0.59              |
| 21:N:490:LEU:HD23 | 21:N:491:GLY:N    | 2.17                     | 0.59              |
| 21:N:599:TYR:HD1  | 21:N:634:LEU:HD22 | 1.66                     | 0.59              |
| 25:R:167:LYS:HE2  | 25:R:197:MET:CE   | 2.32                     | 0.59              |
| 33:Z:190:THR:O    | 33:Z:190:THR:HG22 | 2.02                     | 0.59              |
| 33:Z:217:GLU:OE1  | 33:Z:244:ARG:NE   | 2.31                     | 0.59              |
| 9:B:174:PHE:HB3   | 9:B:178:ARG:NH2   | 2.17                     | 0.59              |
| 10:C:70:ASN:ND2   | 10:C:95:ALA:HB1   | 2.18                     | 0.59              |
| 13:F:22:VAL:O     | 13:F:26:LEU:HG    | 2.02                     | 0.59              |
| 13:F:34:VAL:HG21  | 13:F:200:SER:OG   | 2.02                     | 0.59              |
| 19:L:102:GLY:HA3  | 20:M:153:TYR:HD2  | 1.67                     | 0.59              |
| 19:L:149:ASP:CG   | 19:L:152:THR:HB   | 2.28                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:L:264:ARG:HA   | 19:L:311:GLN:HE22 | 1.66                     | 0.59              |
| 28:U:66:TRP:CZ3   | 28:U:68:LEU:HB3   | 2.37                     | 0.59              |
| 33:Z:64:TYR:CD2   | 33:Z:111:LEU:CG   | 2.81                     | 0.59              |
| 33:Z:278:LEU:CD1  | 33:Z:297:VAL:HG13 | 2.32                     | 0.59              |
| 33:Z:279:THR:HG21 | 33:Z:977:ILE:HD13 | 1.83                     | 0.59              |
| 33:Z:303:ASP:C    | 33:Z:307:HIS:CD2  | 2.80                     | 0.59              |
| 1:1:4:VAL:HG11    | 1:1:49:ALA:HB3    | 1.83                     | 0.59              |
| 2:2:210:THR:OG1   | 3:3:160:GLN:NE2   | 2.35                     | 0.59              |
| 11:D:11:PHE:CE2   | 12:E:26:TYR:HB2   | 2.37                     | 0.59              |
| 13:F:12:THR:CG2   | 13:F:19:LEU:HD13  | 2.06                     | 0.59              |
| 18:K:177:LEU:HB2  | 18:K:181:LYS:HE3  | 1.85                     | 0.59              |
| 19:L:85:GLU:HA    | 20:M:58:MET:HE2   | 1.85                     | 0.59              |
| 20:M:253:GLN:HG3  | 20:M:258:GLU:CB   | 2.32                     | 0.59              |
| 21:N:43:LEU:HD21  | 21:N:69:TYR:HE1   | 1.66                     | 0.59              |
| 22:O:44:SER:OG    | 22:O:73:ILE:HG13  | 2.01                     | 0.59              |
| 22:O:59:LEU:CD2   | 22:O:85:SER:CB    | 2.76                     | 0.59              |
| 22:O:291:ILE:HD12 | 22:O:294:MET:HE2  | 1.85                     | 0.59              |
| 23:P:332:GLU:N    | 23:P:337:HIS:NE2  | 2.50                     | 0.59              |
| 23:P:391:ALA:O    | 24:Q:354:PHE:CD1  | 2.55                     | 0.59              |
| 28:U:67:PHE:CE1   | 30:W:97:THR:CB    | 2.85                     | 0.59              |
| 6:6:70:HIS:CD2    | 12:E:111:SER:HB2  | 2.38                     | 0.59              |
| 8:A:117:LEU:HD23  | 8:A:143:PHE:CD1   | 2.37                     | 0.59              |
| 17:J:329:ARG:HH12 | 17:J:333:ARG:NH1  | 2.01                     | 0.59              |
| 19:L:360:ILE:HG23 | 19:L:391:ILE:HG21 | 1.84                     | 0.59              |
| 22:O:266:PHE:CE1  | 22:O:280:LEU:HD21 | 2.38                     | 0.59              |
| 23:P:79:LEU:HD13  | 23:P:100:VAL:HG21 | 1.83                     | 0.59              |
| 24:Q:179:LEU:HD13 | 24:Q:218:LEU:HD23 | 1.83                     | 0.59              |
| 24:Q:190:ASN:ND2  | 24:Q:193:LYS:HD2  | 2.18                     | 0.59              |
| 25:R:70:TYR:O     | 25:R:70:TYR:CD2   | 2.55                     | 0.59              |
| 28:U:37:ILE:HG23  | 28:U:93:TYR:HD2   | 1.66                     | 0.59              |
| 7:7:163:GLN:O     | 7:7:167:GLU:HG3   | 2.03                     | 0.59              |
| 10:C:162:ALA:HB1  | 10:C:176:LEU:HD21 | 1.83                     | 0.59              |
| 12:E:165:TYR:HB3  | 12:E:167:TYR:CZ   | 2.38                     | 0.59              |
| 15:H:50:LYS:HZ1   | 33:Z:791:LYS:HG2  | 1.67                     | 0.59              |
| 21:N:302:PHE:CE2  | 21:N:757:THR:HB   | 2.37                     | 0.59              |
| 21:N:371:LEU:O    | 21:N:375:HIS:ND1  | 2.18                     | 0.59              |
| 21:N:406:TYR:HD1  | 21:N:448:LEU:HB2  | 1.66                     | 0.59              |
| 21:N:470:LEU:HD11 | 21:N:485:MET:HE1  | 1.85                     | 0.59              |
| 24:Q:83:GLU:HA    | 24:Q:86:MET:CG    | 2.33                     | 0.59              |
| 33:Z:74:SER:HB2   | 33:Z:79:THR:CG2   | 2.25                     | 0.59              |
| 33:Z:748:LEU:CG   | 33:Z:783:VAL:HA   | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:193:TYR:CD1   | 1:1:194:GLU:N     | 2.71                     | 0.59              |
| 2:2:8:PHE:CZ      | 2:2:11:GLY:N      | 2.68                     | 0.59              |
| 10:C:42:ASP:HA    | 10:C:218:LYS:NZ   | 2.17                     | 0.59              |
| 21:N:394:ARG:HG2  | 21:N:395:ALA:O    | 2.03                     | 0.59              |
| 25:R:65:TYR:O     | 25:R:69:GLU:HG2   | 2.03                     | 0.59              |
| 25:R:73:ASN:H     | 25:R:76:GLN:HE21  | 1.50                     | 0.59              |
| 28:U:100:ARG:N    | 28:U:103:ASP:OD2  | 2.35                     | 0.59              |
| 29:V:127:LYS:HE3  | 29:V:194:ARG:CD   | 2.32                     | 0.59              |
| 1:1:14:LEU:CG     | 1:1:100:ALA:CB    | 2.80                     | 0.59              |
| 1:1:174:ARG:HH12  | 1:1:185:ARG:NH2   | 1.98                     | 0.59              |
| 8:A:13:ASP:OD1    | 8:A:14:ARG:HG3    | 2.02                     | 0.59              |
| 8:A:64:LEU:HD13   | 14:G:157:TRP:HD1  | 1.66                     | 0.59              |
| 15:H:334:LEU:HD13 | 20:M:285:ALA:HB2  | 1.84                     | 0.59              |
| 16:I:76:VAL:HG12  | 33:Z:621:LEU:HD13 | 1.85                     | 0.59              |
| 16:I:205:PRO:O    | 16:I:208:TYR:CD2  | 2.56                     | 0.59              |
| 17:J:214:SER:CB   | 17:J:217:GLU:OE1  | 2.51                     | 0.59              |
| 18:K:239:GLY:HA2  | 18:K:242:PHE:CE2  | 2.38                     | 0.59              |
| 21:N:490:LEU:HD21 | 21:N:526:TYR:CG   | 2.37                     | 0.59              |
| 21:N:656:ALA:O    | 21:N:660:LEU:HG   | 2.02                     | 0.59              |
| 22:O:199:LEU:HD11 | 22:O:204:SER:O    | 2.03                     | 0.59              |
| 25:R:170:VAL:CG1  | 25:R:194:VAL:CG2  | 2.80                     | 0.59              |
| 26:S:461:PHE:CE2  | 28:U:274:MET:CA   | 2.78                     | 0.59              |
| 31:X:47:ASP:OD1   | 31:X:67:ILE:HG22  | 2.02                     | 0.59              |
| 31:X:79:LYS:HE2   | 31:X:98:PHE:CZ    | 2.28                     | 0.59              |
| 33:Z:50:GLU:OE2   | 33:Z:55:ARG:CZ    | 2.48                     | 0.59              |
| 33:Z:138:ARG:NH2  | 33:Z:157:LEU:CG   | 2.63                     | 0.59              |
| 5:5:40:PHE:CB     | 5:5:73:ARG:HH21   | 2.13                     | 0.58              |
| 5:5:185:TRP:HZ3   | 5:5:187:TYR:HB3   | 1.68                     | 0.58              |
| 12:E:221:CYS:N    | 12:E:231:TYR:CE1  | 2.71                     | 0.58              |
| 13:F:91:GLN:NE2   | 13:F:108:ALA:HA   | 2.18                     | 0.58              |
| 21:N:315:ASN:HA   | 21:N:318:LYS:HZ2  | 1.68                     | 0.58              |
| 26:S:242:LEU:HD21 | 26:S:279:ILE:CG1  | 2.33                     | 0.58              |
| 11:D:96:HIS:CD2   | 11:D:100:LEU:HD22 | 2.38                     | 0.58              |
| 12:E:165:TYR:HB3  | 12:E:167:TYR:CE1  | 2.36                     | 0.58              |
| 13:F:84:LEU:CD1   | 13:F:112:LEU:HD22 | 2.33                     | 0.58              |
| 25:R:154:LEU:CD1  | 25:R:173:THR:OG1  | 2.52                     | 0.58              |
| 25:R:167:LYS:NZ   | 25:R:199:GLU:HG2  | 2.17                     | 0.58              |
| 33:Z:241:THR:HG22 | 33:Z:244:ARG:H    | 1.69                     | 0.58              |
| 3:3:-2:ASN:HD21   | 3:3:48:ALA:H      | 1.49                     | 0.58              |
| 15:H:217:GLN:HE21 | 15:H:248:LEU:HD13 | 1.68                     | 0.58              |
| 27:T:63:GLU:OE2   | 27:T:89:TYR:OH    | 2.19                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:923:ILE:CD1  | 33:Z:985:LYS:HE2  | 2.25                     | 0.58              |
| 4:4:102:LEU:HD21  | 4:4:132:HIS:NE2   | 2.19                     | 0.58              |
| 11:D:193:LYS:HE3  | 11:D:197:ARG:NH2  | 2.17                     | 0.58              |
| 11:D:193:LYS:CG   | 11:D:197:ARG:NH1  | 2.63                     | 0.58              |
| 15:H:284:VAL:CA   | 20:M:254:MET:HB3  | 2.32                     | 0.58              |
| 16:I:96:LEU:O     | 16:I:100:ARG:HG3  | 2.03                     | 0.58              |
| 18:K:227:ALA:CB   | 18:K:268:ILE:HD12 | 2.34                     | 0.58              |
| 18:K:280:LYS:HE3  | 18:K:296:LEU:HD22 | 1.86                     | 0.58              |
| 19:L:163:THR:HG21 | 19:L:264:ARG:HH22 | 1.68                     | 0.58              |
| 19:L:389:ALA:HB2  | 20:M:339:ARG:HH21 | 1.69                     | 0.58              |
| 22:O:325:GLU:HB3  | 23:P:364:ARG:NH2  | 2.19                     | 0.58              |
| 33:Z:188:ALA:CA   | 33:Z:201:LEU:HD11 | 2.33                     | 0.58              |
| 33:Z:286:VAL:O    | 33:Z:287:ARG:HB2  | 2.01                     | 0.58              |
| 33:Z:522:THR:HG23 | 33:Z:559:LYS:NZ   | 2.19                     | 0.58              |
| 5:5:159:ARG:NH1   | 5:5:200:VAL:HA    | 2.13                     | 0.58              |
| 6:6:-5:TYR:CE1    | 6:6:97:TYR:CG     | 2.92                     | 0.58              |
| 6:6:66:TYR:CD2    | 6:6:73:LYS:O      | 2.56                     | 0.58              |
| 8:A:148:GLU:OE1   | 8:A:230:LYS:HE2   | 2.03                     | 0.58              |
| 12:E:138:PHE:HB3  | 12:E:140:VAL:HG12 | 1.86                     | 0.58              |
| 14:G:168:ARG:CG   | 14:G:172:LYS:HE3  | 2.33                     | 0.58              |
| 22:O:250:TRP:HZ2  | 22:O:271:LYS:CB   | 2.17                     | 0.58              |
| 23:P:263:HIS:HE1  | 23:P:325:ASP:HA   | 1.67                     | 0.58              |
| 25:R:167:LYS:NZ   | 25:R:198:ILE:HB   | 2.18                     | 0.58              |
| 25:R:237:THR:C    | 25:R:246:TYR:CE1  | 2.82                     | 0.58              |
| 1:1:3:ILE:HG13    | 1:1:98:ILE:HD12   | 1.85                     | 0.58              |
| 8:A:252:ASP:C     | 23:P:44:LYS:HZ3   | 2.04                     | 0.58              |
| 9:B:159:TRP:CZ2   | 10:C:57:LEU:HD13  | 2.39                     | 0.58              |
| 9:B:159:TRP:HZ3   | 10:C:54:SER:HB2   | 1.69                     | 0.58              |
| 12:E:198:LEU:CD1  | 12:E:243:LEU:HD13 | 2.33                     | 0.58              |
| 12:E:198:LEU:HD11 | 12:E:243:LEU:HD13 | 1.85                     | 0.58              |
| 13:F:145:LEU:HD21 | 13:F:153:VAL:HG13 | 1.84                     | 0.58              |
| 14:G:215:ILE:HG22 | 14:G:235:LEU:HD13 | 1.85                     | 0.58              |
| 16:I:126:PRO:HB2  | 16:I:128:TYR:HE2  | 1.54                     | 0.58              |
| 24:Q:179:LEU:HD21 | 24:Q:217:GLU:HB3  | 1.84                     | 0.58              |
| 24:Q:299:MET:HE3  | 24:Q:335:PHE:HZ   | 1.67                     | 0.58              |
| 24:Q:343:LEU:HD11 | 24:Q:368:LEU:CD1  | 2.30                     | 0.58              |
| 25:R:258:LEU:CD1  | 25:R:288:SER:HB2  | 2.32                     | 0.58              |
| 26:S:188:TYR:HE2  | 26:S:239:ARG:NH1  | 1.94                     | 0.58              |
| 28:U:280:ASN:HB2  | 29:V:291:ASN:OD1  | 2.03                     | 0.58              |
| 31:X:10:PHE:HE2   | 31:X:101:LEU:CD1  | 2.17                     | 0.58              |
| 8:A:34:ALA:O      | 8:A:35:THR:HG23   | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:98:TYR:HE1   | 10:C:104:GLU:HG3  | 1.68                     | 0.58              |
| 14:G:53:ILE:CD1   | 14:G:212:GLU:HB2  | 2.29                     | 0.58              |
| 15:H:105:ILE:HD12 | 15:H:169:GLU:OE2  | 2.03                     | 0.58              |
| 17:J:370:LEU:HD23 | 17:J:370:LEU:C    | 2.29                     | 0.58              |
| 26:S:322:LEU:HD21 | 26:S:349:THR:HG23 | 1.85                     | 0.58              |
| 27:T:266:TYR:C    | 27:T:266:TYR:CD1  | 2.82                     | 0.58              |
| 28:U:293:GLU:HG2  | 29:V:277:LYS:NZ   | 2.19                     | 0.58              |
| 3:3:177:VAL:HG12  | 3:3:190:TYR:CE1   | 2.38                     | 0.58              |
| 6:6:141:LEU:HD12  | 6:6:145:VAL:CG2   | 2.34                     | 0.58              |
| 7:7:129:TYR:CE1   | 7:7:134:LEU:CD2   | 2.69                     | 0.58              |
| 21:N:353:LEU:H    | 21:N:354:PRO:CD   | 2.17                     | 0.58              |
| 23:P:218:LEU:HD22 | 23:P:256:LYS:HZ2  | 1.69                     | 0.58              |
| 23:P:366:ASN:ND2  | 23:P:373:GLU:CA   | 2.60                     | 0.58              |
| 24:Q:146:TYR:CD1  | 24:Q:184:VAL:HA   | 2.33                     | 0.58              |
| 31:X:79:LYS:CD    | 31:X:98:PHE:HE2   | 2.16                     | 0.58              |
| 33:Z:278:LEU:CG   | 33:Z:297:VAL:HG13 | 2.34                     | 0.58              |
| 3:3:57:MET:HE2    | 3:3:89:ARG:HH21   | 1.69                     | 0.58              |
| 12:E:207:VAL:CA   | 15:H:409:ARG:HH12 | 2.17                     | 0.58              |
| 13:F:51:ARG:HD3   | 13:F:204:GLU:OE1  | 2.03                     | 0.58              |
| 15:H:102:CYS:HB3  | 15:H:105:ILE:HD13 | 1.86                     | 0.58              |
| 15:H:105:ILE:HG23 | 15:H:169:GLU:OE2  | 2.04                     | 0.58              |
| 22:O:250:TRP:HZ2  | 22:O:271:LYS:HB2  | 1.68                     | 0.58              |
| 24:Q:249:LEU:C    | 24:Q:250:THR:HG22 | 2.25                     | 0.58              |
| 25:R:283:THR:O    | 25:R:289:ILE:HD11 | 2.03                     | 0.58              |
| 8:A:163:TYR:C     | 8:A:164:VAL:HG13  | 2.28                     | 0.58              |
| 11:D:203:VAL:O    | 11:D:204:GLN:HB2  | 2.03                     | 0.58              |
| 12:E:31:ILE:CD1   | 12:E:141:ALA:HB2  | 2.34                     | 0.58              |
| 12:E:207:VAL:HB   | 15:H:409:ARG:NH1  | 2.18                     | 0.58              |
| 13:F:18:ARG:NH1   | 13:F:23:GLU:HB2   | 2.18                     | 0.58              |
| 14:G:122:HIS:CE1  | 14:G:128:VAL:CG1  | 2.87                     | 0.58              |
| 15:H:74:THR:HG22  | 15:H:74:THR:O     | 2.04                     | 0.58              |
| 16:I:103:PRO:HG3  | 17:J:120:TYR:OH   | 2.03                     | 0.58              |
| 19:L:145:ARG:NH2  | 19:L:163:THR:HA   | 2.18                     | 0.58              |
| 20:M:203:ARG:HD3  | 20:M:206:LYS:CD   | 2.33                     | 0.58              |
| 20:M:203:ARG:HD3  | 20:M:206:LYS:NZ   | 2.19                     | 0.58              |
| 23:P:425:HIS:HA   | 28:U:228:LYS:NZ   | 2.18                     | 0.58              |
| 25:R:73:ASN:H     | 25:R:76:GLN:NE2   | 2.01                     | 0.58              |
| 25:R:107:GLU:CG   | 25:R:111:LYS:HE2  | 2.19                     | 0.58              |
| 26:S:234:ILE:O    | 26:S:238:LEU:HG   | 2.04                     | 0.58              |
| 26:S:416:GLU:O    | 26:S:417:GLN:NE2  | 2.37                     | 0.58              |
| 30:W:140:ASP:OD2  | 30:W:190:ILE:HD12 | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:X:67:ILE:HD12  | 31:X:69:ILE:CD1   | 2.29                     | 0.58              |
| 33:Z:242:PHE:CB   | 33:Z:275:GLN:HG3  | 2.34                     | 0.58              |
| 2:2:27:ALA:O      | 2:2:28:ASP:OD1    | 2.22                     | 0.57              |
| 4:4:66:TYR:CD2    | 10:C:102:TYR:OH   | 2.56                     | 0.57              |
| 6:6:68:PHE:HZ     | 13:F:67:ASP:HA    | 1.69                     | 0.57              |
| 8:A:91:ARG:HH21   | 14:G:113:ASP:CG   | 2.11                     | 0.57              |
| 15:H:206:VAL:HG23 | 15:H:261:ARG:HH21 | 1.69                     | 0.57              |
| 16:I:340:ARG:HH12 | 16:I:343:ARG:HG2  | 1.67                     | 0.57              |
| 17:J:212:ARG:CZ   | 17:J:246:PHE:CE2  | 2.88                     | 0.57              |
| 17:J:374:ARG:NH2  | 17:J:381:ASP:OD2  | 2.36                     | 0.57              |
| 20:M:119:VAL:HG11 | 20:M:155:ILE:CD1  | 2.31                     | 0.57              |
| 23:P:180:ILE:CG2  | 23:P:184:MET:HE3  | 2.34                     | 0.57              |
| 23:P:234:TYR:CE1  | 23:P:270:LEU:HD13 | 2.38                     | 0.57              |
| 23:P:264:ILE:CG2  | 23:P:280:LEU:HD11 | 2.34                     | 0.57              |
| 27:T:119:THR:CG2  | 27:T:123:HIS:HE1  | 2.12                     | 0.57              |
| 10:C:62:SER:OG    | 10:C:231:LYS:HD3  | 2.04                     | 0.57              |
| 13:F:50:LYS:HE3   | 13:F:212:SER:HB3  | 1.86                     | 0.57              |
| 14:G:11:ASN:HB2   | 14:G:126:ASN:HA   | 1.86                     | 0.57              |
| 15:H:294:LEU:HD12 | 15:H:297:MET:HE3  | 1.85                     | 0.57              |
| 15:H:357:ARG:CZ   | 15:H:359:ASN:HD22 | 2.17                     | 0.57              |
| 27:T:161:TRP:CE3  | 27:T:162:ASP:OD1  | 2.56                     | 0.57              |
| 33:Z:64:TYR:O     | 33:Z:68:LEU:HG    | 2.04                     | 0.57              |
| 33:Z:312:TYR:OH   | 33:Z:348:LEU:HD21 | 2.04                     | 0.57              |
| 33:Z:497:PHE:CB   | 33:Z:533:VAL:HG22 | 2.34                     | 0.57              |
| 2:2:50:ALA:CB     | 3:3:118:ILE:HG21  | 2.30                     | 0.57              |
| 2:2:59:ILE:HD11   | 2:2:86:HIS:CE1    | 2.40                     | 0.57              |
| 8:A:72:ILE:HG12   | 8:A:82:VAL:HG22   | 1.87                     | 0.57              |
| 10:C:123:THR:CG2  | 10:C:130:PRO:HB3  | 2.34                     | 0.57              |
| 16:I:136:VAL:HG11 | 16:I:159:VAL:HG12 | 1.86                     | 0.57              |
| 17:J:277:ASN:ND2  | 17:J:309:ARG:CZ   | 2.59                     | 0.57              |
| 19:L:117:TYR:HE1  | 19:L:131:VAL:HG11 | 1.68                     | 0.57              |
| 21:N:328:PHE:CZ   | 21:N:693:GLY:HA2  | 2.35                     | 0.57              |
| 22:O:4:ASN:HB2    | 22:O:39:PHE:CE1   | 2.39                     | 0.57              |
| 23:P:203:ILE:HG21 | 23:P:220:TYR:CZ   | 2.39                     | 0.57              |
| 27:T:164:LEU:HD21 | 27:T:178:THR:HA   | 1.86                     | 0.57              |
| 33:Z:321:PHE:CE1  | 33:Z:349:THR:HA   | 2.39                     | 0.57              |
| 33:Z:322:GLU:HG2  | 33:Z:464:ASP:CG   | 2.29                     | 0.57              |
| 8:A:52:VAL:HG11   | 8:A:203:VAL:HG22  | 1.87                     | 0.57              |
| 9:B:245:ASP:HA    | 24:Q:95:LYS:HD3   | 1.85                     | 0.57              |
| 16:I:102:ASN:HD21 | 17:J:97:ASP:H     | 1.52                     | 0.57              |
| 16:I:170:VAL:H    | 17:J:227:SER:HB3  | 1.70                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:395:MET:CE   | 16:I:420:LYS:HE2  | 2.34                     | 0.57              |
| 17:J:59:LYS:HG2   | 17:J:63:ARG:NH1   | 2.19                     | 0.57              |
| 17:J:115:LEU:HD13 | 17:J:122:LEU:HD23 | 1.86                     | 0.57              |
| 17:J:277:ASN:HD21 | 17:J:309:ARG:NH2  | 2.03                     | 0.57              |
| 17:J:316:PHE:CG   | 17:J:317:PRO:HD2  | 2.39                     | 0.57              |
| 27:T:151:TRP:HD1  | 27:T:154:GLU:OE2  | 1.88                     | 0.57              |
| 28:U:67:PHE:CZ    | 30:W:97:THR:CG2   | 2.86                     | 0.57              |
| 33:Z:99:LEU:CB    | 33:Z:119:LEU:HD21 | 2.34                     | 0.57              |
| 33:Z:748:LEU:CD1  | 33:Z:783:VAL:HA   | 2.34                     | 0.57              |
| 3:3:109:LYS:HE3   | 3:3:125:LYS:HZ3   | 1.69                     | 0.57              |
| 13:F:43:HIS:CD2   | 13:F:217:GLY:HA3  | 2.39                     | 0.57              |
| 17:J:369:ALA:HB1  | 17:J:374:ARG:HG3  | 1.86                     | 0.57              |
| 18:K:211:LEU:HD23 | 18:K:338:ILE:HB   | 1.85                     | 0.57              |
| 20:M:167:VAL:HG11 | 20:M:170:MET:HE3  | 1.87                     | 0.57              |
| 20:M:251:LEU:O    | 20:M:252:VAL:CA   | 2.36                     | 0.57              |
| 21:N:355:TRP:CH2  | 21:N:356:LEU:CD2  | 2.87                     | 0.57              |
| 24:Q:74:LEU:CD2   | 24:Q:104:PHE:HD1  | 2.15                     | 0.57              |
| 25:R:262:GLU:HA   | 25:R:336:LYS:HZ3  | 1.68                     | 0.57              |
| 28:U:54:LEU:HD23  | 28:U:72:TYR:CE2   | 2.39                     | 0.57              |
| 28:U:89:LEU:HD23  | 28:U:113:TYR:O    | 2.05                     | 0.57              |
| 6:6:39:ASP:O      | 6:6:40:ASN:CB     | 2.50                     | 0.57              |
| 9:B:158:PRO:O     | 10:C:57:LEU:HD12  | 2.05                     | 0.57              |
| 10:C:59:GLN:O     | 10:C:232:PRO:HG2  | 2.05                     | 0.57              |
| 11:D:120:TYR:CE2  | 11:D:129:PHE:CZ   | 2.93                     | 0.57              |
| 13:F:12:THR:HG21  | 13:F:19:LEU:HD11  | 1.85                     | 0.57              |
| 13:F:65:LYS:HE2   | 13:F:222:PHE:CD2  | 2.37                     | 0.57              |
| 15:H:244:LYS:HE3  | 15:H:340:LEU:O    | 2.04                     | 0.57              |
| 16:I:104:LEU:HD23 | 16:I:149:LEU:O    | 2.01                     | 0.57              |
| 18:K:216:GLY:HA3  | 19:L:342:ARG:HH21 | 1.68                     | 0.57              |
| 18:K:393:ARG:NH2  | 19:L:345:ARG:HH12 | 2.03                     | 0.57              |
| 19:L:401:PHE:HD1  | 19:L:404:ARG:CZ   | 2.16                     | 0.57              |
| 22:O:30:GLU:HB3   | 22:O:58:ARG:NH1   | 2.20                     | 0.57              |
| 22:O:228:TYR:HA   | 22:O:290:LYS:HZ3  | 1.67                     | 0.57              |
| 24:Q:6:SER:O      | 24:Q:10:GLU:HG3   | 2.04                     | 0.57              |
| 25:R:140:TYR:HD2  | 25:R:141:TYR:CD1  | 2.22                     | 0.57              |
| 26:S:151:GLU:OE1  | 26:S:154:GLN:HB2  | 2.04                     | 0.57              |
| 1:1:83:LYS:HZ3    | 1:1:118:SER:HA    | 0.77                     | 0.57              |
| 2:2:196:ARG:HH21  | 2:2:199:LYS:HD3   | 1.69                     | 0.57              |
| 3:3:42:LEU:HD21   | 3:3:44:ILE:HD11   | 1.86                     | 0.57              |
| 5:5:40:PHE:CG     | 5:5:73:ARG:NH2    | 2.73                     | 0.57              |
| 9:B:48:GLU:HG2    | 9:B:196:LEU:HD11  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:50:ARG:NH2   | 10:C:209:ASP:HA   | 2.19                     | 0.57              |
| 13:F:65:LYS:CB    | 13:F:222:PHE:CE2  | 2.87                     | 0.57              |
| 25:R:70:TYR:OH    | 25:R:76:GLN:CA    | 2.52                     | 0.57              |
| 1:1:30:VAL:CG2    | 1:1:172:VAL:HG21  | 2.35                     | 0.57              |
| 3:3:68:LYS:HG2    | 10:C:92:ARG:HH11  | 1.70                     | 0.57              |
| 5:5:162:LEU:CD2   | 5:5:200:VAL:HG21  | 2.34                     | 0.57              |
| 7:7:187:PHE:HE1   | 7:7:205:GLN:C     | 2.12                     | 0.57              |
| 8:A:41:ASN:OD1    | 8:A:173:PRO:HD2   | 2.05                     | 0.57              |
| 8:A:163:TYR:O     | 8:A:164:VAL:HG13  | 2.04                     | 0.57              |
| 19:L:165:PRO:HA   | 19:L:265:GLU:OE2  | 2.04                     | 0.57              |
| 21:N:331:ALA:HB2  | 21:N:697:PHE:CD1  | 2.39                     | 0.57              |
| 24:Q:148:LYS:O    | 24:Q:149:LYS:HB2  | 2.04                     | 0.57              |
| 24:Q:268:SER:O    | 24:Q:272:LEU:HG   | 2.04                     | 0.57              |
| 25:R:107:GLU:HG2  | 25:R:111:LYS:CE   | 2.21                     | 0.57              |
| 25:R:203:ASP:OD1  | 25:R:204:TRP:N    | 2.38                     | 0.57              |
| 28:U:21:HIS:CE1   | 28:U:93:TYR:CZ    | 2.92                     | 0.57              |
| 28:U:67:PHE:CE2   | 30:W:100:HIS:CE1  | 2.92                     | 0.57              |
| 31:X:90:VAL:HB    | 31:X:96:ARG:HD3   | 1.86                     | 0.57              |
| 33:Z:71:LEU:HD23  | 33:Z:118:VAL:HG11 | 1.85                     | 0.57              |
| 33:Z:321:PHE:CZ   | 33:Z:349:THR:HA   | 2.40                     | 0.57              |
| 1:1:75:THR:HG22   | 1:1:111:TYR:HD1   | 1.69                     | 0.57              |
| 10:C:140:TYR:HD1  | 10:C:146:TYR:CE1  | 2.23                     | 0.57              |
| 17:J:218:LEU:HD12 | 17:J:229:MET:HB3  | 1.86                     | 0.57              |
| 20:M:56:ASN:O     | 20:M:60:GLU:HG2   | 2.04                     | 0.57              |
| 21:N:31:VAL:CG2   | 21:N:35:LEU:HD12  | 2.34                     | 0.57              |
| 21:N:114:SER:HA   | 21:N:161:TYR:CE2  | 2.40                     | 0.57              |
| 21:N:593:PHE:HA   | 21:N:596:LEU:HG   | 1.86                     | 0.57              |
| 30:W:186:ALA:HB1  | 30:W:191:ILE:HG23 | 1.85                     | 0.57              |
| 31:X:14:VAL:HG13  | 31:X:50:TRP:CE2   | 2.39                     | 0.57              |
| 33:Z:75:ILE:CG2   | 33:Z:121:ILE:CG2  | 2.56                     | 0.57              |
| 7:7:131:SER:OG    | 7:7:132:PRO:HD2   | 2.04                     | 0.57              |
| 14:G:200:TYR:CZ   | 14:G:246:ILE:HG22 | 2.39                     | 0.57              |
| 17:J:166:LEU:C    | 17:J:174:PHE:CE1  | 2.83                     | 0.57              |
| 18:K:393:ARG:HH21 | 19:L:345:ARG:HH12 | 1.51                     | 0.57              |
| 21:N:657:MET:HB3  | 21:N:682:PHE:CE1  | 2.40                     | 0.57              |
| 21:N:717:LEU:O    | 21:N:725:LEU:HD22 | 2.04                     | 0.57              |
| 22:O:250:TRP:HA   | 22:O:269:LEU:HG   | 1.86                     | 0.57              |
| 25:R:50:VAL:HG12  | 25:R:54:ILE:HD12  | 1.84                     | 0.57              |
| 27:T:11:LEU:HD22  | 27:T:30:ILE:CD1   | 2.30                     | 0.57              |
| 1:1:-4:VAL:HG12   | 1:1:49:ALA:CB     | 2.35                     | 0.56              |
| 3:3:37:TYR:CZ     | 3:3:59:ARG:CB     | 2.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:6:29:ARG:HA     | 6:6:191:ASP:OD2   | 2.04                     | 0.56              |
| 6:6:85:GLN:HG3    | 6:6:122:TYR:CD1   | 2.35                     | 0.56              |
| 16:I:104:LEU:HD21 | 16:I:149:LEU:C    | 2.29                     | 0.56              |
| 16:I:246:ARG:HH21 | 17:J:274:GLU:HG2  | 1.70                     | 0.56              |
| 18:K:242:PHE:C    | 18:K:243:VAL:HA   | 2.30                     | 0.56              |
| 19:L:365:THR:OG1  | 19:L:376:PHE:CZ   | 2.57                     | 0.56              |
| 20:M:167:VAL:HG23 | 20:M:269:LEU:HD12 | 1.86                     | 0.56              |
| 20:M:203:ARG:NH1  | 20:M:206:LYS:NZ   | 2.53                     | 0.56              |
| 21:N:162:ARG:HE   | 21:N:164:ASP:HB3  | 1.70                     | 0.56              |
| 21:N:353:LEU:H    | 21:N:354:PRO:HD3  | 1.69                     | 0.56              |
| 22:O:250:TRP:CG   | 22:O:269:LEU:CD2  | 2.88                     | 0.56              |
| 25:R:335:ARG:HD3  | 25:R:376:GLN:HB3  | 1.84                     | 0.56              |
| 27:T:119:THR:HG23 | 27:T:123:HIS:CE1  | 2.38                     | 0.56              |
| 28:U:5:HIS:ND1    | 28:U:6:GLU:O      | 2.37                     | 0.56              |
| 33:Z:354:PRO:O    | 33:Z:357:ILE:HG12 | 2.05                     | 0.56              |
| 33:Z:612:GLY:N    | 33:Z:746:ILE:HG23 | 2.20                     | 0.56              |
| 1:1:5:ALA:HB2     | 1:1:14:LEU:HG     | 1.87                     | 0.56              |
| 1:1:12:VAL:HG22   | 1:1:14:LEU:HD12   | 1.86                     | 0.56              |
| 1:1:83:LYS:NZ     | 1:1:117:GLY:O     | 2.38                     | 0.56              |
| 1:1:173:ILE:HD12  | 1:1:193:TYR:CB    | 2.35                     | 0.56              |
| 15:H:97:LEU:HB2   | 15:H:173:ARG:HD3  | 1.86                     | 0.56              |
| 15:H:152:ILE:HB   | 16:I:125:MET:HE1  | 1.86                     | 0.56              |
| 17:J:25:GLN:NE2   | 21:N:99:GLU:HB3   | 2.20                     | 0.56              |
| 17:J:218:LEU:HD11 | 17:J:229:MET:C    | 2.30                     | 0.56              |
| 20:M:290:ARG:CD   | 20:M:294:GLU:HB3  | 2.31                     | 0.56              |
| 22:O:260:VAL:HG11 | 22:O:262:ASP:OD2  | 2.05                     | 0.56              |
| 23:P:288:ASN:O    | 23:P:289:ASN:HB2  | 2.06                     | 0.56              |
| 25:R:170:VAL:HG11 | 25:R:194:VAL:CG2  | 2.35                     | 0.56              |
| 28:U:83:ILE:HD11  | 29:V:87:PHE:HZ    | 1.69                     | 0.56              |
| 33:Z:269:TYR:OH   | 33:Z:293:MET:HB3  | 2.04                     | 0.56              |
| 1:1:10:ASP:O      | 1:1:102:TYR:HE1   | 1.87                     | 0.56              |
| 1:1:11:GLY:HA3    | 1:1:102:TYR:CD1   | 2.41                     | 0.56              |
| 1:1:13:ILE:HD12   | 1:1:151:THR:CG2   | 2.35                     | 0.56              |
| 1:1:82:PHE:CB     | 1:1:113:ILE:HD13  | 2.36                     | 0.56              |
| 1:1:83:LYS:CD     | 1:1:119:VAL:CG2   | 2.69                     | 0.56              |
| 3:3:53:THR:O      | 3:3:57:MET:HG2    | 2.06                     | 0.56              |
| 5:5:7:ARG:HE      | 5:5:110:PRO:HG2   | 1.69                     | 0.56              |
| 11:D:67:ILE:HD13  | 11:D:109:LEU:HD21 | 1.86                     | 0.56              |
| 12:E:14:THR:HG21  | 12:E:22:PHE:HE2   | 1.69                     | 0.56              |
| 13:F:87:TYR:HE2   | 13:F:128:TYR:OH   | 1.88                     | 0.56              |
| 14:G:111:PHE:HA   | 14:G:114:ARG:CZ   | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:62:ARG:HB2   | 16:I:134:SER:HB2  | 1.86                     | 0.56              |
| 16:I:257:LEU:HD12 | 16:I:258:GLY:N    | 2.21                     | 0.56              |
| 17:J:367:MET:O    | 17:J:371:ARG:HG3  | 2.05                     | 0.56              |
| 19:L:82:ARG:HG2   | 19:L:86:LYS:HE3   | 1.86                     | 0.56              |
| 21:N:602:VAL:CG1  | 21:N:625:LEU:HD23 | 2.36                     | 0.56              |
| 22:O:30:GLU:CD    | 22:O:58:ARG:NH1   | 2.63                     | 0.56              |
| 22:O:131:SER:O    | 22:O:135:ARG:HG3  | 2.05                     | 0.56              |
| 22:O:222:LEU:HB3  | 22:O:280:LEU:HD11 | 1.87                     | 0.56              |
| 23:P:425:HIS:CB   | 28:U:228:LYS:HZ1  | 2.18                     | 0.56              |
| 24:Q:100:LEU:HD23 | 24:Q:103:LYS:HD2  | 1.87                     | 0.56              |
| 25:R:105:LYS:CE   | 25:R:109:LYS:HZ1  | 2.16                     | 0.56              |
| 25:R:134:TRP:CZ3  | 25:R:156:LYS:NZ   | 2.70                     | 0.56              |
| 25:R:137:LEU:CB   | 25:R:141:TYR:CE2  | 2.80                     | 0.56              |
| 25:R:167:LYS:HZ1  | 25:R:198:ILE:HB   | 1.70                     | 0.56              |
| 26:S:267:SER:OG   | 26:S:305:LYS:HE3  | 2.05                     | 0.56              |
| 27:T:28:PRO:HB2   | 27:T:29:PRO:HD3   | 1.88                     | 0.56              |
| 28:U:50:ASN:ND2   | 28:U:87:GLU:OE2   | 2.37                     | 0.56              |
| 29:V:53:MET:CG    | 29:V:108:TYR:HD1  | 2.19                     | 0.56              |
| 33:Z:64:TYR:CE1   | 33:Z:68:LEU:HD11  | 2.40                     | 0.56              |
| 33:Z:221:VAL:CG2  | 33:Z:245:VAL:HG13 | 2.34                     | 0.56              |
| 33:Z:320:SER:O    | 33:Z:326:VAL:HG11 | 2.05                     | 0.56              |
| 33:Z:912:PHE:CE2  | 33:Z:980:VAL:HG23 | 2.39                     | 0.56              |
| 33:Z:929:VAL:CG2  | 33:Z:957:LEU:HD23 | 2.35                     | 0.56              |
| 10:C:140:TYR:HD1  | 10:C:146:TYR:CD1  | 2.23                     | 0.56              |
| 10:C:177:GLN:HE22 | 11:D:52:LEU:HD22  | 1.70                     | 0.56              |
| 18:K:67:TYR:HD1   | 21:N:572:LEU:HB3  | 1.70                     | 0.56              |
| 19:L:214:PRO:HD2  | 19:L:216:LYS:HZ2  | 1.71                     | 0.56              |
| 20:M:170:MET:SD   | 20:M:244:LEU:HD22 | 2.45                     | 0.56              |
| 24:Q:61:LEU:HD11  | 24:Q:65:TYR:OH    | 2.06                     | 0.56              |
| 27:T:27:LEU:O     | 27:T:31:LYS:HG3   | 2.04                     | 0.56              |
| 27:T:62:LEU:HB2   | 27:T:85:LEU:HD13  | 1.87                     | 0.56              |
| 4:4:117:GLN:HE22  | 4:4:130:GLY:HA3   | 1.69                     | 0.56              |
| 5:5:144:TYR:O     | 5:5:145:LYS:HB2   | 2.05                     | 0.56              |
| 7:7:178:TYR:HD2   | 7:7:179:ARG:HG3   | 1.70                     | 0.56              |
| 8:A:162:TYR:CZ    | 8:A:164:VAL:CG1   | 2.88                     | 0.56              |
| 13:F:157:TYR:HH   | 14:G:59:VAL:HG23  | 1.70                     | 0.56              |
| 15:H:308:PHE:CD1  | 15:H:351:VAL:HG13 | 2.40                     | 0.56              |
| 15:H:428:MET:HG3  | 16:I:346:ARG:HH21 | 1.70                     | 0.56              |
| 19:L:386:PHE:HD1  | 19:L:390:ASP:HB3  | 1.70                     | 0.56              |
| 20:M:424:ALA:O    | 20:M:425:ARG:HB2  | 2.05                     | 0.56              |
| 24:Q:74:LEU:HD21  | 24:Q:104:PHE:HD1  | 1.69                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:81:SER:HA    | 24:Q:84:TYR:CD2   | 2.41                     | 0.56              |
| 24:Q:343:LEU:HD12 | 24:Q:366:ILE:HD11 | 1.88                     | 0.56              |
| 33:Z:463:HIS:HA   | 33:Z:466:GLU:CD   | 2.31                     | 0.56              |
| 33:Z:762:GLY:HA2  | 33:Z:765:MET:HE3  | 1.87                     | 0.56              |
| 3:3:1:GLY:HA3     | 3:3:33:LYS:NZ     | 2.20                     | 0.56              |
| 5:5:8:PHE:CZ      | 5:5:13:ILE:CG1    | 2.88                     | 0.56              |
| 5:5:35:ILE:HD11   | 5:5:45:MET:CE     | 2.22                     | 0.56              |
| 10:C:140:TYR:CD1  | 10:C:146:TYR:CE1  | 2.93                     | 0.56              |
| 13:F:87:TYR:CE2   | 13:F:128:TYR:OH   | 2.59                     | 0.56              |
| 15:H:50:LYS:NZ    | 33:Z:791:LYS:HG2  | 2.21                     | 0.56              |
| 15:H:249:TYR:HE2  | 15:H:374:LYS:HG2  | 1.70                     | 0.56              |
| 17:J:77:LYS:HG2   | 17:J:78:ILE:O     | 2.06                     | 0.56              |
| 17:J:96:VAL:HG11  | 17:J:115:LEU:HD21 | 1.87                     | 0.56              |
| 19:L:163:THR:CG2  | 19:L:264:ARG:HH22 | 2.19                     | 0.56              |
| 22:O:41:LEU:H     | 22:O:58:ARG:HD2   | 1.71                     | 0.56              |
| 23:P:431:HIS:CE1  | 28:U:137:TYR:HE1  | 2.24                     | 0.56              |
| 24:Q:220:LEU:HD12 | 24:Q:239:PHE:HE1  | 1.69                     | 0.56              |
| 25:R:137:LEU:HD22 | 25:R:141:TYR:CE2  | 2.41                     | 0.56              |
| 26:S:294:ILE:CG1  | 26:S:317:HIS:HE1  | 2.18                     | 0.56              |
| 33:Z:371:SER:O    | 33:Z:372:ALA:HB2  | 2.05                     | 0.56              |
| 5:5:158:LYS:HB2   | 5:5:177:LEU:HD11  | 1.87                     | 0.56              |
| 6:6:66:TYR:OH     | 6:6:73:LYS:CD     | 2.54                     | 0.56              |
| 12:E:85:ALA:HB2   | 12:E:140:VAL:HG21 | 1.88                     | 0.56              |
| 14:G:168:ARG:HG3  | 14:G:172:LYS:HE3  | 1.88                     | 0.56              |
| 16:I:81:ILE:HG12  | 33:Z:766:HIS:CE1  | 2.39                     | 0.56              |
| 20:M:82:VAL:HG21  | 20:M:140:LEU:HD22 | 1.87                     | 0.56              |
| 20:M:203:ARG:CZ   | 20:M:206:LYS:NZ   | 2.69                     | 0.56              |
| 21:N:315:ASN:CG   | 21:N:318:LYS:HZ2  | 2.11                     | 0.56              |
| 21:N:749:LEU:HD23 | 21:N:753:PHE:HZ   | 1.70                     | 0.56              |
| 24:Q:355:GLU:HG2  | 24:Q:397:LEU:HG   | 1.87                     | 0.56              |
| 27:T:185:ILE:HG22 | 27:T:189:ILE:CD1  | 2.35                     | 0.56              |
| 30:W:186:ALA:HA   | 30:W:191:ILE:HG22 | 0.65                     | 0.56              |
| 2:2:6:VAL:HG21    | 2:2:154:LEU:HD23  | 1.87                     | 0.56              |
| 3:3:150:GLU:HB3   | 3:3:151:PRO:HD2   | 1.88                     | 0.56              |
| 4:4:166:GLU:HB3   | 4:4:170:ARG:NH2   | 2.15                     | 0.56              |
| 8:A:75:ILE:HD13   | 8:A:117:LEU:CD2   | 2.36                     | 0.56              |
| 11:D:19:GLN:CD    | 11:D:128:PRO:CD   | 2.79                     | 0.56              |
| 15:H:173:ARG:NH2  | 16:I:119:ILE:HG21 | 2.21                     | 0.56              |
| 15:H:295:PHE:HZ   | 15:H:336:LEU:CD1  | 2.17                     | 0.56              |
| 16:I:326:MET:SD   | 16:I:344:ILE:HD11 | 2.46                     | 0.56              |
| 17:J:337:LEU:CD2  | 17:J:382:PHE:CZ   | 2.47                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:K:184:ILE:HD12 | 18:K:222:LEU:HD13 | 1.86                     | 0.56              |
| 22:O:217:LEU:CD1  | 22:O:238:ILE:HG21 | 2.35                     | 0.56              |
| 23:P:130:ILE:HG22 | 23:P:136:ARG:NH2  | 2.21                     | 0.56              |
| 23:P:131:PHE:CB   | 23:P:136:ARG:HH11 | 2.18                     | 0.56              |
| 23:P:269:VAL:O    | 23:P:344:ARG:HG3  | 2.06                     | 0.56              |
| 24:Q:9:GLU:HG2    | 24:Q:13:ARG:HH12  | 1.70                     | 0.56              |
| 26:S:218:LEU:C    | 26:S:256:LYS:HZ3  | 2.14                     | 0.56              |
| 27:T:253:GLU:O    | 27:T:254:ASP:CB   | 2.54                     | 0.56              |
| 30:W:12:ASN:H     | 30:W:55:ALA:HB3   | 1.70                     | 0.56              |
| 33:Z:317:GLN:HE22 | 33:Z:874:ASN:HA   | 1.71                     | 0.56              |
| 4:4:143:LEU:HD23  | 4:4:159:LEU:HD21  | 1.85                     | 0.56              |
| 8:A:83:VAL:HG22   | 8:A:141:LEU:HD22  | 1.87                     | 0.56              |
| 10:C:152:ASN:HB2  | 10:C:153:PRO:HD2  | 1.88                     | 0.56              |
| 13:F:105:VAL:CG2  | 13:F:145:LEU:HD13 | 2.21                     | 0.56              |
| 19:L:289:ARG:NH1  | 19:L:333:LEU:C    | 2.63                     | 0.56              |
| 21:N:220:CYS:SG   | 21:N:225:LEU:HD11 | 2.46                     | 0.56              |
| 28:U:62:ASN:ND2   | 28:U:65:VAL:HG23  | 2.21                     | 0.56              |
| 1:1:31:THR:HG21   | 1:1:33:LYS:HE2    | 1.87                     | 0.56              |
| 6:6:66:TYR:HH     | 6:6:73:LYS:HG2    | 1.71                     | 0.56              |
| 11:D:111:ARG:HG2  | 11:D:156:TYR:OH   | 2.06                     | 0.56              |
| 11:D:193:LYS:NZ   | 11:D:236:ILE:HG13 | 2.21                     | 0.56              |
| 15:H:328:GLU:HA   | 15:H:331:ARG:NH2  | 2.21                     | 0.56              |
| 17:J:316:PHE:CD1  | 17:J:317:PRO:HD2  | 2.41                     | 0.56              |
| 18:K:137:VAL:HB   | 18:K:146:LEU:HD13 | 1.87                     | 0.56              |
| 18:K:326:PRO:O    | 18:K:330:ARG:HG3  | 2.06                     | 0.56              |
| 20:M:62:ILE:HG13  | 20:M:66:LYS:HE3   | 1.87                     | 0.56              |
| 20:M:81:ASN:HB2   | 20:M:163:PHE:CD1  | 2.41                     | 0.56              |
| 22:O:179:PHE:HB3  | 22:O:188:PHE:HB2  | 1.86                     | 0.56              |
| 24:Q:385:ILE:HG22 | 24:Q:386:PHE:CE1  | 2.40                     | 0.56              |
| 25:R:252:TYR:CE1  | 25:R:319:CYS:SG   | 2.96                     | 0.56              |
| 27:T:86:LYS:CE    | 27:T:128:TYR:CD2  | 2.81                     | 0.56              |
| 27:T:194:GLU:HB2  | 27:T:226:TRP:HZ2  | 1.71                     | 0.56              |
| 31:X:94:ASN:O     | 31:X:95:GLU:HB2   | 2.05                     | 0.56              |
| 1:1:-8:LYS:HZ3    | 2:2:117:GLY:CA    | 2.08                     | 0.55              |
| 1:1:175:MET:HE1   | 1:1:188:PHE:CE1   | 2.41                     | 0.55              |
| 15:H:172:MET:C    | 16:I:129:TYR:CZ   | 2.71                     | 0.55              |
| 16:I:117:HIS:HB3  | 16:I:129:TYR:O    | 2.06                     | 0.55              |
| 16:I:222:TYR:OH   | 16:I:349:LEU:CB   | 2.43                     | 0.55              |
| 21:N:338:PHE:CZ   | 21:N:749:LEU:HD23 | 2.41                     | 0.55              |
| 21:N:777:ALA:HA   | 21:N:878:GLN:HE21 | 1.71                     | 0.55              |
| 22:O:15:ARG:HB3   | 30:W:20:ASP:OD1   | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:264:TYR:CZ   | 24:Q:330:LEU:HD23 | 2.41                     | 0.55              |
| 26:S:257:LEU:CD2  | 26:S:272:TYR:CE1  | 2.89                     | 0.55              |
| 26:S:258:GLU:O    | 26:S:259:TYR:CD1  | 2.59                     | 0.55              |
| 26:S:452:TYR:HA   | 26:S:456:ASP:OD2  | 2.05                     | 0.55              |
| 27:T:185:ILE:HG22 | 27:T:189:ILE:HD12 | 1.88                     | 0.55              |
| 27:T:247:ASP:CG   | 27:T:248:GLU:H    | 2.13                     | 0.55              |
| 29:V:266:LEU:HD23 | 29:V:266:LEU:C    | 2.30                     | 0.55              |
| 3:3:89:ARG:HB3    | 3:3:94:TYR:CD1    | 2.41                     | 0.55              |
| 3:3:109:LYS:HG2   | 3:3:110:PRO:O     | 2.07                     | 0.55              |
| 4:4:17:SER:HB3    | 4:4:33:LYS:CE     | 2.37                     | 0.55              |
| 6:6:-5:TYR:HE1    | 6:6:97:TYR:HB3    | 1.71                     | 0.55              |
| 8:A:19:PHE:HA     | 8:A:25:LEU:CD2    | 2.34                     | 0.55              |
| 13:F:101:ARG:CZ   | 13:F:103:LEU:HA   | 2.32                     | 0.55              |
| 13:F:201:LEU:C    | 13:F:202:ARG:HG3  | 2.30                     | 0.55              |
| 15:H:340:LEU:HD13 | 15:H:370:ARG:CG   | 2.25                     | 0.55              |
| 19:L:389:ALA:HB1  | 20:M:339:ARG:HE   | 1.72                     | 0.55              |
| 22:O:69:PHE:CE2   | 22:O:73:ILE:O     | 2.60                     | 0.55              |
| 24:Q:86:MET:SD    | 24:Q:93:THR:HG21  | 2.46                     | 0.55              |
| 24:Q:425:GLN:HB3  | 29:V:269:ARG:HG2  | 1.86                     | 0.55              |
| 25:R:137:LEU:O    | 25:R:141:TYR:HD2  | 1.85                     | 0.55              |
| 26:S:286:TYR:CE1  | 26:S:323:LEU:HD13 | 2.39                     | 0.55              |
| 28:U:52:PHE:CZ    | 28:U:76:MET:HE2   | 2.42                     | 0.55              |
| 33:Z:168:GLN:OE1  | 33:Z:195:PHE:CE1  | 2.59                     | 0.55              |
| 6:6:141:LEU:CD1   | 6:6:145:VAL:HG21  | 2.37                     | 0.55              |
| 8:A:75:ILE:HD13   | 8:A:117:LEU:HD21  | 1.87                     | 0.55              |
| 8:A:163:TYR:O     | 8:A:164:VAL:CG1   | 2.54                     | 0.55              |
| 10:C:65:LYS:HA    | 10:C:67:TYR:HE1   | 1.71                     | 0.55              |
| 11:D:146:LYS:HE2  | 11:D:148:TYR:HE2  | 1.71                     | 0.55              |
| 15:H:365:LEU:HD22 | 15:H:370:ARG:HH22 | 1.70                     | 0.55              |
| 17:J:166:LEU:C    | 17:J:174:PHE:CZ   | 2.85                     | 0.55              |
| 17:J:331:HIS:CE1  | 17:J:359:LYS:HE2  | 2.41                     | 0.55              |
| 21:N:308:ASN:HB2  | 21:N:711:ARG:HD2  | 1.88                     | 0.55              |
| 31:X:66:LEU:CD2   | 31:X:97:TYR:CD1   | 2.89                     | 0.55              |
| 33:Z:149:TRP:CD1  | 33:Z:214:HIS:CE1  | 2.95                     | 0.55              |
| 33:Z:553:ARG:NH1  | 33:Z:595:MET:CE   | 2.66                     | 0.55              |
| 33:Z:557:GLU:CD   | 33:Z:562:TRP:HZ3  | 2.13                     | 0.55              |
| 33:Z:973:TYR:HA   | 33:Z:984:LYS:HD3  | 1.88                     | 0.55              |
| 4:4:37:LEU:CD1    | 4:4:60:GLN:HA     | 2.37                     | 0.55              |
| 10:C:3:SER:CB     | 11:D:6:ARG:HH21   | 2.18                     | 0.55              |
| 12:E:15:PHE:HE1   | 13:F:126:ARG:HE   | 1.54                     | 0.55              |
| 13:F:117:GLN:HG3  | 13:F:121:GLN:NE2  | 2.21                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:343:PHE:HZ   | 20:M:233:ARG:NH2  | 2.04                     | 0.55              |
| 17:J:62:LEU:CD1   | 18:K:89:ILE:HG13  | 2.27                     | 0.55              |
| 17:J:219:VAL:HB   | 18:K:281:ARG:CG   | 2.36                     | 0.55              |
| 18:K:258:PHE:HB2  | 18:K:302:GLN:OE1  | 2.06                     | 0.55              |
| 23:P:416:SER:OG   | 29:V:245:VAL:HG22 | 2.07                     | 0.55              |
| 24:Q:426:LEU:CD2  | 28:U:293:GLU:OE1  | 2.53                     | 0.55              |
| 28:U:65:VAL:HG12  | 30:W:96:LEU:HD11  | 1.86                     | 0.55              |
| 4:4:17:SER:HB3    | 4:4:33:LYS:HE2    | 1.89                     | 0.55              |
| 11:D:193:LYS:HZ3  | 11:D:235:GLN:HB2  | 1.71                     | 0.55              |
| 16:I:377:LEU:O    | 16:I:381:VAL:HG23 | 2.06                     | 0.55              |
| 21:N:406:TYR:OH   | 21:N:748:PHE:HE1  | 1.76                     | 0.55              |
| 22:O:157:LEU:HD22 | 22:O:171:PHE:CG   | 2.41                     | 0.55              |
| 24:Q:167:LYS:O    | 24:Q:168:LEU:HD23 | 2.06                     | 0.55              |
| 25:R:354:ALA:HA   | 25:R:364:LEU:HD22 | 1.88                     | 0.55              |
| 26:S:323:LEU:CD2  | 26:S:383:LEU:HD23 | 2.37                     | 0.55              |
| 27:T:186:ARG:NH1  | 27:T:220:PHE:HE2  | 2.00                     | 0.55              |
| 30:W:25:ARG:NH1   | 30:W:144:PHE:CD2  | 2.61                     | 0.55              |
| 33:Z:205:LEU:HA   | 33:Z:236:PHE:CZ   | 2.41                     | 0.55              |
| 1:1:82:PHE:HB3    | 1:1:113:ILE:HD13  | 1.88                     | 0.55              |
| 7:7:8:TYR:CZ      | 7:7:11:GLY:HA3    | 2.41                     | 0.55              |
| 7:7:92:MET:CE     | 7:7:122:VAL:HG22  | 2.37                     | 0.55              |
| 9:B:75:TYR:CD1    | 9:B:82:TYR:CD1    | 2.94                     | 0.55              |
| 10:C:136:ILE:HD11 | 10:C:165:VAL:CG2  | 2.36                     | 0.55              |
| 13:F:206:LEU:HD21 | 13:F:211:LEU:HD11 | 1.88                     | 0.55              |
| 18:K:258:PHE:HZ   | 18:K:299:LEU:CD1  | 2.19                     | 0.55              |
| 19:L:178:ILE:HD13 | 19:L:230:LEU:HD23 | 1.87                     | 0.55              |
| 21:N:43:LEU:HD11  | 21:N:69:TYR:CE1   | 2.42                     | 0.55              |
| 21:N:588:VAL:CG1  | 21:N:621:THR:CG2  | 2.57                     | 0.55              |
| 24:Q:74:LEU:HD21  | 24:Q:104:PHE:CD1  | 2.42                     | 0.55              |
| 28:U:283:ARG:NH1  | 29:V:291:ASN:CG   | 2.65                     | 0.55              |
| 33:Z:92:LEU:HD23  | 33:Z:122:LEU:HD13 | 1.88                     | 0.55              |
| 33:Z:301:THR:C    | 33:Z:307:HIS:CE1  | 2.84                     | 0.55              |
| 1:1:17:ASP:HB3    | 1:1:163:ILE:HD11  | 1.89                     | 0.55              |
| 2:2:99:ILE:HG12   | 2:2:127:LEU:HD12  | 1.88                     | 0.55              |
| 2:2:223:ILE:HG12  | 10:C:222:ASP:OD2  | 2.06                     | 0.55              |
| 6:6:91:LYS:CB     | 6:6:96:TYR:HE1    | 2.00                     | 0.55              |
| 11:D:17:ILE:CG2   | 11:D:19:GLN:HG2   | 2.36                     | 0.55              |
| 16:I:214:LYS:HZ2  | 16:I:318:ASP:CA   | 2.16                     | 0.55              |
| 17:J:27:ILE:HG21  | 18:K:50:LYS:HE2   | 1.87                     | 0.55              |
| 17:J:223:ILE:O    | 17:J:225:GLU:N    | 2.40                     | 0.55              |
| 19:L:117:TYR:HE1  | 19:L:131:VAL:CG1  | 2.19                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:L:145:ARG:NH2  | 19:L:163:THR:CA   | 2.68                     | 0.55              |
| 20:M:431:SER:O    | 20:M:432:PHE:CD1  | 2.59                     | 0.55              |
| 21:N:325:PHE:H    | 29:V:185:ILE:HG21 | 1.72                     | 0.55              |
| 21:N:749:LEU:CD2  | 21:N:753:PHE:HZ   | 2.19                     | 0.55              |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:HD21 | 1.71                     | 0.55              |
| 26:S:286:TYR:HB3  | 26:S:324:MET:HB3  | 1.89                     | 0.55              |
| 27:T:103:SER:HB3  | 27:T:141:LEU:HD12 | 1.89                     | 0.55              |
| 28:U:104:LEU:HD11 | 28:U:152:LYS:HD2  | 1.88                     | 0.55              |
| 29:V:127:LYS:HE3  | 29:V:194:ARG:CZ   | 2.37                     | 0.55              |
| 33:Z:850:LEU:HD23 | 33:Z:850:LEU:C    | 2.31                     | 0.55              |
| 12:E:68:VAL:HG12  | 12:E:93:ARG:HH21  | 1.71                     | 0.55              |
| 12:E:109:VAL:HG11 | 12:E:156:PHE:CD1  | 2.42                     | 0.55              |
| 13:F:47:VAL:HG21  | 13:F:193:GLY:HA3  | 1.89                     | 0.55              |
| 14:G:233:ASP:O    | 14:G:237:GLU:HG3  | 2.06                     | 0.55              |
| 15:H:345:PRO:HD2  | 15:H:349:ILE:HD12 | 1.87                     | 0.55              |
| 18:K:395:VAL:HG13 | 19:L:206:ILE:HG22 | 1.88                     | 0.55              |
| 20:M:216:LYS:HZ2  | 20:M:321:VAL:HB   | 1.72                     | 0.55              |
| 21:N:355:TRP:CZ3  | 21:N:356:LEU:HD23 | 2.41                     | 0.55              |
| 22:O:250:TRP:CZ2  | 22:O:271:LYS:HG3  | 2.41                     | 0.55              |
| 25:R:170:VAL:HG11 | 25:R:194:VAL:HG22 | 1.89                     | 0.55              |
| 28:U:83:ILE:HG22  | 28:U:84:ASN:ND2   | 2.22                     | 0.55              |
| 28:U:92:TRP:CE2   | 28:U:120:LEU:HG   | 2.41                     | 0.55              |
| 28:U:275:VAL:C    | 28:U:278:ILE:HG22 | 2.27                     | 0.55              |
| 33:Z:56:LEU:CD2   | 33:Z:68:LEU:CD2   | 2.79                     | 0.55              |
| 4:4:84:ARG:HD2    | 4:4:124:LYS:HB3   | 1.89                     | 0.55              |
| 6:6:1:GLY:C       | 6:6:46:ASN:HD21   | 2.15                     | 0.55              |
| 8:A:83:VAL:HG22   | 8:A:141:LEU:HD23  | 1.89                     | 0.55              |
| 13:F:159:THR:CA   | 13:F:169:LYS:HZ2  | 2.18                     | 0.55              |
| 15:H:326:ASP:HA   | 15:H:329:VAL:CG2  | 2.37                     | 0.55              |
| 16:I:174:ASP:CG   | 17:J:282:PHE:HB2  | 2.31                     | 0.55              |
| 20:M:385:GLU:O    | 20:M:385:GLU:OE1  | 2.25                     | 0.55              |
| 21:N:358:LYS:HD2  | 29:V:183:ALA:HA   | 1.88                     | 0.55              |
| 23:P:271:SER:O    | 23:P:344:ARG:CD   | 2.55                     | 0.55              |
| 23:P:344:ARG:NH2  | 23:P:347:GLU:CD   | 2.61                     | 0.55              |
| 25:R:167:LYS:HZ3  | 25:R:199:GLU:HG2  | 1.71                     | 0.55              |
| 25:R:251:THR:O    | 25:R:255:VAL:HG23 | 2.06                     | 0.55              |
| 28:U:83:ILE:HD11  | 29:V:87:PHE:CZ    | 2.41                     | 0.55              |
| 30:W:180:LEU:HD13 | 30:W:182:TYR:HE1  | 1.72                     | 0.55              |
| 33:Z:497:PHE:CZ   | 33:Z:505:VAL:HG12 | 2.41                     | 0.55              |
| 33:Z:549:ASN:HD22 | 33:Z:562:TRP:HH2  | 1.53                     | 0.55              |
| 33:Z:604:GLY:O    | 33:Z:608:TYR:CD2  | 2.57                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:75:THR:CG2    | 1:1:111:TYR:HD1   | 2.20                     | 0.55              |
| 8:A:128:TYR:CE1   | 8:A:134:MET:CE    | 2.90                     | 0.55              |
| 9:B:43:VAL:CG1    | 9:B:137:ALA:HB1   | 2.36                     | 0.55              |
| 10:C:13:PHE:HA    | 10:C:19:LEU:HD23  | 1.88                     | 0.55              |
| 16:I:340:ARG:HH12 | 16:I:343:ARG:CG   | 2.19                     | 0.55              |
| 17:J:33:LYS:O     | 17:J:37:LYS:HG2   | 2.07                     | 0.55              |
| 18:K:389:GLU:HB3  | 18:K:414:GLN:NE2  | 2.22                     | 0.55              |
| 19:L:115:GLU:HG2  | 19:L:137:ARG:NH2  | 2.21                     | 0.55              |
| 19:L:289:ARG:HD3  | 19:L:334:ASP:OD1  | 2.06                     | 0.55              |
| 21:N:302:PHE:CD1  | 21:N:306:ASN:ND2  | 2.75                     | 0.55              |
| 22:O:217:LEU:HD12 | 22:O:238:ILE:HG21 | 1.89                     | 0.55              |
| 27:T:112:ASN:HA   | 27:T:177:PHE:CE1  | 2.42                     | 0.55              |
| 33:Z:79:THR:O     | 33:Z:80:SER:CB    | 2.55                     | 0.55              |
| 33:Z:851:ALA:O    | 33:Z:855:LEU:HG   | 2.06                     | 0.55              |
| 15:H:69:VAL:HG21  | 16:I:133:LEU:HG   | 1.87                     | 0.54              |
| 15:H:172:MET:CG   | 16:I:129:TYR:HD2  | 2.06                     | 0.54              |
| 16:I:214:LYS:NZ   | 16:I:318:ASP:CA   | 2.70                     | 0.54              |
| 18:K:161:MET:CE   | 18:K:237:VAL:HG13 | 2.31                     | 0.54              |
| 21:N:16:ASN:HA    | 21:N:21:LYS:HZ1   | 1.72                     | 0.54              |
| 21:N:130:ASP:HB3  | 21:N:133:LEU:HD12 | 1.89                     | 0.54              |
| 21:N:717:LEU:HD21 | 21:N:733:LEU:HD13 | 1.88                     | 0.54              |
| 22:O:165:LEU:HD12 | 22:O:202:SER:HB3  | 1.90                     | 0.54              |
| 28:U:14:VAL:HG21  | 28:U:48:VAL:HG12  | 1.88                     | 0.54              |
| 33:Z:887:GLY:H    | 33:Z:893:PHE:HD2  | 1.55                     | 0.54              |
| 2:2:124:TYR:CZ    | 2:2:139:GLU:CB    | 2.87                     | 0.54              |
| 8:A:81:MET:SD     | 8:A:143:PHE:HE1   | 2.29                     | 0.54              |
| 9:B:151:ASP:HB3   | 9:B:152:PRO:HD2   | 1.88                     | 0.54              |
| 11:D:6:ARG:HA     | 12:E:125:GLU:OE1  | 2.08                     | 0.54              |
| 14:G:217:TRP:NE1  | 14:G:228:LYS:HB2  | 2.19                     | 0.54              |
| 15:H:208:TYR:CD1  | 15:H:211:VAL:CG1  | 2.90                     | 0.54              |
| 16:I:220:ILE:CG1  | 16:I:344:ILE:HG21 | 2.38                     | 0.54              |
| 17:J:156:GLN:HE22 | 17:J:314:ILE:HG21 | 1.72                     | 0.54              |
| 19:L:226:THR:HA   | 19:L:389:ALA:HB2  | 1.88                     | 0.54              |
| 20:M:253:GLN:CG   | 20:M:258:GLU:HB2  | 2.37                     | 0.54              |
| 21:N:16:ASN:O     | 21:N:17:GLN:CG    | 2.55                     | 0.54              |
| 22:O:117:ASN:ND2  | 22:O:167:ILE:HA   | 2.22                     | 0.54              |
| 22:O:250:TRP:CA   | 22:O:269:LEU:HD21 | 2.37                     | 0.54              |
| 23:P:105:LYS:HB2  | 23:P:115:ARG:NH1  | 2.22                     | 0.54              |
| 25:R:62:TYR:CE2   | 25:R:180:PHE:HB3  | 2.42                     | 0.54              |
| 28:U:52:PHE:CD2   | 28:U:72:TYR:CE2   | 2.88                     | 0.54              |
| 29:V:121:VAL:HG13 | 29:V:122:ASP:N    | 2.23                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:493:LEU:HD21 | 33:Z:497:PHE:CE2  | 2.42                     | 0.54              |
| 33:Z:550:PHE:CE1  | 33:Z:566:LEU:HB2  | 2.42                     | 0.54              |
| 33:Z:867:PHE:O    | 33:Z:909:ARG:NH2  | 2.40                     | 0.54              |
| 1:1:75:THR:CG2    | 1:1:111:TYR:CD1   | 2.91                     | 0.54              |
| 4:4:106:TYR:CZ    | 4:4:185:LYS:CB    | 2.90                     | 0.54              |
| 5:5:8:PHE:HZ      | 5:5:13:ILE:HD11   | 1.70                     | 0.54              |
| 10:C:2:GLY:N      | 14:G:126:ASN:HD21 | 2.06                     | 0.54              |
| 14:G:199:ILE:HD13 | 14:G:213:LEU:HG   | 1.90                     | 0.54              |
| 17:J:212:ARG:CZ   | 17:J:246:PHE:HE2  | 2.19                     | 0.54              |
| 18:K:209:VAL:HG22 | 18:K:336:ARG:HB2  | 1.88                     | 0.54              |
| 21:N:174:LEU:HD12 | 21:N:182:ASN:CG   | 2.33                     | 0.54              |
| 21:N:529:GLN:NE2  | 21:N:559:TYR:HA   | 2.21                     | 0.54              |
| 24:Q:322:GLU:HG3  | 24:Q:326:MET:HE2  | 1.88                     | 0.54              |
| 27:T:270:ILE:HD11 | 29:V:288:LEU:HD21 | 1.88                     | 0.54              |
| 33:Z:102:ILE:CG2  | 33:Z:115:LEU:HD13 | 2.38                     | 0.54              |
| 1:1:83:LYS:HZ2    | 1:1:117:GLY:C     | 2.15                     | 0.54              |
| 3:3:1:GLY:HA3     | 3:3:33:LYS:HZ3    | 1.71                     | 0.54              |
| 4:4:13:ILE:HG12   | 4:4:182:ILE:HG12  | 1.88                     | 0.54              |
| 7:7:41:THR:HG21   | 7:7:84:ILE:HD12   | 1.90                     | 0.54              |
| 7:7:48:ASP:OD1    | 7:7:50:SER:HB2    | 2.08                     | 0.54              |
| 8:A:128:TYR:CZ    | 8:A:134:MET:HE2   | 2.41                     | 0.54              |
| 13:F:101:ARG:HH22 | 13:F:103:LEU:HD13 | 1.72                     | 0.54              |
| 16:I:220:ILE:HD11 | 16:I:344:ILE:HD13 | 1.90                     | 0.54              |
| 17:J:186:ILE:HD11 | 17:J:300:LEU:HD11 | 1.89                     | 0.54              |
| 17:J:305:LEU:HB3  | 17:J:313:LYS:HE2  | 1.87                     | 0.54              |
| 21:N:158:LEU:HD12 | 21:N:202:PHE:CE2  | 2.38                     | 0.54              |
| 21:N:649:VAL:HG11 | 21:N:651:PHE:CE2  | 2.42                     | 0.54              |
| 21:N:720:ALA:O    | 21:N:721:ASP:CG   | 2.50                     | 0.54              |
| 21:N:919:THR:CG2  | 21:N:921:ARG:HG2  | 2.36                     | 0.54              |
| 22:O:167:ILE:HG23 | 22:O:168:THR:N    | 2.22                     | 0.54              |
| 29:V:71:MET:HA    | 29:V:87:PHE:CE2   | 2.42                     | 0.54              |
| 33:Z:562:TRP:CD2  | 33:Z:566:LEU:CD1  | 2.87                     | 0.54              |
| 33:Z:812:ILE:HD11 | 33:Z:834:LEU:HD22 | 1.89                     | 0.54              |
| 1:1:57:ASP:CB     | 8:A:106:TYR:HE1   | 2.17                     | 0.54              |
| 3:3:19:ARG:NH2    | 3:3:171:LEU:HD23  | 2.22                     | 0.54              |
| 8:A:75:ILE:HD11   | 8:A:81:MET:HB2    | 1.89                     | 0.54              |
| 9:B:174:PHE:HB3   | 9:B:178:ARG:HH22  | 1.71                     | 0.54              |
| 11:D:138:PHE:HE1  | 11:D:215:VAL:HG12 | 1.72                     | 0.54              |
| 14:G:122:HIS:CE1  | 14:G:128:VAL:HG11 | 2.42                     | 0.54              |
| 21:N:736:PHE:CD1  | 21:N:749:LEU:HB2  | 2.43                     | 0.54              |
| 22:O:40:GLN:NE2   | 22:O:55:THR:O     | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:509:LEU:HD13 | 33:Z:530:LEU:HD23 | 1.88                     | 0.54              |
| 33:Z:957:LEU:C    | 33:Z:957:LEU:HD12 | 2.32                     | 0.54              |
| 4:4:8:VAL:CG2     | 4:4:11:SER:OG     | 2.55                     | 0.54              |
| 5:5:76:VAL:HG21   | 5:5:103:GLY:HA3   | 1.90                     | 0.54              |
| 7:7:8:TYR:CE2     | 7:7:10:ASN:C      | 2.85                     | 0.54              |
| 11:D:17:ILE:HG22  | 11:D:19:GLN:HG2   | 1.90                     | 0.54              |
| 11:D:82:SER:OG    | 11:D:131:VAL:HG11 | 2.08                     | 0.54              |
| 12:E:165:TYR:HB2  | 12:E:167:TYR:HH   | 1.70                     | 0.54              |
| 18:K:84:GLU:O     | 18:K:88:ARG:HG3   | 2.08                     | 0.54              |
| 19:L:113:SER:OG   | 19:L:116:LYS:HB2  | 2.08                     | 0.54              |
| 21:N:654:GLN:HG3  | 21:N:698:GLY:CA   | 2.37                     | 0.54              |
| 24:Q:353:PRO:C    | 24:Q:354:PHE:CD1  | 2.86                     | 0.54              |
| 31:X:29:VAL:HG21  | 31:X:59:ARG:HH12  | 1.72                     | 0.54              |
| 33:Z:168:GLN:CD   | 33:Z:195:PHE:CE1  | 2.86                     | 0.54              |
| 33:Z:385:PHE:HE2  | 33:Z:389:PHE:HE2  | 1.48                     | 0.54              |
| 1:1:89:ASN:HB3    | 1:1:92:ASN:OD1    | 2.07                     | 0.54              |
| 3:3:59:ARG:HH21   | 10:C:100:LYS:HA   | 1.71                     | 0.54              |
| 3:3:63:ASN:CB     | 10:C:96:GLN:HE22  | 2.20                     | 0.54              |
| 5:5:6:PHE:CZ      | 5:5:13:ILE:CB     | 2.89                     | 0.54              |
| 5:5:174:SER:CB    | 5:5:190:ASN:HD21  | 2.21                     | 0.54              |
| 6:6:31:GLU:CD     | 7:7:129:TYR:HA    | 2.33                     | 0.54              |
| 6:6:68:PHE:CZ     | 13:F:66:CYS:O     | 2.61                     | 0.54              |
| 7:7:103:TRP:CE3   | 7:7:124:LEU:HD22  | 2.43                     | 0.54              |
| 8:A:57:LYS:NZ     | 8:A:66:PRO:HB2    | 2.23                     | 0.54              |
| 11:D:37:LYS:CE    | 11:D:160:SER:HA   | 2.38                     | 0.54              |
| 11:D:159:TRP:CZ2  | 12:E:59:LEU:CD1   | 2.89                     | 0.54              |
| 16:I:253:ILE:CD1  | 16:I:287:ILE:HA   | 2.37                     | 0.54              |
| 17:J:338:THR:HA   | 17:J:376:HIS:NE2  | 2.22                     | 0.54              |
| 21:N:77:SER:O     | 21:N:81:TYR:CD1   | 2.52                     | 0.54              |
| 21:N:363:ALA:HB2  | 29:V:182:LYS:NZ   | 2.23                     | 0.54              |
| 21:N:641:LEU:CD1  | 21:N:660:LEU:HD23 | 2.36                     | 0.54              |
| 22:O:30:GLU:CD    | 22:O:58:ARG:HH11  | 2.14                     | 0.54              |
| 22:O:384:MET:CE   | 28:U:190:LEU:N    | 2.70                     | 0.54              |
| 25:R:259:PHE:HE1  | 25:R:332:GLU:HB2  | 1.72                     | 0.54              |
| 27:T:50:ILE:HD13  | 27:T:96:LEU:HB3   | 1.88                     | 0.54              |
| 32:Y:82:ASP:O     | 32:Y:86:ARG:HG3   | 2.07                     | 0.54              |
| 33:Z:223:LEU:O    | 33:Z:227:ILE:HG23 | 2.08                     | 0.54              |
| 33:Z:318:LYS:HB2  | 33:Z:874:ASN:HD21 | 1.72                     | 0.54              |
| 33:Z:557:GLU:OE1  | 33:Z:562:TRP:HZ3  | 1.86                     | 0.54              |
| 33:Z:774:ARG:O    | 33:Z:777:PRO:HD2  | 2.07                     | 0.54              |
| 1:1:70:TYR:CD1    | 14:G:110:ALA:CB   | 2.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:32:ASP:CB     | 4:4:35:ARG:HH12   | 2.18                     | 0.54              |
| 14:G:111:PHE:CB   | 14:G:114:ARG:NH2  | 2.71                     | 0.54              |
| 14:G:192:VAL:HG13 | 14:G:215:ILE:CD1  | 2.33                     | 0.54              |
| 15:H:306:ILE:HG21 | 15:H:308:PHE:CE1  | 2.39                     | 0.54              |
| 23:P:130:ILE:O    | 23:P:136:ARG:CZ   | 2.55                     | 0.54              |
| 24:Q:50:ARG:NH2   | 24:Q:53:GLU:OE1   | 2.41                     | 0.54              |
| 24:Q:419:LEU:HD22 | 28:U:289:ASP:OD2  | 2.08                     | 0.54              |
| 25:R:276:LEU:O    | 25:R:280:ILE:HG23 | 2.07                     | 0.54              |
| 26:S:256:LYS:O    | 26:S:259:TYR:CD1  | 2.61                     | 0.54              |
| 27:T:126:LEU:CD2  | 27:T:136:LEU:CD2  | 2.79                     | 0.54              |
| 33:Z:119:LEU:HD13 | 33:Z:137:TYR:CE2  | 2.43                     | 0.54              |
| 33:Z:286:VAL:HG11 | 33:Z:317:GLN:HG2  | 1.89                     | 0.54              |
| 33:Z:601:VAL:HB   | 33:Z:620:LEU:HD23 | 1.90                     | 0.54              |
| 2:2:59:ILE:HD12   | 2:2:82:MET:CB     | 2.37                     | 0.54              |
| 2:2:109:HIS:HB3   | 2:2:111:PHE:CE2   | 2.43                     | 0.54              |
| 2:2:124:TYR:CZ    | 2:2:139:GLU:CA    | 2.90                     | 0.54              |
| 3:3:57:MET:HE2    | 3:3:89:ARG:HH22   | 1.72                     | 0.54              |
| 11:D:10:ILE:CD1   | 12:E:10:ARG:HB3   | 2.38                     | 0.54              |
| 12:E:20:ARG:CG    | 20:M:432:PHE:HZ   | 2.20                     | 0.54              |
| 15:H:344:ASP:OD1  | 15:H:345:PRO:HD2  | 2.08                     | 0.54              |
| 17:J:363:THR:OG1  | 18:K:203:ILE:HD11 | 2.08                     | 0.54              |
| 17:J:377:VAL:HG12 | 17:J:378:THR:N    | 2.23                     | 0.54              |
| 18:K:126:LEU:HD22 | 18:K:149:ILE:HD12 | 1.90                     | 0.54              |
| 21:N:909:GLU:HB3  | 21:N:911:LYS:HZ3  | 1.73                     | 0.54              |
| 22:O:215:TYR:CZ   | 22:O:219:ILE:HD11 | 2.43                     | 0.54              |
| 23:P:72:TRP:CZ2   | 23:P:103:TYR:HB3  | 2.38                     | 0.54              |
| 23:P:163:LEU:O    | 23:P:167:THR:HG23 | 2.08                     | 0.54              |
| 2:2:126:SER:OG    | 2:2:135:MET:HB3   | 2.07                     | 0.54              |
| 3:3:41:PHE:CE1    | 3:3:181:ILE:HD13  | 2.42                     | 0.54              |
| 6:6:61:ASN:O      | 6:6:65:TRP:HD1    | 1.91                     | 0.54              |
| 7:7:145:PRO:HA    | 7:7:148:ARG:NE    | 2.12                     | 0.54              |
| 15:H:333:MET:HE1  | 15:H:362:ASP:OD2  | 2.08                     | 0.54              |
| 20:M:72:ASN:CB    | 20:M:156:LEU:CD2  | 2.86                     | 0.54              |
| 22:O:217:LEU:HD12 | 22:O:238:ILE:CG2  | 2.38                     | 0.54              |
| 22:O:250:TRP:CG   | 22:O:269:LEU:HD21 | 2.40                     | 0.54              |
| 25:R:262:GLU:HA   | 25:R:336:LYS:NZ   | 2.23                     | 0.54              |
| 27:T:112:ASN:CB   | 27:T:177:PHE:CZ   | 2.90                     | 0.54              |
| 33:Z:149:TRP:CG   | 33:Z:214:HIS:CE1  | 2.96                     | 0.54              |
| 33:Z:316:ALA:HB1  | 33:Z:868:ASN:OD1  | 2.08                     | 0.54              |
| 1:1:120:HIS:HB2   | 7:7:28:PHE:CE1    | 2.44                     | 0.53              |
| 3:3:37:TYR:CE1    | 3:3:59:ARG:CB     | 2.92                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:32:ASP:HB3    | 4:4:35:ARG:NH1    | 2.21                     | 0.53              |
| 4:4:129:TYR:CG    | 4:4:143:LEU:HD13  | 2.43                     | 0.53              |
| 5:5:135:PHE:CB    | 5:5:167:ARG:NH2   | 2.65                     | 0.53              |
| 7:7:145:PRO:HG3   | 7:7:148:ARG:NH2   | 2.23                     | 0.53              |
| 8:A:84:ASN:HD22   | 8:A:171:THR:HG23  | 1.74                     | 0.53              |
| 18:K:374:ARG:HH12 | 18:K:408:GLU:HG2  | 1.73                     | 0.53              |
| 20:M:216:LYS:HE3  | 20:M:267:PHE:HE1  | 1.73                     | 0.53              |
| 21:N:585:ARG:HH21 | 21:N:623:PHE:HE2  | 1.43                     | 0.53              |
| 23:P:241:LEU:HD23 | 23:P:264:ILE:CG1  | 2.37                     | 0.53              |
| 24:Q:158:ILE:HG23 | 24:Q:177:VAL:CG1  | 2.38                     | 0.53              |
| 28:U:16:LEU:HA    | 28:U:19:LEU:HD12  | 1.90                     | 0.53              |
| 33:Z:582:ASP:HA   | 33:Z:585:LEU:HD12 | 1.90                     | 0.53              |
| 2:2:99:ILE:HG13   | 2:2:127:LEU:HD12  | 1.90                     | 0.53              |
| 4:4:34:THR:HG21   | 4:4:181:LYS:NZ    | 2.23                     | 0.53              |
| 4:4:84:ARG:HD2    | 4:4:124:LYS:CB    | 2.38                     | 0.53              |
| 4:4:161:LYS:HE2   | 4:4:165:GLN:HE21  | 1.72                     | 0.53              |
| 7:7:118:PHE:CE2   | 7:7:120:ARG:CD    | 2.89                     | 0.53              |
| 8:A:189:SER:OG    | 8:A:191:ILE:HG12  | 2.08                     | 0.53              |
| 16:I:148:LEU:HD23 | 16:I:160:LEU:HD22 | 1.90                     | 0.53              |
| 17:J:61:GLU:O     | 17:J:65:LEU:HG    | 2.08                     | 0.53              |
| 18:K:132:LYS:HB2  | 18:K:135:MET:CG   | 2.36                     | 0.53              |
| 18:K:183:GLU:HG2  | 18:K:338:ILE:HG12 | 1.89                     | 0.53              |
| 21:N:340:HIS:CB   | 21:N:374:ILE:HG12 | 2.38                     | 0.53              |
| 27:T:59:LYS:HG3   | 27:T:85:LEU:HD11  | 1.90                     | 0.53              |
| 31:X:38:ASN:ND2   | 31:X:43:LEU:HG    | 2.23                     | 0.53              |
| 33:Z:303:ASP:C    | 33:Z:307:HIS:HD2  | 2.15                     | 0.53              |
| 2:2:72:ARG:NH1    | 8:A:113:PRO:HB3   | 2.23                     | 0.53              |
| 2:2:112:SER:HB2   | 2:2:127:LEU:HD11  | 1.89                     | 0.53              |
| 3:3:83:SER:HB2    | 3:3:121:ILE:HD11  | 1.90                     | 0.53              |
| 3:3:129:VAL:CG2   | 3:3:138:PHE:CZ    | 2.91                     | 0.53              |
| 5:5:3:THR:HG23    | 5:5:16:VAL:HG12   | 1.89                     | 0.53              |
| 10:C:40:ALA:CA    | 10:C:184:MET:SD   | 2.84                     | 0.53              |
| 11:D:10:ILE:HG22  | 11:D:18:PHE:CE2   | 2.43                     | 0.53              |
| 12:E:17:PRO:CA    | 13:F:24:TYR:CE2   | 2.89                     | 0.53              |
| 23:P:97:ILE:O     | 23:P:101:MET:HG2  | 2.08                     | 0.53              |
| 23:P:144:VAL:HG12 | 23:P:148:LYS:HE3  | 1.90                     | 0.53              |
| 24:Q:4:PRO:HB3    | 24:Q:50:ARG:NH1   | 2.23                     | 0.53              |
| 33:Z:106:TRP:HB2  | 33:Z:112:LYS:HZ2  | 1.73                     | 0.53              |
| 33:Z:126:TYR:O    | 33:Z:127:SER:HB2  | 2.08                     | 0.53              |
| 33:Z:497:PHE:CD2  | 33:Z:505:VAL:HB   | 2.43                     | 0.53              |
| 4:4:81:SER:CA     | 4:4:124:LYS:NZ    | 2.68                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:158:THR:OG1  | 10:C:160:TRP:NE1  | 2.40                     | 0.53              |
| 12:E:207:VAL:CB   | 15:H:409:ARG:NH1  | 2.71                     | 0.53              |
| 17:J:153:LEU:O    | 17:J:157:ILE:HG13 | 2.08                     | 0.53              |
| 21:N:145:LEU:HD22 | 21:N:173:LYS:NZ   | 2.21                     | 0.53              |
| 21:N:362:TRP:CH2  | 29:V:23:THR:HB    | 2.44                     | 0.53              |
| 22:O:80:LYS:HE2   | 22:O:81:TYR:HE1   | 1.74                     | 0.53              |
| 25:R:301:TYR:CZ   | 25:R:305:PHE:CZ   | 2.94                     | 0.53              |
| 27:T:249:MET:O    | 27:T:250:MET:CB   | 2.56                     | 0.53              |
| 30:W:186:ALA:HB1  | 30:W:191:ILE:HG21 | 1.76                     | 0.53              |
| 33:Z:865:ASP:CG   | 33:Z:909:ARG:CZ   | 2.81                     | 0.53              |
| 1:1:5:ALA:CB      | 1:1:14:LEU:HG     | 2.39                     | 0.53              |
| 1:1:14:LEU:CD1    | 1:1:100:ALA:HB1   | 2.32                     | 0.53              |
| 4:4:66:TYR:CZ     | 10:C:102:TYR:OH   | 2.61                     | 0.53              |
| 10:C:209:ASP:OD1  | 10:C:210:ARG:HG3  | 2.09                     | 0.53              |
| 13:F:101:ARG:HH12 | 13:F:103:LEU:HA   | 1.67                     | 0.53              |
| 15:H:365:LEU:HD23 | 15:H:370:ARG:CZ   | 2.38                     | 0.53              |
| 18:K:105:GLN:O    | 18:K:106:ASN:HB2  | 2.09                     | 0.53              |
| 20:M:197:ILE:HG13 | 20:M:198:VAL:N    | 2.24                     | 0.53              |
| 21:N:117:TYR:CZ   | 21:N:202:PHE:HB2  | 2.43                     | 0.53              |
| 23:P:426:ILE:HA   | 23:P:429:ILE:HD12 | 1.89                     | 0.53              |
| 24:Q:50:ARG:CZ    | 24:Q:53:GLU:OE1   | 2.57                     | 0.53              |
| 24:Q:99:THR:CG2   | 24:Q:103:LYS:HE3  | 2.37                     | 0.53              |
| 25:R:31:PHE:CZ    | 25:R:320:LYS:HA   | 2.43                     | 0.53              |
| 25:R:70:TYR:OH    | 25:R:76:GLN:HA    | 2.08                     | 0.53              |
| 33:Z:493:LEU:CD1  | 33:Z:497:PHE:CE2  | 2.88                     | 0.53              |
| 33:Z:915:ALA:HB1  | 33:Z:983:LEU:CD1  | 2.38                     | 0.53              |
| 6:6:70:HIS:CD2    | 12:E:111:SER:CB   | 2.92                     | 0.53              |
| 9:B:40:THR:HG21   | 9:B:182:GLU:HG2   | 1.91                     | 0.53              |
| 14:G:136:ILE:HG12 | 14:G:149:MET:CG   | 2.39                     | 0.53              |
| 14:G:136:ILE:HG12 | 14:G:149:MET:HG3  | 1.90                     | 0.53              |
| 17:J:134:VAL:CG1  | 17:J:135:SER:N    | 2.34                     | 0.53              |
| 17:J:234:PHE:HZ   | 17:J:279:LEU:HD21 | 1.74                     | 0.53              |
| 17:J:338:THR:O    | 17:J:341:ILE:HG22 | 2.08                     | 0.53              |
| 18:K:242:PHE:C    | 18:K:244:HIS:N    | 2.66                     | 0.53              |
| 19:L:167:VAL:HG23 | 20:M:142:PRO:CG   | 2.33                     | 0.53              |
| 21:N:130:ASP:OD2  | 21:N:132:LYS:HB2  | 2.09                     | 0.53              |
| 23:P:95:TYR:CD2   | 23:P:96:MET:HE3   | 2.35                     | 0.53              |
| 26:S:436:ILE:HG23 | 27:T:197:TYR:CE2  | 2.43                     | 0.53              |
| 28:U:20:ASP:CG    | 28:U:24:ARG:HE    | 2.12                     | 0.53              |
| 29:V:181:ASN:C    | 29:V:182:LYS:HG2  | 2.34                     | 0.53              |
| 33:Z:57:LYS:HE2   | 33:Z:98:ASP:OD2   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:246:CYS:O    | 33:Z:250:VAL:HG23 | 2.08                     | 0.53              |
| 33:Z:394:TYR:HB3  | 33:Z:859:LYS:HE3  | 1.90                     | 0.53              |
| 33:Z:550:PHE:HZ   | 33:Z:566:LEU:CB   | 2.13                     | 0.53              |
| 4:4:43:MET:HE3    | 4:4:103:ILE:HG12  | 1.89                     | 0.53              |
| 9:B:219:PRO:CA    | 9:B:222:LEU:HD12  | 2.32                     | 0.53              |
| 11:D:18:PHE:CG    | 11:D:19:GLN:N     | 2.76                     | 0.53              |
| 12:E:68:VAL:CG1   | 12:E:93:ARG:NH2   | 2.71                     | 0.53              |
| 15:H:157:VAL:HG12 | 15:H:159:LEU:H    | 1.74                     | 0.53              |
| 16:I:354:ASP:OD1  | 16:I:357:THR:HG23 | 2.08                     | 0.53              |
| 17:J:370:LEU:HD23 | 17:J:370:LEU:O    | 2.07                     | 0.53              |
| 19:L:386:PHE:CD1  | 19:L:390:ASP:HB3  | 2.43                     | 0.53              |
| 21:N:223:LEU:CD2  | 21:N:897:LYS:HB2  | 2.39                     | 0.53              |
| 21:N:539:MET:HE2  | 21:N:551:GLY:N    | 2.23                     | 0.53              |
| 21:N:719:ASN:N    | 21:N:726:ASP:OD2  | 2.41                     | 0.53              |
| 23:P:202:LYS:HE2  | 23:P:206:LYS:HZ2  | 1.72                     | 0.53              |
| 23:P:431:HIS:CE1  | 28:U:156:HIS:H    | 2.27                     | 0.53              |
| 24:Q:201:ALA:HB1  | 24:Q:218:LEU:HD21 | 1.89                     | 0.53              |
| 27:T:26:LEU:O     | 27:T:29:PRO:HD2   | 2.08                     | 0.53              |
| 27:T:119:THR:HG22 | 27:T:123:HIS:CE1  | 2.44                     | 0.53              |
| 30:W:131:THR:HG23 | 30:W:134:LYS:HD2  | 1.89                     | 0.53              |
| 33:Z:385:PHE:HZ   | 33:Z:389:PHE:CZ   | 2.20                     | 0.53              |
| 33:Z:397:ASP:OD1  | 33:Z:425:ILE:HD12 | 2.09                     | 0.53              |
| 33:Z:846:PHE:CE2  | 33:Z:901:PHE:HE2  | 2.27                     | 0.53              |
| 1:1:59:VAL:HG21   | 1:1:82:PHE:CE1    | 2.44                     | 0.53              |
| 1:1:66:TYR:CE2    | 1:1:73:PRO:CB     | 2.89                     | 0.53              |
| 3:3:54:LEU:CD1    | 3:3:96:VAL:HG11   | 2.38                     | 0.53              |
| 10:C:120:GLN:OE1  | 11:D:80:ALA:HB1   | 2.09                     | 0.53              |
| 12:E:219:LEU:HB2  | 12:E:236:THR:CG2  | 2.39                     | 0.53              |
| 15:H:200:VAL:HG13 | 15:H:270:THR:CG2  | 2.38                     | 0.53              |
| 15:H:224:VAL:O    | 15:H:228:PRO:HG3  | 2.07                     | 0.53              |
| 20:M:75:LEU:HD23  | 20:M:77:TYR:HB2   | 1.89                     | 0.53              |
| 21:N:221:ASP:HA   | 21:N:894:ARG:HH12 | 1.74                     | 0.53              |
| 21:N:919:THR:HG23 | 21:N:921:ARG:HG2  | 1.89                     | 0.53              |
| 23:P:425:HIS:O    | 23:P:429:ILE:HG13 | 2.09                     | 0.53              |
| 26:S:339:GLN:HA   | 26:S:342:LEU:HD12 | 1.91                     | 0.53              |
| 33:Z:609:THR:HG21 | 33:Z:878:LEU:HD13 | 1.91                     | 0.53              |
| 33:Z:761:PHE:CG   | 33:Z:780:MET:HE2  | 2.43                     | 0.53              |
| 33:Z:809:MET:HG2  | 33:Z:847:ILE:CD1  | 2.38                     | 0.53              |
| 1:1:120:HIS:CE1   | 7:7:31:VAL:HG22   | 2.44                     | 0.53              |
| 2:2:36:ARG:NH2    | 2:2:39:PRO:CD     | 2.72                     | 0.53              |
| 5:5:32:LYS:O      | 5:5:33:ARG:NH1    | 2.36                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:99:VAL:O     | 15:H:173:ARG:HD3  | 2.08                     | 0.53              |
| 16:I:193:GLU:O    | 16:I:346:ARG:NH1  | 2.42                     | 0.53              |
| 18:K:393:ARG:HH21 | 19:L:345:ARG:NH1  | 2.06                     | 0.53              |
| 20:M:264:ARG:HG2  | 20:M:311:GLN:HE21 | 1.74                     | 0.53              |
| 21:N:619:CYS:SG   | 21:N:655:ALA:HB2  | 2.49                     | 0.53              |
| 21:N:649:VAL:CG1  | 21:N:651:PHE:CE2  | 2.91                     | 0.53              |
| 21:N:768:ILE:HD13 | 21:N:871:MET:HE3  | 1.90                     | 0.53              |
| 22:O:15:ARG:CB    | 30:W:20:ASP:OD1   | 2.57                     | 0.53              |
| 22:O:26:PHE:HZ    | 22:O:64:ASN:ND2   | 2.05                     | 0.53              |
| 22:O:138:LEU:HD23 | 22:O:138:LEU:C    | 2.33                     | 0.53              |
| 22:O:384:MET:HE3  | 28:U:190:LEU:HA   | 1.90                     | 0.53              |
| 29:V:140:VAL:CG1  | 29:V:156:PHE:HE2  | 2.22                     | 0.53              |
| 30:W:179:ARG:NE   | 30:W:184:ASN:OD1  | 2.37                     | 0.53              |
| 31:X:104:LYS:NZ   | 31:X:107:GLY:O    | 2.40                     | 0.53              |
| 33:Z:51:LEU:HB3   | 33:Z:91:PHE:CZ    | 2.34                     | 0.53              |
| 33:Z:298:PHE:HZ   | 33:Z:314:LEU:HD22 | 1.74                     | 0.53              |
| 33:Z:383:SER:HA   | 33:Z:849:ARG:HH11 | 1.74                     | 0.53              |
| 33:Z:463:HIS:NE2  | 33:Z:497:PHE:CE1  | 2.77                     | 0.53              |
| 4:4:7:ARG:HH11    | 4:4:114:GLU:HA    | 1.74                     | 0.53              |
| 4:4:45:PHE:HB3    | 4:4:99:VAL:HG11   | 1.92                     | 0.53              |
| 8:A:46:ARG:HD2    | 8:A:152:PRO:HB2   | 1.90                     | 0.53              |
| 10:C:41:SER:HB3   | 10:C:184:MET:CE   | 2.38                     | 0.53              |
| 10:C:98:TYR:CE1   | 10:C:105:ASP:O    | 2.62                     | 0.53              |
| 15:H:379:LEU:HD21 | 15:H:415:THR:HG22 | 1.89                     | 0.53              |
| 15:H:385:ARG:HB3  | 15:H:389:PHE:CE2  | 2.44                     | 0.53              |
| 18:K:423:LYS:HG3  | 18:K:424:PHE:CD2  | 2.43                     | 0.53              |
| 19:L:228:LYS:HB2  | 19:L:349:ILE:HD11 | 1.90                     | 0.53              |
| 22:O:188:PHE:CD2  | 22:O:220:SER:HB3  | 2.44                     | 0.53              |
| 24:Q:104:PHE:HE2  | 24:Q:114:GLN:HA   | 1.74                     | 0.53              |
| 25:R:70:TYR:HE2   | 25:R:77:SER:H     | 1.57                     | 0.53              |
| 25:R:110:ILE:HD11 | 25:R:140:TYR:OH   | 2.09                     | 0.53              |
| 26:S:378:GLN:CB   | 26:S:382:ARG:HH12 | 2.21                     | 0.53              |
| 27:T:8:THR:HG23   | 27:T:61:ILE:CG1   | 2.38                     | 0.53              |
| 30:W:6:THR:HG23   | 30:W:111:VAL:HG23 | 1.90                     | 0.53              |
| 33:Z:263:ALA:O    | 33:Z:267:THR:HG23 | 2.08                     | 0.53              |
| 33:Z:419:VAL:HG21 | 33:Z:447:VAL:HA   | 1.91                     | 0.53              |
| 33:Z:773:ARG:O    | 33:Z:776:VAL:HG12 | 2.09                     | 0.53              |
| 3:3:16:CYS:SG     | 3:3:34:ILE:HD12   | 2.49                     | 0.52              |
| 5:5:111:THR:HG21  | 5:5:113:TYR:OH    | 2.07                     | 0.52              |
| 8:A:88:PRO:O      | 14:G:120:GLN:NE2  | 2.42                     | 0.52              |
| 12:E:207:VAL:CB   | 15:H:409:ARG:HH12 | 2.22                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:308:PHE:HE1  | 15:H:351:VAL:HG13 | 1.73                     | 0.52              |
| 17:J:62:LEU:HD13  | 18:K:86:VAL:HA    | 1.90                     | 0.52              |
| 17:J:206:THR:O    | 17:J:207:ASP:HB2  | 2.09                     | 0.52              |
| 18:K:168:ASP:OD1  | 19:L:315:PHE:CE1  | 2.62                     | 0.52              |
| 18:K:239:GLY:HA2  | 18:K:242:PHE:CD2  | 2.44                     | 0.52              |
| 21:N:762:ARG:HB2  | 21:N:769:PRO:HG3  | 1.90                     | 0.52              |
| 22:O:245:ASP:HA   | 22:O:249:ASP:OD1  | 2.09                     | 0.52              |
| 24:Q:331:THR:CG2  | 24:Q:335:PHE:CE2  | 2.92                     | 0.52              |
| 25:R:222:ARG:HA   | 25:R:224:PHE:CZ   | 2.45                     | 0.52              |
| 26:S:145:PHE:HD2  | 26:S:152:LEU:CD2  | 2.21                     | 0.52              |
| 33:Z:65:GLU:CA    | 33:Z:111:LEU:HD21 | 2.38                     | 0.52              |
| 33:Z:550:PHE:HZ   | 33:Z:566:LEU:C    | 2.18                     | 0.52              |
| 14:G:161:GLY:HA3  | 14:G:175:LEU:HD21 | 1.90                     | 0.52              |
| 15:H:284:VAL:N    | 20:M:254:MET:HB3  | 2.25                     | 0.52              |
| 17:J:228:ARG:NH1  | 17:J:232:GLU:CD   | 2.66                     | 0.52              |
| 17:J:236:MET:O    | 17:J:240:HIS:HD2  | 1.91                     | 0.52              |
| 19:L:85:GLU:HG3   | 20:M:58:MET:HE2   | 1.92                     | 0.52              |
| 19:L:178:ILE:HD12 | 19:L:183:ILE:HG21 | 1.91                     | 0.52              |
| 19:L:247:PRO:HB3  | 20:M:303:ARG:NH2  | 2.24                     | 0.52              |
| 19:L:312:MET:SD   | 19:L:342:ARG:HA   | 2.48                     | 0.52              |
| 22:O:301:PHE:CZ   | 28:U:234:ASN:HA   | 2.43                     | 0.52              |
| 27:T:236:ASN:OD1  | 27:T:238:GLN:HB2  | 2.10                     | 0.52              |
| 31:X:14:VAL:HG13  | 31:X:50:TRP:CZ2   | 2.44                     | 0.52              |
| 31:X:75:TRP:NE1   | 31:X:125:MET:CB   | 2.63                     | 0.52              |
| 33:Z:138:ARG:HH12 | 33:Z:160:GLU:HB3  | 1.73                     | 0.52              |
| 1:1:18:SER:HB3    | 1:1:31:THR:HG22   | 1.91                     | 0.52              |
| 2:2:25:ILE:HG21   | 3:3:138:PHE:HB3   | 1.92                     | 0.52              |
| 7:7:-7:GLN:CG     | 7:7:101:PRO:HD2   | 2.35                     | 0.52              |
| 7:7:124:LEU:HD12  | 7:7:124:LEU:C     | 2.34                     | 0.52              |
| 10:C:26:LEU:HD23  | 10:C:153:PRO:CG   | 2.39                     | 0.52              |
| 12:E:207:VAL:CA   | 15:H:409:ARG:NH1  | 2.70                     | 0.52              |
| 19:L:170:MET:HG2  | 19:L:266:MET:CE   | 2.39                     | 0.52              |
| 19:L:257:GLY:HA2  | 19:L:303:ARG:NH2  | 2.24                     | 0.52              |
| 22:O:255:LEU:HD23 | 22:O:255:LEU:C    | 2.34                     | 0.52              |
| 26:S:188:TYR:OH   | 26:S:240:ASP:HB2  | 2.09                     | 0.52              |
| 26:S:250:ALA:CB   | 26:S:279:ILE:HD13 | 2.39                     | 0.52              |
| 30:W:172:LEU:CD1  | 30:W:190:ILE:HB   | 2.37                     | 0.52              |
| 33:Z:53:VAL:HG23  | 33:Z:91:PHE:CD2   | 2.44                     | 0.52              |
| 33:Z:474:LEU:HD23 | 33:Z:493:LEU:HD23 | 1.68                     | 0.52              |
| 33:Z:805:LEU:HD22 | 33:Z:841:GLU:CG   | 2.39                     | 0.52              |
| 3:3:169:ASP:HB2   | 3:3:172:SER:OG    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:138:PHE:CZ    | 7:7:142:MET:HG3   | 2.45                     | 0.52              |
| 15:H:174:VAL:HG13 | 15:H:183:ILE:CG2  | 2.24                     | 0.52              |
| 16:I:106:ILE:HD13 | 16:I:160:LEU:HD21 | 1.89                     | 0.52              |
| 16:I:278:ILE:CG2  | 16:I:325:ILE:HD12 | 2.39                     | 0.52              |
| 18:K:170:THR:HG23 | 18:K:172:ALA:H    | 1.74                     | 0.52              |
| 20:M:129:LEU:HD13 | 20:M:130:PRO:O    | 2.09                     | 0.52              |
| 20:M:167:VAL:CG2  | 20:M:269:LEU:HD12 | 2.39                     | 0.52              |
| 21:N:232:LEU:HD12 | 21:N:237:LEU:CD1  | 2.40                     | 0.52              |
| 22:O:4:ASN:HB2    | 22:O:39:PHE:CE2   | 2.44                     | 0.52              |
| 22:O:117:ASN:HD22 | 22:O:167:ILE:HD12 | 1.74                     | 0.52              |
| 22:O:228:TYR:HE2  | 22:O:231:GLY:H    | 1.57                     | 0.52              |
| 23:P:319:GLU:HB3  | 23:P:323:ASN:OD1  | 2.09                     | 0.52              |
| 23:P:440:HIS:ND1  | 28:U:209:GLU:HB3  | 2.24                     | 0.52              |
| 24:Q:122:ILE:HG22 | 24:Q:126:LYS:HE3  | 1.90                     | 0.52              |
| 24:Q:395:GLY:O    | 24:Q:396:TRP:HD1  | 1.93                     | 0.52              |
| 25:R:179:PHE:CE1  | 25:R:321:TYR:OH   | 2.62                     | 0.52              |
| 27:T:202:LEU:O    | 27:T:205:ILE:HG22 | 2.08                     | 0.52              |
| 28:U:37:ILE:CG2   | 28:U:93:TYR:HD2   | 2.23                     | 0.52              |
| 29:V:52:LEU:HD12  | 29:V:69:PHE:CZ    | 2.45                     | 0.52              |
| 31:X:104:LYS:HE3  | 31:X:108:ASN:CG   | 2.34                     | 0.52              |
| 33:Z:809:MET:HG2  | 33:Z:847:ILE:HD12 | 1.91                     | 0.52              |
| 33:Z:809:MET:HE3  | 33:Z:847:ILE:HD11 | 1.92                     | 0.52              |
| 8:A:156:LYS:HB3   | 8:A:166:TYR:CZ    | 2.43                     | 0.52              |
| 15:H:284:VAL:HG13 | 20:M:252:VAL:HG12 | 1.91                     | 0.52              |
| 16:I:222:TYR:CD1  | 16:I:348:ILE:O    | 2.63                     | 0.52              |
| 19:L:88:TYR:CE1   | 20:M:62:ILE:HG21  | 2.45                     | 0.52              |
| 19:L:88:TYR:CE1   | 20:M:62:ILE:CG2   | 2.92                     | 0.52              |
| 19:L:170:MET:HE2  | 19:L:266:MET:HB2  | 1.92                     | 0.52              |
| 20:M:197:ILE:CB   | 20:M:322:LYS:HD3  | 2.32                     | 0.52              |
| 21:N:150:LEU:HD21 | 21:N:173:LYS:HG3  | 1.90                     | 0.52              |
| 21:N:363:ALA:HB2  | 29:V:182:LYS:HZ3  | 1.72                     | 0.52              |
| 21:N:645:THR:HG21 | 21:N:660:LEU:HD11 | 1.90                     | 0.52              |
| 21:N:745:LEU:O    | 21:N:748:PHE:HD1  | 1.92                     | 0.52              |
| 23:P:333:ALA:HB3  | 23:P:336:HIS:HB2  | 1.91                     | 0.52              |
| 24:Q:250:THR:HG23 | 24:Q:251:THR:H    | 1.72                     | 0.52              |
| 26:S:237:ILE:HG21 | 26:S:253:PHE:CZ   | 2.45                     | 0.52              |
| 27:T:89:TYR:CG    | 27:T:102:LYS:CD   | 2.92                     | 0.52              |
| 33:Z:81:SER:O     | 33:Z:82:MET:CB    | 2.57                     | 0.52              |
| 33:Z:392:LEU:HD11 | 33:Z:427:GLN:HB3  | 1.90                     | 0.52              |
| 33:Z:886:VAL:CA   | 33:Z:893:PHE:CE2  | 2.82                     | 0.52              |
| 4:4:145:HIS:CD2   | 4:4:146:HIS:CE1   | 2.96                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:6:-5:TYR:CD1    | 6:6:97:TYR:CG     | 2.97                     | 0.52              |
| 7:7:49:ILE:HG23   | 7:7:52:MET:HE3    | 1.92                     | 0.52              |
| 9:B:139:HIS:CE1   | 9:B:145:PHE:CZ    | 2.98                     | 0.52              |
| 11:D:34:VAL:HG12  | 11:D:163:THR:OG1  | 2.08                     | 0.52              |
| 13:F:11:VAL:HA    | 14:G:129:ARG:HG2  | 1.91                     | 0.52              |
| 15:H:215:LYS:O    | 15:H:219:GLU:HG3  | 2.09                     | 0.52              |
| 15:H:286:GLU:CD   | 15:H:289:ARG:HH21 | 2.18                     | 0.52              |
| 15:H:295:PHE:CD1  | 15:H:339:GLN:HG3  | 2.44                     | 0.52              |
| 15:H:302:LYS:HD2  | 15:H:348:ASN:HD22 | 1.73                     | 0.52              |
| 15:H:389:PHE:HZ   | 15:H:419:LEU:CD2  | 2.18                     | 0.52              |
| 16:I:217:LYS:HD3  | 16:I:343:ARG:HD2  | 1.91                     | 0.52              |
| 17:J:219:VAL:CG1  | 18:K:281:ARG:HD2  | 2.39                     | 0.52              |
| 20:M:218:ALA:HB3  | 20:M:324:LEU:HD22 | 1.92                     | 0.52              |
| 24:Q:222:SER:O    | 24:Q:226:HIS:ND1  | 2.30                     | 0.52              |
| 24:Q:289:GLU:CD   | 24:Q:291:TYR:CE1  | 2.86                     | 0.52              |
| 26:S:230:LYS:NZ   | 26:S:256:LYS:O    | 2.37                     | 0.52              |
| 28:U:54:LEU:CD2   | 28:U:72:TYR:HD2   | 2.22                     | 0.52              |
| 29:V:135:ARG:NE   | 29:V:157:ARG:NH1  | 2.08                     | 0.52              |
| 33:Z:272:TYR:CE2  | 33:Z:284:LEU:HD11 | 2.39                     | 0.52              |
| 1:1:14:LEU:CD1    | 1:1:100:ALA:CB    | 2.87                     | 0.52              |
| 3:3:26:GLY:HA3    | 3:3:174:TRP:CE2   | 2.44                     | 0.52              |
| 6:6:66:TYR:OH     | 6:6:73:LYS:HE2    | 2.10                     | 0.52              |
| 6:6:136:LEU:HD21  | 6:6:185:ARG:HD2   | 1.90                     | 0.52              |
| 12:E:98:THR:HG22  | 12:E:102:TYR:CD2  | 2.45                     | 0.52              |
| 18:K:395:VAL:HG11 | 19:L:207:PHE:CD1  | 2.44                     | 0.52              |
| 21:N:490:LEU:HD23 | 21:N:490:LEU:C    | 2.35                     | 0.52              |
| 21:N:602:VAL:HG12 | 21:N:625:LEU:HD23 | 1.92                     | 0.52              |
| 23:P:287:ASP:HB3  | 23:P:297:GLU:OE1  | 2.09                     | 0.52              |
| 25:R:266:LEU:HA   | 25:R:270:VAL:HG21 | 1.80                     | 0.52              |
| 26:S:257:LEU:HD23 | 26:S:272:TYR:CZ   | 2.44                     | 0.52              |
| 26:S:311:GLN:NE2  | 26:S:338:MET:H    | 2.08                     | 0.52              |
| 26:S:315:LYS:HD3  | 26:S:345:TYR:HE1  | 1.58                     | 0.52              |
| 27:T:24:GLU:HA    | 27:T:27:LEU:HD12  | 1.92                     | 0.52              |
| 31:X:87:PHE:HE2   | 31:X:121:ILE:HG21 | 1.75                     | 0.52              |
| 33:Z:518:LEU:HD23 | 33:Z:523:ALA:O    | 2.09                     | 0.52              |
| 33:Z:531:ALA:HA   | 33:Z:573:LEU:HD21 | 1.91                     | 0.52              |
| 33:Z:612:GLY:CA   | 33:Z:746:ILE:HG21 | 2.37                     | 0.52              |
| 33:Z:821:GLY:O    | 33:Z:962:ARG:NH2  | 2.42                     | 0.52              |
| 5:5:111:THR:CG2   | 5:5:113:TYR:CE1   | 2.92                     | 0.52              |
| 10:C:29:ILE:CD1   | 10:C:153:PRO:HD3  | 2.40                     | 0.52              |
| 12:E:109:VAL:CG1  | 12:E:156:PHE:CE1  | 2.93                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:324:GLY:HA2  | 20:M:290:ARG:NH2  | 2.09                     | 0.52              |
| 15:H:330:GLN:O    | 15:H:334:LEU:HG   | 2.09                     | 0.52              |
| 17:J:345:LYS:O    | 17:J:349:LYS:HG3  | 2.10                     | 0.52              |
| 21:N:269:LEU:O    | 21:N:273:LEU:HG   | 2.10                     | 0.52              |
| 21:N:318:LYS:HA   | 29:V:180:LEU:CD1  | 2.40                     | 0.52              |
| 21:N:654:GLN:HG3  | 21:N:698:GLY:HA3  | 1.90                     | 0.52              |
| 22:O:150:LEU:HD22 | 22:O:175:ASN:OD1  | 2.09                     | 0.52              |
| 24:Q:220:LEU:HD12 | 24:Q:239:PHE:CE1  | 2.45                     | 0.52              |
| 27:T:104:LYS:N    | 27:T:141:LEU:HD13 | 2.25                     | 0.52              |
| 28:U:54:LEU:HD22  | 28:U:72:TYR:HD2   | 1.74                     | 0.52              |
| 33:Z:601:VAL:HB   | 33:Z:620:LEU:CD2  | 2.40                     | 0.52              |
| 2:2:8:PHE:CE1     | 2:2:11:GLY:CA     | 2.92                     | 0.52              |
| 6:6:58:ARG:CD     | 6:6:87:LEU:HD22   | 2.39                     | 0.52              |
| 8:A:135:ARG:HH21  | 14:G:14:PHE:HD2   | 1.56                     | 0.52              |
| 11:D:68:ASP:CG    | 11:D:97:ARG:NH2   | 2.50                     | 0.52              |
| 15:H:412:PRO:HG2  | 15:H:451:ILE:HG13 | 1.91                     | 0.52              |
| 16:I:204:HIS:CD2  | 16:I:207:LEU:HD11 | 2.13                     | 0.52              |
| 18:K:209:VAL:HG11 | 18:K:338:ILE:HD12 | 1.91                     | 0.52              |
| 18:K:281:ARG:HD3  | 18:K:286:THR:HB   | 1.92                     | 0.52              |
| 20:M:354:GLU:HG2  | 20:M:357:ARG:NH2  | 2.25                     | 0.52              |
| 21:N:759:ILE:HG12 | 21:N:871:MET:SD   | 2.50                     | 0.52              |
| 26:S:425:ARG:NH1  | 27:T:155:GLY:CA   | 2.72                     | 0.52              |
| 27:T:236:ASN:CG   | 27:T:238:GLN:HB2  | 2.34                     | 0.52              |
| 29:V:180:LEU:O    | 29:V:181:ASN:HB2  | 2.10                     | 0.52              |
| 33:Z:327:GLN:HG3  | 33:Z:349:THR:O    | 2.10                     | 0.52              |
| 4:4:26:VAL:CG1    | 4:4:29:ASP:HB3    | 2.31                     | 0.52              |
| 7:7:131:SER:HB3   | 7:7:134:LEU:HD21  | 1.91                     | 0.52              |
| 10:C:177:GLN:CG   | 11:D:54:LEU:HD21  | 2.27                     | 0.52              |
| 11:D:146:LYS:HB3  | 11:D:148:TYR:HE2  | 1.75                     | 0.52              |
| 13:F:81:ALA:HB2   | 13:F:130:VAL:HG21 | 1.92                     | 0.52              |
| 16:I:380:LEU:HD13 | 16:I:420:LYS:CE   | 2.40                     | 0.52              |
| 17:J:329:ARG:HH11 | 17:J:333:ARG:NH2  | 2.07                     | 0.52              |
| 22:O:59:LEU:CD2   | 22:O:85:SER:HB3   | 2.32                     | 0.52              |
| 22:O:102:LEU:O    | 22:O:103:LYS:HG2  | 2.09                     | 0.52              |
| 23:P:104:LEU:HD13 | 23:P:115:ARG:HG2  | 1.90                     | 0.52              |
| 26:S:141:LEU:O    | 26:S:145:PHE:CE1  | 2.62                     | 0.52              |
| 28:U:54:LEU:HD23  | 28:U:72:TYR:CD2   | 2.45                     | 0.52              |
| 29:V:57:PHE:HE2   | 29:V:59:ASP:O     | 1.92                     | 0.52              |
| 33:Z:419:VAL:O    | 33:Z:422:ILE:CG1  | 2.34                     | 0.52              |
| 33:Z:957:LEU:HB2  | 33:Z:961:GLU:CD   | 2.35                     | 0.52              |
| 1:1:36:ARG:HB2    | 1:1:42:TRP:CZ3    | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:103:VAL:O     | 2:2:104:ASP:OD1   | 2.28                     | 0.51              |
| 2:2:160:GLN:O     | 2:2:164:TRP:CD1   | 2.63                     | 0.51              |
| 2:2:210:THR:CG2   | 3:3:160:GLN:HE21  | 2.22                     | 0.51              |
| 4:4:45:PHE:HB3    | 4:4:99:VAL:CG1    | 2.41                     | 0.51              |
| 6:6:13:VAL:HG12   | 6:6:197:ILE:HG23  | 1.92                     | 0.51              |
| 8:A:252:ASP:HB2   | 23:P:85:LYS:HE3   | 1.92                     | 0.51              |
| 9:B:94:HIS:HA     | 9:B:98:LYS:HE2    | 1.92                     | 0.51              |
| 10:C:15:PRO:HB2   | 16:I:332:GLU:OE1  | 2.10                     | 0.51              |
| 12:E:157:HIS:ND1  | 12:E:170:LYS:HE2  | 2.25                     | 0.51              |
| 14:G:111:PHE:HA   | 14:G:114:ARG:NH2  | 2.25                     | 0.51              |
| 14:G:122:HIS:NE2  | 14:G:128:VAL:CG1  | 2.63                     | 0.51              |
| 17:J:167:PRO:N    | 17:J:174:PHE:CE1  | 2.77                     | 0.51              |
| 18:K:421:VAL:O    | 18:K:422:ASP:HB2  | 2.09                     | 0.51              |
| 20:M:76:PRO:C     | 20:M:77:TYR:CD1   | 2.89                     | 0.51              |
| 21:N:273:LEU:O    | 21:N:277:LEU:CG   | 2.50                     | 0.51              |
| 21:N:654:GLN:HE21 | 21:N:697:PHE:HD2  | 1.55                     | 0.51              |
| 21:N:717:LEU:HD22 | 21:N:733:LEU:HD12 | 1.92                     | 0.51              |
| 23:P:218:LEU:HD22 | 23:P:256:LYS:NZ   | 2.25                     | 0.51              |
| 24:Q:146:TYR:CD1  | 24:Q:151:TYR:CE1  | 2.97                     | 0.51              |
| 24:Q:302:VAL:HG13 | 24:Q:314:PHE:CE1  | 2.45                     | 0.51              |
| 25:R:335:ARG:HA   | 25:R:371:PHE:CE2  | 2.45                     | 0.51              |
| 26:S:151:GLU:OE1  | 26:S:154:GLN:N    | 2.39                     | 0.51              |
| 28:U:39:GLY:HA2   | 28:U:49:THR:OG1   | 2.10                     | 0.51              |
| 28:U:283:ARG:CD   | 29:V:287:THR:HG22 | 2.39                     | 0.51              |
| 33:Z:495:ILE:HD11 | 33:Z:903:MET:HG2  | 1.92                     | 0.51              |
| 33:Z:957:LEU:CD1  | 33:Z:958:ASN:O    | 2.59                     | 0.51              |
| 4:4:102:LEU:CD2   | 4:4:117:GLN:HG2   | 2.36                     | 0.51              |
| 6:6:-2:ASN:OD1    | 6:6:48:PHE:CD1    | 2.64                     | 0.51              |
| 9:B:160:LYS:HE2   | 10:C:56:LEU:HA    | 1.92                     | 0.51              |
| 12:E:154:GLN:HE22 | 12:E:166:ARG:HH21 | 1.57                     | 0.51              |
| 15:H:331:ARG:CD   | 20:M:252:VAL:HG11 | 2.40                     | 0.51              |
| 16:I:397:THR:HG22 | 17:J:312:ARG:HH22 | 1.75                     | 0.51              |
| 16:I:433:GLU:OE1  | 16:I:433:GLU:N    | 2.40                     | 0.51              |
| 18:K:160:VAL:HG12 | 18:K:238:ASN:ND2  | 2.25                     | 0.51              |
| 20:M:179:THR:HG1  | 20:M:182:ASP:CG   | 2.17                     | 0.51              |
| 20:M:394:VAL:HA   | 20:M:423:GLN:NE2  | 2.19                     | 0.51              |
| 21:N:94:LYS:HE2   | 21:N:143:LYS:HZ1  | 1.72                     | 0.51              |
| 22:O:23:HIS:CE1   | 22:O:24:PRO:HD2   | 2.43                     | 0.51              |
| 22:O:189:TYR:CZ   | 22:O:193:LEU:HD11 | 2.44                     | 0.51              |
| 23:P:333:ALA:O    | 23:P:337:HIS:CD2  | 2.64                     | 0.51              |
| 24:Q:114:GLN:HG3  | 24:Q:144:LEU:HD11 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:309:ARG:HH21 | 24:Q:345:SER:C    | 2.14                     | 0.51              |
| 27:T:111:LEU:HG   | 27:T:145:PRO:HG3  | 1.90                     | 0.51              |
| 33:Z:86:PRO:HG2   | 33:Z:87:LYS:HG3   | 1.92                     | 0.51              |
| 33:Z:99:LEU:HB3   | 33:Z:119:LEU:HD21 | 1.92                     | 0.51              |
| 33:Z:443:ASP:CB   | 33:Z:447:VAL:CB   | 2.84                     | 0.51              |
| 33:Z:955:VAL:HG12 | 33:Z:956:LEU:HG   | 1.92                     | 0.51              |
| 1:1:6:VAL:HG13    | 1:1:142:PHE:CE1   | 2.46                     | 0.51              |
| 1:1:51:ASP:CG     | 1:1:93:LEU:HD22   | 2.35                     | 0.51              |
| 2:2:75:ARG:HB3    | 2:2:77:VAL:HG22   | 1.91                     | 0.51              |
| 5:5:58:TRP:CH2    | 5:5:62:GLN:NE2    | 2.78                     | 0.51              |
| 12:E:165:TYR:CB   | 12:E:167:TYR:OH   | 2.58                     | 0.51              |
| 12:E:196:ALA:O    | 12:E:200:VAL:HG23 | 2.11                     | 0.51              |
| 15:H:272:ILE:HD13 | 15:H:297:MET:HE1  | 1.92                     | 0.51              |
| 16:I:317:ASP:HB3  | 16:I:343:ARG:CZ   | 2.40                     | 0.51              |
| 21:N:749:LEU:HD12 | 21:N:752:SER:OG   | 2.10                     | 0.51              |
| 23:P:241:LEU:CD2  | 23:P:264:ILE:HG13 | 2.41                     | 0.51              |
| 25:R:121:GLU:HG2  | 25:R:130:GLN:HE22 | 1.76                     | 0.51              |
| 33:Z:278:LEU:HB3  | 33:Z:297:VAL:HG11 | 1.93                     | 0.51              |
| 33:Z:550:PHE:HE1  | 33:Z:566:LEU:HB2  | 1.76                     | 0.51              |
| 1:1:11:GLY:CA     | 1:1:102:TYR:CE1   | 2.93                     | 0.51              |
| 5:5:158:LYS:HE3   | 5:5:196:LEU:CD1   | 2.40                     | 0.51              |
| 9:B:239:THR:HG22  | 9:B:240:SER:N     | 2.25                     | 0.51              |
| 12:E:121:LEU:HD22 | 13:F:79:PRO:CB    | 2.41                     | 0.51              |
| 13:F:65:LYS:HA    | 13:F:222:PHE:CE2  | 2.45                     | 0.51              |
| 15:H:59:ILE:HD11  | 16:I:92:GLU:OE1   | 2.06                     | 0.51              |
| 19:L:290:ARG:NH1  | 19:L:293:GLU:C    | 2.65                     | 0.51              |
| 21:N:308:ASN:CB   | 21:N:711:ARG:HD2  | 2.41                     | 0.51              |
| 22:O:79:VAL:HB    | 22:O:83:LEU:HD12  | 1.92                     | 0.51              |
| 22:O:250:TRP:CZ2  | 22:O:271:LYS:CB   | 2.94                     | 0.51              |
| 22:O:280:LEU:HD23 | 22:O:280:LEU:O    | 2.11                     | 0.51              |
| 23:P:154:ASP:OD2  | 23:P:190:LYS:NZ   | 2.43                     | 0.51              |
| 30:W:95:GLN:HA    | 30:W:98:LEU:HD12  | 1.91                     | 0.51              |
| 33:Z:124:MET:C    | 33:Z:124:MET:SD   | 2.94                     | 0.51              |
| 33:Z:363:ASP:O    | 33:Z:366:LYS:HD3  | 2.10                     | 0.51              |
| 33:Z:821:GLY:HA2  | 33:Z:863:THR:CG2  | 2.24                     | 0.51              |
| 2:2:191:LEU:C     | 2:2:193:PRO:HD3   | 2.35                     | 0.51              |
| 4:4:65:LEU:CD1    | 4:4:69:ARG:HE     | 2.23                     | 0.51              |
| 8:A:232:LYS:CG    | 8:A:234:PHE:HE1   | 2.23                     | 0.51              |
| 13:F:7:ASP:CB     | 13:F:21:GLN:NE2   | 2.74                     | 0.51              |
| 14:G:200:TYR:CD1  | 14:G:246:ILE:HG21 | 2.46                     | 0.51              |
| 15:H:49:LEU:HD21  | 33:Z:759:ARG:HA   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:220:ILE:HG13 | 16:I:344:ILE:CG2  | 2.38                     | 0.51              |
| 17:J:218:LEU:CD2  | 17:J:230:VAL:HG22 | 2.40                     | 0.51              |
| 19:L:214:PRO:HD2  | 19:L:216:LYS:NZ   | 2.24                     | 0.51              |
| 19:L:290:ARG:NH1  | 19:L:293:GLU:HA   | 2.24                     | 0.51              |
| 21:N:83:LEU:HD11  | 21:N:133:LEU:CD2  | 2.41                     | 0.51              |
| 21:N:508:THR:HG22 | 21:N:510:HIS:N    | 2.25                     | 0.51              |
| 23:P:130:ILE:CG2  | 23:P:136:ARG:NH2  | 2.73                     | 0.51              |
| 24:Q:88:PHE:CE2   | 24:Q:89:ALA:HB2   | 2.46                     | 0.51              |
| 26:S:388:ILE:HG21 | 26:S:422:MET:CE   | 2.40                     | 0.51              |
| 30:W:21:PHE:CD1   | 30:W:25:ARG:HG3   | 2.44                     | 0.51              |
| 33:Z:138:ARG:HH21 | 33:Z:157:LEU:HD11 | 1.69                     | 0.51              |
| 33:Z:338:HIS:CD2  | 33:Z:339:PHE:CZ   | 2.94                     | 0.51              |
| 1:1:55:ILE:HG23   | 1:1:85:LEU:HD13   | 1.93                     | 0.51              |
| 2:2:36:ARG:CZ     | 2:2:38:SER:CA     | 2.88                     | 0.51              |
| 3:3:28:SER:CB     | 4:4:127:LEU:HD21  | 2.40                     | 0.51              |
| 5:5:179:HIS:HB3   | 5:5:188:HIS:NE2   | 2.26                     | 0.51              |
| 8:A:54:ILE:CG2    | 8:A:210:MET:CE    | 2.86                     | 0.51              |
| 8:A:54:ILE:HD13   | 8:A:207:ILE:HG13  | 1.92                     | 0.51              |
| 12:E:15:PHE:HD1   | 12:E:21:LEU:CD1   | 2.18                     | 0.51              |
| 19:L:196:VAL:HG11 | 19:L:345:ARG:HE   | 1.75                     | 0.51              |
| 19:L:264:ARG:HA   | 19:L:311:GLN:NE2  | 2.26                     | 0.51              |
| 22:O:15:ARG:HH11  | 22:O:72:LYS:HG2   | 1.76                     | 0.51              |
| 22:O:41:LEU:HG    | 22:O:58:ARG:HG3   | 1.91                     | 0.51              |
| 24:Q:146:TYR:CZ   | 24:Q:183:LYS:O    | 2.64                     | 0.51              |
| 26:S:315:LYS:HB2  | 26:S:345:TYR:OH   | 2.11                     | 0.51              |
| 26:S:399:TYR:CD2  | 26:S:401:LYS:O    | 2.50                     | 0.51              |
| 30:W:76:LEU:O     | 30:W:79:THR:HG23  | 2.10                     | 0.51              |
| 33:Z:71:LEU:CD2   | 33:Z:118:VAL:CG1  | 2.89                     | 0.51              |
| 33:Z:497:PHE:CD2  | 33:Z:505:VAL:HG11 | 2.45                     | 0.51              |
| 33:Z:866:VAL:HB   | 33:Z:873:LEU:CG   | 2.36                     | 0.51              |
| 6:6:141:LEU:HD11  | 6:6:145:VAL:HG21  | 1.93                     | 0.51              |
| 8:A:54:ILE:HD12   | 8:A:206:ALA:CB    | 2.41                     | 0.51              |
| 9:B:184:GLU:HG2   | 9:B:185:LEU:N     | 2.26                     | 0.51              |
| 18:K:244:HIS:CD2  | 19:L:256:ILE:HG23 | 2.46                     | 0.51              |
| 19:L:281:ASP:OD2  | 19:L:282:GLU:HG2  | 2.11                     | 0.51              |
| 21:N:349:ILE:O    | 21:N:353:LEU:HD23 | 2.11                     | 0.51              |
| 26:S:157:GLU:HG2  | 26:S:161:LYS:HE3  | 1.93                     | 0.51              |
| 27:T:151:TRP:CZ3  | 27:T:159:LYS:HB3  | 2.45                     | 0.51              |
| 28:U:83:ILE:HG21  | 29:V:70:ALA:HB3   | 1.93                     | 0.51              |
| 29:V:168:LEU:CD1  | 29:V:188:LEU:HG   | 2.41                     | 0.51              |
| 33:Z:138:ARG:CZ   | 33:Z:157:LEU:CD1  | 2.86                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:208:VAL:HG11 | 33:Z:236:PHE:CG   | 2.44                     | 0.51              |
| 4:4:17:SER:HB3    | 4:4:33:LYS:CD     | 2.40                     | 0.51              |
| 8:A:205:PHE:HZ    | 8:A:209:HIS:CE1   | 2.09                     | 0.51              |
| 9:B:219:PRO:HA    | 9:B:222:LEU:CD1   | 2.33                     | 0.51              |
| 9:B:248:GLU:OE1   | 24:Q:95:LYS:HD2   | 2.11                     | 0.51              |
| 14:G:106:ILE:HG13 | 14:G:107:PRO:O    | 2.11                     | 0.51              |
| 18:K:243:VAL:O    | 18:K:243:VAL:HG12 | 2.09                     | 0.51              |
| 19:L:178:ILE:HD11 | 19:L:230:LEU:CA   | 2.41                     | 0.51              |
| 23:P:156:ALA:O    | 23:P:159:ILE:HG22 | 2.10                     | 0.51              |
| 23:P:395:ARG:HD2  | 24:Q:357:VAL:CB   | 2.41                     | 0.51              |
| 25:R:168:ILE:HG13 | 25:R:206:ARG:HH21 | 1.75                     | 0.51              |
| 33:Z:301:THR:O    | 33:Z:307:HIS:HE1  | 1.94                     | 0.51              |
| 33:Z:491:LEU:O    | 33:Z:495:ILE:HG13 | 2.11                     | 0.51              |
| 33:Z:591:ILE:HG22 | 33:Z:593:HIS:CD2  | 2.46                     | 0.51              |
| 7:7:48:ASP:OD1    | 7:7:50:SER:N      | 2.43                     | 0.51              |
| 8:A:164:VAL:HG12  | 9:B:61:LEU:CD2    | 2.39                     | 0.51              |
| 13:F:157:TYR:CZ   | 14:G:59:VAL:HB    | 2.45                     | 0.51              |
| 19:L:246:SER:OG   | 19:L:280:MET:HA   | 2.11                     | 0.51              |
| 21:N:121:GLU:O    | 21:N:122:GLN:NE2  | 2.44                     | 0.51              |
| 21:N:235:ALA:HA   | 21:N:273:LEU:HD21 | 1.92                     | 0.51              |
| 25:R:222:ARG:CA   | 25:R:224:PHE:CE2  | 2.93                     | 0.51              |
| 8:A:117:LEU:CD2   | 8:A:143:PHE:CE1   | 2.94                     | 0.51              |
| 13:F:80:ASP:OD2   | 13:F:128:TYR:O    | 2.29                     | 0.51              |
| 14:G:118:TYR:HE2  | 14:G:131:PHE:HZ   | 1.58                     | 0.51              |
| 15:H:308:PHE:CE1  | 15:H:351:VAL:CG1  | 2.94                     | 0.51              |
| 16:I:204:HIS:CD2  | 33:Z:930:GLY:HA2  | 2.46                     | 0.51              |
| 17:J:248:ASP:O    | 17:J:249:GLU:HB3  | 2.11                     | 0.51              |
| 17:J:328:LEU:CD2  | 17:J:343:LEU:HD22 | 2.41                     | 0.51              |
| 20:M:384:ASP:N    | 20:M:386:PHE:CE1  | 2.77                     | 0.51              |
| 21:N:70:TYR:CE1   | 21:N:100:THR:HB   | 2.46                     | 0.51              |
| 21:N:207:LEU:HB3  | 21:N:232:LEU:HD21 | 1.91                     | 0.51              |
| 21:N:394:ARG:HA   | 21:N:401:LYS:HZ1  | 1.76                     | 0.51              |
| 22:O:151:ASP:O    | 22:O:154:GLU:HB2  | 2.11                     | 0.51              |
| 24:Q:273:ASN:OD1  | 24:Q:306:TYR:OH   | 2.26                     | 0.51              |
| 24:Q:311:LEU:HD21 | 24:Q:343:LEU:HD13 | 1.91                     | 0.51              |
| 24:Q:391:ASP:OD1  | 25:R:347:THR:HB   | 2.11                     | 0.51              |
| 33:Z:493:LEU:CD1  | 33:Z:497:PHE:CE1  | 2.84                     | 0.51              |
| 33:Z:562:TRP:CD1  | 33:Z:566:LEU:CG   | 2.81                     | 0.51              |
| 1:1:11:GLY:CA     | 1:1:102:TYR:CD1   | 2.94                     | 0.50              |
| 3:3:63:ASN:HB3    | 10:C:96:GLN:HE22  | 1.76                     | 0.50              |
| 3:3:83:SER:CB     | 3:3:121:ILE:HD11  | 2.40                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:17:SER:HB3    | 4:4:33:LYS:HD2    | 1.93                     | 0.50              |
| 5:5:179:HIS:CB    | 5:5:188:HIS:NE2   | 2.74                     | 0.50              |
| 6:6:66:TYR:CE2    | 6:6:73:LYS:C      | 2.84                     | 0.50              |
| 8:A:15:HIS:HB3    | 10:C:6:TYR:CE1    | 2.46                     | 0.50              |
| 10:C:38:ILE:HD12  | 10:C:193:ALA:HB2  | 1.93                     | 0.50              |
| 15:H:382:LEU:HD23 | 15:H:385:ARG:NH1  | 2.25                     | 0.50              |
| 16:I:349:LEU:C    | 16:I:349:LEU:HD12 | 2.37                     | 0.50              |
| 18:K:100:LEU:HB3  | 18:K:109:ILE:O    | 2.12                     | 0.50              |
| 21:N:32:VAL:HG11  | 21:N:67:LYS:HB2   | 1.94                     | 0.50              |
| 21:N:756:THR:HB   | 21:N:900:ASN:ND2  | 2.26                     | 0.50              |
| 31:X:37:PRO:HA    | 31:X:46:TRP:CE3   | 2.46                     | 0.50              |
| 33:Z:96:TYR:HB3   | 33:Z:97:PRO:HD3   | 1.93                     | 0.50              |
| 33:Z:443:ASP:CB   | 33:Z:447:VAL:HB   | 2.38                     | 0.50              |
| 3:3:57:MET:O      | 3:3:61:LYS:HG3    | 2.11                     | 0.50              |
| 5:5:76:VAL:CG2    | 5:5:103:GLY:HA3   | 2.41                     | 0.50              |
| 8:A:203:VAL:O     | 8:A:207:ILE:HG13  | 2.12                     | 0.50              |
| 12:E:165:TYR:CD2  | 20:M:434:ALA:HB2  | 2.46                     | 0.50              |
| 16:I:208:TYR:CE1  | 16:I:209:GLU:CG   | 2.91                     | 0.50              |
| 21:N:521:LEU:HD23 | 21:N:524:ILE:HD12 | 1.92                     | 0.50              |
| 21:N:579:SER:HA   | 21:N:584:ARG:CZ   | 2.41                     | 0.50              |
| 21:N:599:TYR:CE1  | 21:N:634:LEU:HD22 | 2.46                     | 0.50              |
| 26:S:203:SER:O    | 26:S:204:ASP:CB   | 2.60                     | 0.50              |
| 27:T:229:VAL:HG12 | 27:T:230:ASN:H    | 1.75                     | 0.50              |
| 1:1:42:TRP:CD1    | 1:1:178:LEU:HD11  | 2.46                     | 0.50              |
| 2:2:217:ILE:HG22  | 3:3:187:VAL:HG22  | 1.93                     | 0.50              |
| 8:A:156:LYS:CB    | 8:A:166:TYR:CE1   | 2.87                     | 0.50              |
| 11:D:7:ALA:N      | 12:E:125:GLU:OE1  | 2.44                     | 0.50              |
| 15:H:208:TYR:CD1  | 15:H:211:VAL:HG11 | 2.46                     | 0.50              |
| 16:I:255:LYS:HG3  | 18:K:284:ALA:O    | 2.11                     | 0.50              |
| 20:M:196:ALA:HA   | 20:M:345:ARG:HH21 | 1.77                     | 0.50              |
| 21:N:138:GLU:HG2  | 21:N:162:ARG:HH12 | 1.76                     | 0.50              |
| 21:N:749:LEU:HD23 | 21:N:753:PHE:CZ   | 2.46                     | 0.50              |
| 22:O:146:ALA:O    | 22:O:150:LEU:HG   | 2.12                     | 0.50              |
| 23:P:274:GLY:N    | 23:P:277:GLN:HE21 | 2.09                     | 0.50              |
| 24:Q:146:TYR:HE1  | 24:Q:184:VAL:CA   | 2.05                     | 0.50              |
| 25:R:338:TYR:CD1  | 25:R:377:LEU:HD13 | 2.46                     | 0.50              |
| 27:T:229:VAL:HB   | 27:T:234:TYR:CE1  | 2.44                     | 0.50              |
| 3:3:60:TYR:CE2    | 10:C:96:GLN:HB2   | 2.45                     | 0.50              |
| 9:B:35:LEU:C      | 9:B:35:LEU:HD12   | 2.37                     | 0.50              |
| 14:G:168:ARG:NE   | 14:G:172:LYS:HZ2  | 2.06                     | 0.50              |
| 15:H:155:PHE:CE2  | 20:M:76:PRO:CB    | 2.95                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:172:MET:HG3  | 16:I:129:TYR:HD2  | 1.69                     | 0.50              |
| 15:H:358:PRO:HA   | 15:H:361:LEU:HD12 | 1.92                     | 0.50              |
| 18:K:67:TYR:OH    | 21:N:609:LEU:HD21 | 2.12                     | 0.50              |
| 21:N:406:TYR:HE1  | 21:N:448:LEU:HB3  | 1.73                     | 0.50              |
| 21:N:771:PHE:HE2  | 21:N:773:MET:HG2  | 1.73                     | 0.50              |
| 22:O:122:HIS:C    | 22:O:166:ARG:HH12 | 2.20                     | 0.50              |
| 26:S:288:THR:CG2  | 26:S:292:TYR:HE2  | 2.24                     | 0.50              |
| 3:3:155:PHE:CE1   | 3:3:189:ARG:CD    | 2.88                     | 0.50              |
| 7:7:103:TRP:O     | 7:7:103:TRP:CG    | 2.60                     | 0.50              |
| 8:A:229:THR:OG1   | 8:A:232:LYS:HG3   | 2.12                     | 0.50              |
| 14:G:200:TYR:CD1  | 14:G:200:TYR:C    | 2.89                     | 0.50              |
| 16:I:228:GLY:O    | 16:I:232:LEU:HG   | 2.12                     | 0.50              |
| 21:N:536:ILE:HD13 | 21:N:555:ILE:HG13 | 1.89                     | 0.50              |
| 23:P:203:ILE:CG2  | 23:P:220:TYR:CZ   | 2.95                     | 0.50              |
| 26:S:316:LEU:O    | 26:S:320:ILE:HG13 | 2.12                     | 0.50              |
| 27:T:220:PHE:HB3  | 27:T:224:ARG:NH1  | 2.27                     | 0.50              |
| 3:3:100:VAL:HG21  | 3:3:115:PHE:CE1   | 2.47                     | 0.50              |
| 5:5:101:ILE:HD12  | 5:5:115:VAL:HG21  | 1.93                     | 0.50              |
| 6:6:49:ALA:HB3    | 7:7:127:VAL:HG22  | 1.92                     | 0.50              |
| 9:B:139:HIS:HD2   | 9:B:234:ARG:NE    | 2.09                     | 0.50              |
| 14:G:111:PHE:HD1  | 14:G:114:ARG:CZ   | 2.19                     | 0.50              |
| 21:N:16:ASN:HA    | 21:N:21:LYS:NZ    | 2.27                     | 0.50              |
| 21:N:50:TYR:CD1   | 21:N:62:ALA:HB2   | 2.47                     | 0.50              |
| 21:N:756:THR:HB   | 21:N:900:ASN:HD22 | 1.77                     | 0.50              |
| 24:Q:39:SER:OG    | 24:Q:88:PHE:HB2   | 2.11                     | 0.50              |
| 26:S:315:LYS:NZ   | 26:S:345:TYR:HE1  | 2.06                     | 0.50              |
| 31:X:72:GLU:O     | 31:X:91:PHE:CD2   | 2.64                     | 0.50              |
| 33:Z:298:PHE:CZ   | 33:Z:314:LEU:HD22 | 2.46                     | 0.50              |
| 33:Z:577:GLN:O    | 33:Z:580:GLN:HG2  | 2.12                     | 0.50              |
| 7:7:77:GLU:O      | 7:7:77:GLU:HG3    | 2.12                     | 0.50              |
| 9:B:75:TYR:HB3    | 9:B:134:LEU:HD23  | 1.91                     | 0.50              |
| 9:B:249:ALA:HB1   | 24:Q:94:VAL:HG12  | 1.93                     | 0.50              |
| 15:H:295:PHE:CZ   | 15:H:336:LEU:CD1  | 2.91                     | 0.50              |
| 18:K:241:GLU:HA   | 19:L:303:ARG:HH12 | 1.74                     | 0.50              |
| 19:L:178:ILE:HD11 | 19:L:230:LEU:HA   | 1.93                     | 0.50              |
| 19:L:412:PRO:O    | 19:L:416:MET:HG3  | 2.11                     | 0.50              |
| 22:O:30:GLU:HG2   | 22:O:58:ARG:CZ    | 2.42                     | 0.50              |
| 26:S:327:ILE:HG21 | 26:S:349:THR:CG2  | 2.42                     | 0.50              |
| 33:Z:433:LEU:HD13 | 33:Z:468:GLU:HB3  | 1.93                     | 0.50              |
| 4:4:143:LEU:CD2   | 4:4:159:LEU:HD21  | 2.42                     | 0.50              |
| 6:6:17:ASP:OD2    | 6:6:189:VAL:HG22  | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:6:MET:HE1     | 7:7:150:VAL:CG1   | 2.32                     | 0.50              |
| 11:D:11:PHE:HE2   | 12:E:26:TYR:C     | 2.19                     | 0.50              |
| 13:F:43:HIS:CD2   | 13:F:218:LYS:H    | 2.29                     | 0.50              |
| 14:G:193:LYS:HE2  | 14:G:241:PHE:CB   | 2.23                     | 0.50              |
| 18:K:98:GLN:NE2   | 18:K:136:SER:CB   | 2.69                     | 0.50              |
| 19:L:178:ILE:CD1  | 19:L:230:LEU:CD2  | 2.87                     | 0.50              |
| 20:M:75:LEU:HD22  | 20:M:77:TYR:H     | 1.77                     | 0.50              |
| 20:M:203:ARG:HB3  | 20:M:206:LYS:HD2  | 1.94                     | 0.50              |
| 21:N:492:THR:CA   | 21:N:528:ARG:HH11 | 2.24                     | 0.50              |
| 23:P:152:LYS:HD3  | 23:P:155:GLU:OE1  | 2.12                     | 0.50              |
| 25:R:417:TYR:OH   | 28:U:292:ILE:CG2  | 2.60                     | 0.50              |
| 33:Z:64:TYR:HE2   | 33:Z:111:LEU:HB3  | 1.74                     | 0.50              |
| 33:Z:79:THR:O     | 33:Z:80:SER:HB3   | 2.11                     | 0.50              |
| 1:1:-8:LYS:HZ1    | 2:2:117:GLY:CA    | 2.24                     | 0.50              |
| 1:1:19:ARG:CZ     | 1:1:170:GLY:C     | 2.85                     | 0.50              |
| 4:4:106:TYR:CE1   | 4:4:185:LYS:HA    | 2.47                     | 0.50              |
| 8:A:18:ILE:HA     | 9:B:128:ARG:HH11  | 1.76                     | 0.50              |
| 8:A:130:GLN:HG2   | 9:B:128:ARG:HG2   | 1.93                     | 0.50              |
| 17:J:349:LYS:HZ3  | 17:J:383:GLU:CG   | 2.25                     | 0.50              |
| 18:K:55:GLU:O     | 18:K:59:GLU:HG3   | 2.11                     | 0.50              |
| 18:K:159:SER:HG   | 18:K:244:HIS:CE1  | 2.18                     | 0.50              |
| 21:N:84:ALA:O     | 21:N:86:LYS:HG3   | 2.11                     | 0.50              |
| 21:N:353:LEU:N    | 21:N:354:PRO:CD   | 2.75                     | 0.50              |
| 22:O:30:GLU:CB    | 22:O:58:ARG:NH1   | 2.75                     | 0.50              |
| 23:P:160:LEU:HD12 | 23:P:186:LEU:HD12 | 1.93                     | 0.50              |
| 23:P:343:LYS:O    | 23:P:347:GLU:HG3  | 2.12                     | 0.50              |
| 24:Q:9:GLU:HG2    | 24:Q:13:ARG:NH1   | 2.26                     | 0.50              |
| 24:Q:38:SER:OG    | 24:Q:88:PHE:CD1   | 2.51                     | 0.50              |
| 24:Q:38:SER:HG    | 24:Q:88:PHE:HE1   | 1.42                     | 0.50              |
| 24:Q:61:LEU:CD2   | 24:Q:65:TYR:CZ    | 2.94                     | 0.50              |
| 26:S:242:LEU:HD13 | 26:S:278:LYS:HD3  | 1.93                     | 0.50              |
| 26:S:250:ALA:HB2  | 26:S:279:ILE:HD13 | 1.94                     | 0.50              |
| 29:V:292:ILE:O    | 29:V:296:LEU:HG   | 2.12                     | 0.50              |
| 33:Z:405:ASN:O    | 33:Z:409:LYS:HG3  | 2.12                     | 0.50              |
| 3:3:-2:ASN:HD21   | 3:3:48:ALA:N      | 2.09                     | 0.49              |
| 4:4:103:ILE:HD12  | 4:4:118:ILE:CD1   | 2.40                     | 0.49              |
| 7:7:1:THR:H       | 7:7:19:LEU:HD23   | 1.77                     | 0.49              |
| 10:C:147:GLN:HB3  | 10:C:149:TYR:CE1  | 2.47                     | 0.49              |
| 11:D:193:LYS:HG3  | 11:D:197:ARG:HH12 | 1.72                     | 0.49              |
| 15:H:147:ILE:HD12 | 15:H:181:TYR:CB   | 2.40                     | 0.49              |
| 15:H:295:PHE:CE1  | 15:H:336:LEU:HD12 | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:J:363:THR:HA   | 18:K:203:ILE:HD11 | 1.93                     | 0.49              |
| 18:K:241:GLU:HA   | 19:L:303:ARG:HH11 | 1.75                     | 0.49              |
| 21:N:221:ASP:HB3  | 21:N:894:ARG:HH22 | 1.77                     | 0.49              |
| 21:N:304:LEU:HD23 | 21:N:343:THR:O    | 2.12                     | 0.49              |
| 22:O:195:TYR:CD2  | 22:O:213:LEU:HD22 | 2.46                     | 0.49              |
| 22:O:199:LEU:HD12 | 22:O:203:THR:O    | 2.11                     | 0.49              |
| 22:O:250:TRP:NE1  | 22:O:269:LEU:O    | 2.44                     | 0.49              |
| 23:P:77:GLU:O     | 23:P:81:LEU:HG    | 2.12                     | 0.49              |
| 25:R:258:LEU:HD11 | 25:R:288:SER:HA   | 1.94                     | 0.49              |
| 30:W:139:VAL:CG1  | 30:W:157:PHE:HE2  | 2.18                     | 0.49              |
| 33:Z:442:VAL:O    | 33:Z:443:ASP:HB2  | 2.12                     | 0.49              |
| 33:Z:562:TRP:CZ2  | 33:Z:566:LEU:HD21 | 2.46                     | 0.49              |
| 33:Z:850:LEU:CD2  | 33:Z:854:LEU:CD1  | 2.89                     | 0.49              |
| 1:1:112:THR:HG22  | 7:7:27:ARG:NH2    | 2.27                     | 0.49              |
| 4:4:37:LEU:HD12   | 4:4:60:GLN:HA     | 1.94                     | 0.49              |
| 5:5:159:ARG:NH1   | 5:5:204:GLU:HB2   | 2.27                     | 0.49              |
| 11:D:13:PRO:HB3   | 12:E:26:TYR:CZ    | 2.46                     | 0.49              |
| 11:D:236:ILE:CG2  | 11:D:240:LYS:HE3  | 2.42                     | 0.49              |
| 14:G:68:VAL:HG12  | 14:G:69:VAL:N     | 2.28                     | 0.49              |
| 15:H:172:MET:HB3  | 16:I:129:TYR:HD2  | 1.48                     | 0.49              |
| 15:H:385:ARG:O    | 15:H:389:PHE:CD2  | 2.65                     | 0.49              |
| 17:J:143:PRO:HB2  | 17:J:204:HIS:HB2  | 1.93                     | 0.49              |
| 18:K:170:THR:N    | 18:K:173:ASP:OD2  | 2.37                     | 0.49              |
| 18:K:329:LEU:HA   | 18:K:334:LEU:HD23 | 1.93                     | 0.49              |
| 21:N:223:LEU:HD22 | 21:N:897:LYS:HB2  | 1.92                     | 0.49              |
| 21:N:338:PHE:CE1  | 21:N:749:LEU:HB3  | 2.47                     | 0.49              |
| 21:N:515:ARG:NH2  | 21:N:741:TYR:CD2  | 2.80                     | 0.49              |
| 24:Q:50:ARG:HH21  | 24:Q:53:GLU:HB2   | 1.74                     | 0.49              |
| 25:R:164:THR:HG21 | 25:R:199:GLU:OE1  | 2.11                     | 0.49              |
| 27:T:1:MET:HB3    | 27:T:9:LYS:NZ     | 2.27                     | 0.49              |
| 28:U:52:PHE:CD2   | 28:U:72:TYR:HE2   | 2.30                     | 0.49              |
| 33:Z:49:LEU:C     | 33:Z:49:LEU:HD12  | 2.37                     | 0.49              |
| 33:Z:165:TYR:CE1  | 33:Z:196:SER:HB3  | 2.47                     | 0.49              |
| 33:Z:502:ASN:O    | 33:Z:505:VAL:HG22 | 2.11                     | 0.49              |
| 33:Z:557:GLU:OE1  | 33:Z:562:TRP:HE3  | 1.95                     | 0.49              |
| 33:Z:805:LEU:CD2  | 33:Z:841:GLU:CD   | 2.72                     | 0.49              |
| 1:1:55:ILE:HG23   | 1:1:85:LEU:CD1    | 2.42                     | 0.49              |
| 6:6:141:LEU:HD12  | 6:6:145:VAL:HG23  | 1.95                     | 0.49              |
| 10:C:41:SER:HB3   | 10:C:184:MET:HE3  | 1.94                     | 0.49              |
| 11:D:31:THR:OG1   | 11:D:76:SER:HA    | 2.12                     | 0.49              |
| 13:F:152:ASN:ND2  | 14:G:81:ILE:HD12  | 2.26                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:J:142:VAL:O    | 17:J:142:VAL:HG12 | 2.12                     | 0.49              |
| 17:J:224:GLY:O    | 17:J:225:GLU:C    | 2.55                     | 0.49              |
| 17:J:247:MET:CE   | 17:J:272:MET:HG3  | 2.42                     | 0.49              |
| 23:P:101:MET:CE   | 23:P:119:ILE:HD11 | 2.42                     | 0.49              |
| 23:P:241:LEU:HD23 | 23:P:264:ILE:HG13 | 1.93                     | 0.49              |
| 23:P:287:ASP:HB3  | 23:P:297:GLU:CD   | 2.37                     | 0.49              |
| 25:R:397:ASN:HD22 | 26:S:451:ILE:C    | 2.20                     | 0.49              |
| 28:U:46:ILE:HG21  | 28:U:119:LEU:HD22 | 1.92                     | 0.49              |
| 28:U:52:PHE:CE2   | 28:U:76:MET:HE2   | 2.47                     | 0.49              |
| 28:U:54:LEU:CD2   | 28:U:72:TYR:CD2   | 2.96                     | 0.49              |
| 30:W:76:LEU:C     | 30:W:79:THR:HG23  | 2.37                     | 0.49              |
| 33:Z:205:LEU:HA   | 33:Z:236:PHE:HZ   | 1.77                     | 0.49              |
| 2:2:109:HIS:HB3   | 2:2:111:PHE:HE2   | 1.77                     | 0.49              |
| 11:D:193:LYS:HE2  | 11:D:197:ARG:NH2  | 2.27                     | 0.49              |
| 15:H:307:PHE:CE2  | 15:H:309:ASP:OD1  | 2.66                     | 0.49              |
| 17:J:29:GLU:O     | 17:J:32:LEU:HB3   | 2.12                     | 0.49              |
| 18:K:346:ARG:CG   | 18:K:349:ARG:NH2  | 2.61                     | 0.49              |
| 20:M:129:LEU:HD21 | 20:M:155:ILE:HG13 | 1.95                     | 0.49              |
| 20:M:338:LEU:HD21 | 20:M:346:LYS:NZ   | 2.27                     | 0.49              |
| 22:O:41:LEU:CD2   | 22:O:62:TYR:HB2   | 2.42                     | 0.49              |
| 22:O:384:MET:HE3  | 28:U:190:LEU:CA   | 2.42                     | 0.49              |
| 23:P:292:LYS:HG2  | 23:P:320:PRO:HB2  | 1.93                     | 0.49              |
| 25:R:338:TYR:CZ   | 25:R:368:LEU:HD11 | 2.48                     | 0.49              |
| 29:V:52:LEU:HD12  | 29:V:69:PHE:HZ    | 1.77                     | 0.49              |
| 29:V:84:ASP:OD2   | 29:V:87:PHE:HB2   | 2.12                     | 0.49              |
| 30:W:9:VAL:HA     | 30:W:52:ILE:HG13  | 1.94                     | 0.49              |
| 30:W:35:PHE:CE2   | 30:W:182:TYR:CE2  | 3.00                     | 0.49              |
| 33:Z:532:HIS:O    | 33:Z:535:VAL:HG23 | 2.11                     | 0.49              |
| 1:1:123:PRO:HG2   | 1:1:124:TYR:CD1   | 2.47                     | 0.49              |
| 5:5:1:THR:HA      | 5:5:17:ASP:OD2    | 2.13                     | 0.49              |
| 7:7:17:ASP:C      | 7:7:17:ASP:OD1    | 2.56                     | 0.49              |
| 8:A:148:GLU:OE2   | 8:A:230:LYS:HG3   | 2.12                     | 0.49              |
| 11:D:181:ARG:NH1  | 12:E:57:PRO:O     | 2.45                     | 0.49              |
| 15:H:274:VAL:HG21 | 15:H:308:PHE:CE2  | 2.48                     | 0.49              |
| 15:H:351:VAL:HG11 | 15:H:353:PHE:CE1  | 2.37                     | 0.49              |
| 16:I:340:ARG:NH1  | 16:I:343:ARG:HG3  | 2.26                     | 0.49              |
| 17:J:162:GLU:HG2  | 17:J:166:LEU:HD12 | 1.94                     | 0.49              |
| 21:N:340:HIS:HB2  | 21:N:374:ILE:HG12 | 1.92                     | 0.49              |
| 21:N:515:ARG:NH2  | 21:N:738:GLN:CD   | 2.65                     | 0.49              |
| 24:Q:176:ASP:O    | 24:Q:180:LEU:HG   | 2.12                     | 0.49              |
| 29:V:254:ARG:O    | 29:V:258:GLU:HG3  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:294:ILE:O    | 33:Z:298:PHE:CD2  | 2.65                     | 0.49              |
| 33:Z:295:ARG:NH2  | 33:Z:325:GLY:HA3  | 2.27                     | 0.49              |
| 33:Z:486:SER:O    | 33:Z:490:ILE:CG1  | 2.25                     | 0.49              |
| 2:2:113:ILE:HG12  | 2:2:119:THR:HG22  | 1.93                     | 0.49              |
| 3:3:100:VAL:HG21  | 3:3:115:PHE:HE1   | 1.78                     | 0.49              |
| 9:B:94:HIS:HA     | 9:B:98:LYS:CE     | 2.43                     | 0.49              |
| 15:H:59:ILE:CD1   | 16:I:92:GLU:CD    | 2.69                     | 0.49              |
| 21:N:162:ARG:CZ   | 21:N:165:ILE:CD1  | 2.91                     | 0.49              |
| 22:O:250:TRP:CZ2  | 22:O:271:LYS:HG2  | 2.47                     | 0.49              |
| 24:Q:246:TYR:HA   | 24:Q:249:LEU:HD12 | 1.93                     | 0.49              |
| 33:Z:463:HIS:CE1  | 33:Z:497:PHE:CD1  | 3.01                     | 0.49              |
| 2:2:59:ILE:O      | 2:2:63:ILE:HG12   | 2.13                     | 0.49              |
| 3:3:109:LYS:CE    | 3:3:125:LYS:NZ    | 2.76                     | 0.49              |
| 5:5:159:ARG:NH2   | 5:5:203:GLU:OE1   | 2.45                     | 0.49              |
| 7:7:-3:VAL:HG23   | 7:7:49:ILE:H      | 1.76                     | 0.49              |
| 7:7:144:ASN:O     | 7:7:148:ARG:HG3   | 2.13                     | 0.49              |
| 9:B:159:TRP:CE2   | 10:C:57:LEU:HD13  | 2.48                     | 0.49              |
| 15:H:392:HIS:CE1  | 15:H:420:ARG:CG   | 2.94                     | 0.49              |
| 16:I:117:HIS:O    | 16:I:118:ALA:HB2  | 2.12                     | 0.49              |
| 17:J:101:ASP:C    | 17:J:102:ILE:HG23 | 2.38                     | 0.49              |
| 18:K:280:LYS:HZ1  | 18:K:296:LEU:CD2  | 2.19                     | 0.49              |
| 19:L:133:ASN:ND2  | 28:U:86:LYS:NZ    | 2.60                     | 0.49              |
| 19:L:165:PRO:HB3  | 19:L:269:TYR:CE2  | 2.48                     | 0.49              |
| 21:N:642:ASP:HB2  | 21:N:643:PRO:CD   | 2.42                     | 0.49              |
| 22:O:188:PHE:HD2  | 22:O:220:SER:HB3  | 1.77                     | 0.49              |
| 23:P:237:VAL:CG1  | 23:P:267:PHE:CE2  | 2.95                     | 0.49              |
| 24:Q:64:LEU:O     | 24:Q:68:MET:HG2   | 2.13                     | 0.49              |
| 27:T:32:ILE:HA    | 27:T:35:ILE:HD12  | 1.95                     | 0.49              |
| 27:T:228:ILE:HG22 | 27:T:229:VAL:O    | 2.13                     | 0.49              |
| 28:U:67:PHE:CE1   | 30:W:97:THR:HG23  | 2.47                     | 0.49              |
| 2:2:73:GLU:O      | 2:2:75:ARG:NH1    | 2.45                     | 0.49              |
| 4:4:37:LEU:HD12   | 4:4:60:GLN:HG2    | 1.95                     | 0.49              |
| 12:E:165:TYR:HE2  | 20:M:433:TYR:O    | 1.96                     | 0.49              |
| 14:G:98:PHE:CE2   | 14:G:104:THR:HG23 | 2.47                     | 0.49              |
| 14:G:149:MET:HE3  | 14:G:151:GLU:OE2  | 2.12                     | 0.49              |
| 16:I:193:GLU:OE1  | 16:I:348:ILE:HG12 | 2.12                     | 0.49              |
| 17:J:151:GLY:HA3  | 17:J:326:GLU:HG3  | 1.95                     | 0.49              |
| 17:J:337:LEU:O    | 25:R:204:TRP:NE1  | 2.46                     | 0.49              |
| 18:K:281:ARG:NH1  | 18:K:287:GLY:O    | 2.46                     | 0.49              |
| 18:K:353:PHE:HD1  | 18:K:387:MET:SD   | 2.36                     | 0.49              |
| 20:M:159:LEU:HB3  | 20:M:160:PRO:HD2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:83:LEU:HD11  | 21:N:133:LEU:HD21 | 1.95                     | 0.49              |
| 21:N:657:MET:CB   | 21:N:682:PHE:CE1  | 2.95                     | 0.49              |
| 22:O:384:MET:HE1  | 28:U:189:ARG:CB   | 2.43                     | 0.49              |
| 23:P:90:LYS:HE3   | 23:P:129:LYS:HB3  | 1.95                     | 0.49              |
| 24:Q:273:ASN:CB   | 24:Q:306:TYR:OH   | 2.59                     | 0.49              |
| 25:R:356:ALA:O    | 32:Y:89:GLN:NE2   | 2.46                     | 0.49              |
| 25:R:417:TYR:CZ   | 28:U:292:ILE:CG2  | 2.95                     | 0.49              |
| 30:W:6:THR:HG21   | 30:W:40:LYS:HZ2   | 1.76                     | 0.49              |
| 31:X:73:THR:HB    | 31:X:129:LEU:HD11 | 1.94                     | 0.49              |
| 2:2:160:GLN:NE2   | 2:2:164:TRP:CE2   | 2.80                     | 0.49              |
| 5:5:145:LYS:HB3   | 5:5:148:LEU:HG    | 1.95                     | 0.49              |
| 15:H:246:ILE:HD11 | 15:H:352:MET:HG2  | 1.95                     | 0.49              |
| 19:L:117:TYR:CE1  | 19:L:131:VAL:HG13 | 2.44                     | 0.49              |
| 19:L:231:LEU:O    | 19:L:235:VAL:HG23 | 2.13                     | 0.49              |
| 21:N:447:SER:HA   | 21:N:450:ILE:HG22 | 1.94                     | 0.49              |
| 22:O:60:ARG:HH21  | 22:O:94:GLU:CD    | 2.20                     | 0.49              |
| 23:P:203:ILE:CG1  | 23:P:220:TYR:CZ   | 2.90                     | 0.49              |
| 23:P:308:LEU:HD21 | 23:P:346:ILE:HA   | 1.95                     | 0.49              |
| 23:P:392:LYS:HG2  | 24:Q:354:PHE:CD2  | 2.47                     | 0.49              |
| 24:Q:59:LEU:HD13  | 24:Q:103:LYS:HG2  | 1.95                     | 0.49              |
| 26:S:343:LEU:HD12 | 26:S:347:HIS:CE1  | 2.48                     | 0.49              |
| 27:T:131:LYS:H    | 27:T:135:ASN:ND2  | 2.11                     | 0.49              |
| 33:Z:889:VAL:HG23 | 33:Z:891:PRO:HD2  | 1.93                     | 0.49              |
| 33:Z:924:LYS:HZ3  | 33:Z:993:GLU:HG3  | 1.74                     | 0.49              |
| 1:1:1:THR:HG22    | 1:1:1:THR:O       | 2.13                     | 0.49              |
| 1:1:120:HIS:CB    | 7:7:28:PHE:CE1    | 2.95                     | 0.49              |
| 6:6:31:GLU:OE1    | 7:7:129:TYR:HB2   | 2.12                     | 0.49              |
| 11:D:7:ALA:CB     | 12:E:125:GLU:OE2  | 2.53                     | 0.49              |
| 12:E:45:GLY:HA2   | 12:E:153:TYR:CE1  | 2.47                     | 0.49              |
| 17:J:56:ARG:NH2   | 21:N:611:LYS:O    | 2.42                     | 0.49              |
| 18:K:216:GLY:HA3  | 19:L:342:ARG:HH22 | 1.75                     | 0.49              |
| 20:M:59:LEU:O     | 20:M:62:ILE:HG22  | 2.13                     | 0.49              |
| 23:P:48:GLN:HE22  | 23:P:86:HIS:CG    | 2.31                     | 0.49              |
| 25:R:113:LEU:HD22 | 25:R:136:ASN:HB3  | 1.94                     | 0.49              |
| 25:R:175:ALA:HB2  | 25:R:209:ARG:HD3  | 1.94                     | 0.49              |
| 26:S:399:TYR:HB3  | 26:S:402:ILE:HD13 | 1.94                     | 0.49              |
| 33:Z:99:LEU:HB2   | 33:Z:119:LEU:HD21 | 1.94                     | 0.49              |
| 33:Z:371:SER:HB3  | 33:Z:399:LEU:HD13 | 1.95                     | 0.49              |
| 33:Z:440:LEU:HD23 | 33:Z:440:LEU:C    | 2.37                     | 0.49              |
| 3:3:-2:ASN:ND2    | 3:3:48:ALA:H      | 2.11                     | 0.48              |
| 8:A:104:PHE:CD1   | 8:A:108:TYR:CD2   | 3.01                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:B:250:LEU:HD22  | 24:Q:132:PHE:CZ   | 2.48                     | 0.48              |
| 11:D:6:ARG:HH12   | 13:F:123:TYR:CB   | 2.26                     | 0.48              |
| 12:E:184:LEU:HD13 | 13:F:56:LEU:HG    | 1.94                     | 0.48              |
| 15:H:65:GLU:O     | 15:H:69:VAL:CG2   | 2.52                     | 0.48              |
| 15:H:418:GLU:O    | 15:H:422:VAL:HG23 | 2.13                     | 0.48              |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:HB   | 1.95                     | 0.48              |
| 17:J:286:LYS:HE3  | 17:J:289:LYS:NZ   | 2.28                     | 0.48              |
| 19:L:228:LYS:HB2  | 19:L:349:ILE:CD1  | 2.43                     | 0.48              |
| 20:M:82:VAL:HG11  | 20:M:140:LEU:HB3  | 1.95                     | 0.48              |
| 21:N:447:SER:O    | 21:N:450:ILE:HG22 | 2.13                     | 0.48              |
| 23:P:72:TRP:HH2   | 23:P:103:TYR:HB2  | 1.56                     | 0.48              |
| 26:S:302:HIS:CD2  | 26:S:303:ASN:CG   | 2.91                     | 0.48              |
| 28:U:293:GLU:CG   | 29:V:277:LYS:HE3  | 2.43                     | 0.48              |
| 29:V:168:LEU:HD11 | 29:V:188:LEU:HG   | 1.95                     | 0.48              |
| 33:Z:74:SER:HB3   | 33:Z:79:THR:CG2   | 2.42                     | 0.48              |
| 33:Z:290:GLU:HB3  | 33:Z:293:MET:HG3  | 1.95                     | 0.48              |
| 33:Z:546:ILE:HG22 | 33:Z:550:PHE:CD2  | 2.48                     | 0.48              |
| 1:1:98:ILE:CD1    | 1:1:127:ALA:HB3   | 2.37                     | 0.48              |
| 4:4:63:ILE:HD11   | 4:4:82:PHE:CD2    | 2.48                     | 0.48              |
| 11:D:120:TYR:CD2  | 11:D:129:PHE:CE1  | 3.01                     | 0.48              |
| 12:E:35:SER:OG    | 12:E:53:ARG:NE    | 2.35                     | 0.48              |
| 12:E:157:HIS:CE1  | 12:E:159:GLU:OE2  | 2.65                     | 0.48              |
| 16:I:362:LEU:CD2  | 16:I:377:LEU:CD2  | 2.91                     | 0.48              |
| 17:J:186:ILE:CG2  | 17:J:313:LYS:HG2  | 2.44                     | 0.48              |
| 17:J:210:PHE:CE2  | 17:J:212:ARG:HG3  | 2.48                     | 0.48              |
| 19:L:92:GLU:CG    | 20:M:65:ASN:HD21  | 2.26                     | 0.48              |
| 19:L:125:PRO:HG2  | 19:L:127:TYR:OH   | 2.13                     | 0.48              |
| 19:L:140:LEU:HD21 | 19:L:158:ILE:HD11 | 1.94                     | 0.48              |
| 19:L:193:LEU:HD21 | 19:L:347:VAL:HG21 | 1.94                     | 0.48              |
| 19:L:357:ARG:HB3  | 19:L:361:PHE:HE2  | 1.77                     | 0.48              |
| 20:M:167:VAL:HG23 | 20:M:269:LEU:CD1  | 2.43                     | 0.48              |
| 22:O:41:LEU:C     | 22:O:41:LEU:HD12  | 2.39                     | 0.48              |
| 23:P:306:ASN:OD1  | 23:P:306:ASN:O    | 2.31                     | 0.48              |
| 23:P:311:TRP:CD1  | 23:P:345:VAL:HG21 | 2.48                     | 0.48              |
| 24:Q:141:LEU:HG   | 24:Q:145:HIS:HD2  | 1.74                     | 0.48              |
| 24:Q:239:PHE:CE2  | 24:Q:264:TYR:HB3  | 2.48                     | 0.48              |
| 31:X:120:GLU:O    | 31:X:124:LYS:HG3  | 2.13                     | 0.48              |
| 33:Z:103:TYR:HE1  | 33:Z:116:ALA:CB   | 2.25                     | 0.48              |
| 33:Z:781:GLY:HA2  | 33:Z:818:CYS:SG   | 2.54                     | 0.48              |
| 1:1:143:ARG:HG2   | 1:1:144:GLU:O     | 2.14                     | 0.48              |
| 2:2:210:THR:HG23  | 3:3:160:GLN:NE2   | 2.27                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:40:HIS:CE1    | 4:4:108:LYS:HD3   | 2.49                     | 0.48              |
| 6:6:17:ASP:C      | 6:6:17:ASP:OD1    | 2.56                     | 0.48              |
| 9:B:66:LEU:CD1    | 9:B:235:PHE:CE2   | 2.87                     | 0.48              |
| 12:E:14:THR:HG22  | 12:E:22:PHE:HE2   | 1.78                     | 0.48              |
| 12:E:121:LEU:HD22 | 13:F:79:PRO:HB3   | 1.95                     | 0.48              |
| 15:H:171:GLY:O    | 16:I:129:TYR:CE1  | 2.66                     | 0.48              |
| 16:I:290:LYS:CE   | 16:I:336:PRO:HD3  | 2.43                     | 0.48              |
| 17:J:326:GLU:OE2  | 17:J:329:ARG:NH2  | 2.43                     | 0.48              |
| 19:L:169:ASN:HD22 | 19:L:262:ILE:HD13 | 1.79                     | 0.48              |
| 21:N:223:LEU:O    | 21:N:227:LYS:HG3  | 2.13                     | 0.48              |
| 21:N:776:TYR:HD2  | 21:N:881:TYR:HB3  | 1.77                     | 0.48              |
| 24:Q:164:GLU:O    | 24:Q:168:LEU:HB2  | 2.12                     | 0.48              |
| 25:R:130:GLN:NE2  | 25:R:134:TRP:NE1  | 2.48                     | 0.48              |
| 27:T:108:LEU:HD23 | 27:T:174:PHE:HE1  | 1.76                     | 0.48              |
| 33:Z:56:LEU:HD23  | 33:Z:68:LEU:CD2   | 2.41                     | 0.48              |
| 6:6:91:LYS:O      | 6:6:96:TYR:CE1    | 2.66                     | 0.48              |
| 8:A:158:ASP:OD2   | 8:A:162:TYR:HB3   | 2.13                     | 0.48              |
| 12:E:70:ILE:HD12  | 12:E:74:ILE:HG22  | 1.95                     | 0.48              |
| 13:F:49:LEU:CD2   | 13:F:201:LEU:HD21 | 2.43                     | 0.48              |
| 15:H:101:ARG:NH2  | 15:H:150:LYS:HD3  | 2.27                     | 0.48              |
| 16:I:141:LEU:HD21 | 16:I:159:VAL:HB   | 1.94                     | 0.48              |
| 17:J:146:THR:HG22 | 17:J:149:MET:HB2  | 1.95                     | 0.48              |
| 18:K:71:GLU:OE2   | 21:N:576:VAL:CG2  | 2.55                     | 0.48              |
| 20:M:129:LEU:C    | 20:M:129:LEU:HD12 | 2.38                     | 0.48              |
| 21:N:14:ARG:HH21  | 21:N:42:GLU:CD    | 2.21                     | 0.48              |
| 21:N:492:THR:C    | 21:N:528:ARG:HH11 | 2.20                     | 0.48              |
| 24:Q:141:LEU:CG   | 24:Q:145:HIS:NE2  | 2.76                     | 0.48              |
| 26:S:390:THR:HA   | 26:S:393:ARG:NH1  | 2.29                     | 0.48              |
| 26:S:425:ARG:HH12 | 27:T:155:GLY:N    | 2.11                     | 0.48              |
| 27:T:220:PHE:HB3  | 27:T:224:ARG:HH12 | 1.78                     | 0.48              |
| 28:U:293:GLU:HG2  | 29:V:277:LYS:HE3  | 1.94                     | 0.48              |
| 33:Z:321:PHE:CZ   | 33:Z:349:THR:O    | 2.67                     | 0.48              |
| 33:Z:481:PRO:O    | 33:Z:482:ASP:HB2  | 2.13                     | 0.48              |
| 1:1:126:ILE:HD12  | 1:1:131:SER:O     | 2.13                     | 0.48              |
| 3:3:64:LEU:CD1    | 10:C:92:ARG:HB3   | 2.43                     | 0.48              |
| 8:A:117:LEU:HD23  | 8:A:143:PHE:CE1   | 2.49                     | 0.48              |
| 10:C:29:ILE:HD11  | 10:C:153:PRO:HD3  | 1.95                     | 0.48              |
| 11:D:64:VAL:HG11  | 11:D:213:THR:HG21 | 1.95                     | 0.48              |
| 13:F:159:THR:HA   | 13:F:169:LYS:CE   | 2.40                     | 0.48              |
| 15:H:381:ASP:C    | 15:H:381:ASP:OD1  | 2.55                     | 0.48              |
| 15:H:428:MET:CG   | 16:I:346:ARG:HH21 | 2.24                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:172:LYS:CD   | 17:J:231:ARG:HH12 | 2.27                     | 0.48              |
| 16:I:384:LYS:CD   | 16:I:420:LYS:HD2  | 2.37                     | 0.48              |
| 17:J:32:LEU:HD22  | 26:S:225:HIS:CE1  | 2.49                     | 0.48              |
| 19:L:371:THR:HG21 | 19:L:411:ASN:HD22 | 1.78                     | 0.48              |
| 20:M:72:ASN:HB3   | 20:M:156:LEU:HD22 | 1.94                     | 0.48              |
| 20:M:207:PHE:CD2  | 20:M:212:ILE:HD11 | 2.49                     | 0.48              |
| 21:N:183:VAL:HG21 | 21:N:221:ASP:OD2  | 2.13                     | 0.48              |
| 23:P:332:GLU:O    | 23:P:333:ALA:HB2  | 2.14                     | 0.48              |
| 24:Q:165:PHE:CE2  | 24:Q:173:SER:OG   | 2.60                     | 0.48              |
| 25:R:70:TYR:O     | 25:R:70:TYR:CG    | 2.63                     | 0.48              |
| 26:S:451:ILE:O    | 26:S:452:TYR:HB2  | 2.13                     | 0.48              |
| 27:T:89:TYR:CE1   | 27:T:102:LYS:HB2  | 2.49                     | 0.48              |
| 28:U:24:ARG:HH22  | 29:V:66:VAL:CG1   | 2.27                     | 0.48              |
| 29:V:186:GLN:HG2  | 29:V:190:HIS:CD2  | 2.48                     | 0.48              |
| 30:W:20:ASP:HB2   | 30:W:25:ARG:CZ    | 2.43                     | 0.48              |
| 30:W:133:LYS:HE3  | 30:W:163:ASN:ND2  | 2.22                     | 0.48              |
| 31:X:87:PHE:CE2   | 31:X:121:ILE:HG21 | 2.47                     | 0.48              |
| 31:X:121:ILE:O    | 31:X:125:MET:HG2  | 2.13                     | 0.48              |
| 3:3:65:TYR:HD2    | 3:3:73:ILE:HG22   | 1.76                     | 0.48              |
| 4:4:72:TYR:OH     | 4:4:109:LYS:HB3   | 2.13                     | 0.48              |
| 6:6:77:ILE:HD11   | 6:6:102:ILE:HB    | 1.95                     | 0.48              |
| 8:A:34:ALA:O      | 8:A:35:THR:CG2    | 2.61                     | 0.48              |
| 10:C:5:ARG:O      | 10:C:6:TYR:HD1    | 1.96                     | 0.48              |
| 13:F:101:ARG:HH11 | 13:F:103:LEU:HA   | 1.65                     | 0.48              |
| 13:F:168:ALA:O    | 13:F:172:LEU:HG   | 2.13                     | 0.48              |
| 17:J:200:ARG:HG2  | 17:J:210:PHE:CD2  | 2.48                     | 0.48              |
| 21:N:328:PHE:HB2  | 29:V:181:ASN:CG   | 2.38                     | 0.48              |
| 21:N:510:HIS:HB2  | 21:N:513:ILE:HD12 | 1.95                     | 0.48              |
| 21:N:657:MET:HG2  | 21:N:682:PHE:CE1  | 2.45                     | 0.48              |
| 21:N:657:MET:HE1  | 21:N:685:VAL:HG21 | 1.96                     | 0.48              |
| 21:N:919:THR:CG2  | 21:N:922:GLN:HG2  | 2.44                     | 0.48              |
| 23:P:308:LEU:HD12 | 23:P:349:ASN:OD1  | 2.08                     | 0.48              |
| 24:Q:50:ARG:NH2   | 24:Q:53:GLU:HB2   | 2.29                     | 0.48              |
| 25:R:209:ARG:NE   | 25:R:243:LEU:HD22 | 2.19                     | 0.48              |
| 25:R:331:ARG:O    | 25:R:371:PHE:CZ   | 2.66                     | 0.48              |
| 27:T:57:ILE:HG23  | 27:T:58:THR:N     | 2.28                     | 0.48              |
| 33:Z:473:LEU:C    | 33:Z:477:TYR:CD2  | 2.92                     | 0.48              |
| 33:Z:924:LYS:HA   | 33:Z:959:HIS:HD2  | 1.79                     | 0.48              |
| 3:3:155:PHE:HB2   | 3:3:180:ILE:CD1   | 2.43                     | 0.48              |
| 8:A:58:LYS:HE2    | 19:L:384:ASP:OD1  | 2.14                     | 0.48              |
| 15:H:144:LYS:HB2  | 20:M:74:GLN:CD    | 2.39                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:M:203:ARG:CZ   | 20:M:206:LYS:HZ1  | 2.27                     | 0.48              |
| 20:M:236:ALA:CA   | 20:M:277:ILE:HD12 | 2.43                     | 0.48              |
| 21:N:657:MET:CG   | 21:N:682:PHE:HE1  | 2.26                     | 0.48              |
| 23:P:363:LEU:HG   | 23:P:398:LYS:HD3  | 1.94                     | 0.48              |
| 25:R:298:ALA:O    | 25:R:299:SER:CB   | 2.60                     | 0.48              |
| 28:U:32:ARG:CD    | 28:U:94:HIS:CE1   | 2.97                     | 0.48              |
| 33:Z:522:THR:HG23 | 33:Z:559:LYS:HZ3  | 1.78                     | 0.48              |
| 33:Z:744:ALA:CB   | 33:Z:783:VAL:HG23 | 2.43                     | 0.48              |
| 33:Z:884:THR:OG1  | 33:Z:904:LEU:CD2  | 2.61                     | 0.48              |
| 2:2:36:ARG:NH1    | 2:2:38:SER:HA     | 2.28                     | 0.48              |
| 4:4:39:PRO:HD2    | 4:4:73:GLU:OE2    | 2.14                     | 0.48              |
| 8:A:160:ALA:HB1   | 18:K:428:LYS:HG2  | 1.95                     | 0.48              |
| 9:B:67:LEU:HD11   | 9:B:73:ALA:CB     | 2.39                     | 0.48              |
| 9:B:123:GLN:HE22  | 10:C:86:ILE:HG13  | 1.78                     | 0.48              |
| 9:B:210:GLU:CG    | 9:B:237:LYS:HE3   | 2.20                     | 0.48              |
| 9:B:217:GLU:HB3   | 9:B:234:ARG:HG2   | 1.95                     | 0.48              |
| 12:E:14:THR:CG2   | 12:E:22:PHE:CE2   | 2.96                     | 0.48              |
| 13:F:12:THR:CG2   | 13:F:19:LEU:CD2   | 2.92                     | 0.48              |
| 19:L:390:ASP:OD1  | 20:M:338:LEU:HD13 | 2.14                     | 0.48              |
| 21:N:263:SER:CB   | 21:N:721:ASP:OD2  | 2.62                     | 0.48              |
| 21:N:758:VAL:H    | 21:N:874:ILE:HD12 | 1.78                     | 0.48              |
| 26:S:381:VAL:HG22 | 27:T:150:ARG:HE   | 1.78                     | 0.48              |
| 28:U:11:ALA:HB3   | 28:U:14:VAL:HG23  | 1.95                     | 0.48              |
| 30:W:99:LYS:NZ    | 30:W:135:ASN:HB3  | 2.29                     | 0.48              |
| 33:Z:233:LEU:O    | 33:Z:271:ILE:HD11 | 2.13                     | 0.48              |
| 1:1:116:GLY:CA    | 7:7:-4:ILE:HD11   | 2.40                     | 0.48              |
| 3:3:155:PHE:HB2   | 3:3:180:ILE:HD11  | 1.96                     | 0.48              |
| 11:D:174:PHE:HZ   | 11:D:197:ARG:HB3  | 1.78                     | 0.48              |
| 15:H:168:ILE:HG12 | 15:H:174:VAL:HB   | 1.96                     | 0.48              |
| 17:J:349:LYS:HZ3  | 17:J:383:GLU:HG3  | 1.78                     | 0.48              |
| 20:M:164:ASP:CG   | 20:M:165:SER:H    | 2.22                     | 0.48              |
| 20:M:384:ASP:O    | 20:M:385:GLU:HB3  | 2.14                     | 0.48              |
| 21:N:314:LEU:HD13 | 21:N:336:ASN:OD1  | 2.14                     | 0.48              |
| 24:Q:61:LEU:HD21  | 24:Q:65:TYR:CZ    | 2.44                     | 0.48              |
| 24:Q:419:LEU:HD21 | 28:U:286:ILE:HG12 | 1.96                     | 0.48              |
| 27:T:89:TYR:CG    | 27:T:102:LYS:HD2  | 2.49                     | 0.48              |
| 30:W:20:ASP:HB2   | 30:W:25:ARG:NH2   | 2.21                     | 0.48              |
| 33:Z:493:LEU:CD2  | 33:Z:497:PHE:CE2  | 2.97                     | 0.48              |
| 33:Z:493:LEU:HG   | 33:Z:497:PHE:CD2  | 2.48                     | 0.48              |
| 33:Z:850:LEU:HD23 | 33:Z:850:LEU:O    | 2.13                     | 0.48              |
| 1:1:138:CYS:HA    | 1:1:154:PHE:HZ    | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:159:ARG:NH1   | 5:5:200:VAL:HG22  | 2.28                     | 0.48              |
| 13:F:190:ILE:HG23 | 13:F:213:ILE:HD13 | 1.95                     | 0.48              |
| 15:H:254:THR:OG1  | 15:H:377:PHE:CZ   | 2.58                     | 0.48              |
| 15:H:299:ARG:HH21 | 15:H:345:PRO:HD3  | 1.77                     | 0.48              |
| 15:H:358:PRO:HB2  | 15:H:374:LYS:NZ   | 2.23                     | 0.48              |
| 16:I:137:ASP:HB2  | 16:I:140:LEU:HG   | 1.96                     | 0.48              |
| 17:J:374:ARG:HH21 | 17:J:381:ASP:CG   | 2.21                     | 0.48              |
| 18:K:83:GLN:O     | 18:K:86:VAL:HG12  | 2.14                     | 0.48              |
| 18:K:150:LEU:HD22 | 19:L:112:LEU:HD21 | 1.96                     | 0.48              |
| 18:K:258:PHE:CG   | 18:K:302:GLN:CB   | 2.92                     | 0.48              |
| 22:O:48:PHE:CD1   | 22:O:80:LYS:NZ    | 2.76                     | 0.48              |
| 24:Q:63:GLN:O     | 24:Q:66:VAL:HG22  | 2.13                     | 0.48              |
| 25:R:237:THR:OG1  | 25:R:238:PHE:CE1  | 2.65                     | 0.48              |
| 26:S:145:PHE:O    | 26:S:146:LEU:HB3  | 2.13                     | 0.48              |
| 28:U:72:TYR:CZ    | 28:U:76:MET:HG3   | 2.49                     | 0.48              |
| 28:U:106:ILE:CG2  | 28:U:110:PHE:HE2  | 2.27                     | 0.48              |
| 29:V:135:ARG:HD2  | 29:V:157:ARG:CZ   | 2.31                     | 0.48              |
| 33:Z:92:LEU:HD12  | 33:Z:95:THR:OG1   | 2.14                     | 0.48              |
| 33:Z:363:ASP:O    | 33:Z:366:LYS:CD   | 2.62                     | 0.48              |
| 33:Z:392:LEU:HD13 | 33:Z:424:SER:C    | 2.38                     | 0.48              |
| 1:1:175:MET:HE1   | 1:1:188:PHE:HE1   | 1.75                     | 0.47              |
| 2:2:197:GLU:HB2   | 3:3:142:GLU:OE2   | 2.14                     | 0.47              |
| 4:4:37:LEU:HD23   | 4:4:41:THR:HG21   | 1.96                     | 0.47              |
| 8:A:219:SER:H     | 8:A:222:ASP:HB2   | 1.79                     | 0.47              |
| 13:F:91:GLN:HE22  | 13:F:108:ALA:HA   | 1.79                     | 0.47              |
| 14:G:168:ARG:HE   | 14:G:172:LYS:CE   | 2.27                     | 0.47              |
| 15:H:422:VAL:HG13 | 15:H:446:ALA:HB3  | 1.95                     | 0.47              |
| 15:H:434:ARG:HG2  | 33:Z:956:LEU:HB3  | 1.95                     | 0.47              |
| 16:I:384:LYS:HD3  | 16:I:420:LYS:CD   | 2.37                     | 0.47              |
| 17:J:85:LEU:HD23  | 17:J:95:ILE:HG13  | 1.96                     | 0.47              |
| 17:J:308:GLY:N    | 17:J:311:ASP:OD1  | 2.45                     | 0.47              |
| 19:L:140:LEU:HD23 | 19:L:158:ILE:HG12 | 1.96                     | 0.47              |
| 21:N:282:TYR:CE2  | 21:N:286:LEU:HB2  | 2.49                     | 0.47              |
| 21:N:666:GLN:HG2  | 21:N:875:LEU:CD2  | 2.43                     | 0.47              |
| 21:N:666:GLN:O    | 21:N:875:LEU:HD22 | 2.13                     | 0.47              |
| 22:O:204:SER:HB3  | 22:O:209:GLU:HG2  | 1.96                     | 0.47              |
| 22:O:366:MET:SD   | 28:U:229:LEU:HD13 | 2.54                     | 0.47              |
| 23:P:270:LEU:HD22 | 23:P:340:ASP:HB2  | 1.96                     | 0.47              |
| 27:T:211:PHE:CZ   | 27:T:220:PHE:CE2  | 3.02                     | 0.47              |
| 28:U:277:TYR:CE1  | 29:V:295:VAL:HG13 | 2.12                     | 0.47              |
| 28:U:293:GLU:HG2  | 29:V:277:LYS:HD2  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:V:49:VAL:HG12  | 29:V:73:GLN:HG2   | 1.95                     | 0.47              |
| 32:Y:82:ASP:HB3   | 32:Y:86:ARG:HH12  | 1.76                     | 0.47              |
| 33:Z:208:VAL:HG21 | 33:Z:236:PHE:CZ   | 2.46                     | 0.47              |
| 33:Z:763:HIS:C    | 33:Z:766:HIS:ND1  | 2.71                     | 0.47              |
| 9:B:106:PRO:HD2   | 9:B:109:LEU:HD12  | 1.96                     | 0.47              |
| 10:C:18:ARG:HH21  | 11:D:29:ARG:NH2   | 2.10                     | 0.47              |
| 15:H:365:LEU:CD2  | 15:H:370:ARG:CZ   | 2.92                     | 0.47              |
| 15:H:456:LYS:HD3  | 16:I:332:GLU:HB3  | 1.95                     | 0.47              |
| 16:I:389:GLY:HA2  | 16:I:392:ILE:HD12 | 1.95                     | 0.47              |
| 21:N:325:PHE:HE1  | 29:V:167:ASN:OD1  | 1.96                     | 0.47              |
| 21:N:585:ARG:CZ   | 21:N:589:ILE:HD11 | 2.44                     | 0.47              |
| 22:O:29:PHE:CE2   | 22:O:61:LEU:HD11  | 2.49                     | 0.47              |
| 24:Q:114:GLN:HG3  | 24:Q:144:LEU:CD1  | 2.44                     | 0.47              |
| 25:R:363:PHE:CE1  | 32:Y:78:LYS:CD    | 2.80                     | 0.47              |
| 26:S:338:MET:O    | 26:S:342:LEU:HG   | 2.14                     | 0.47              |
| 33:Z:474:LEU:O    | 33:Z:478:VAL:HG23 | 2.14                     | 0.47              |
| 33:Z:535:VAL:HG22 | 33:Z:572:ILE:CG2  | 2.44                     | 0.47              |
| 33:Z:846:PHE:HE2  | 33:Z:901:PHE:HE2  | 1.61                     | 0.47              |
| 33:Z:850:LEU:HD21 | 33:Z:854:LEU:CD1  | 2.43                     | 0.47              |
| 1:1:51:ASP:OD1    | 1:1:93:LEU:CD2    | 2.62                     | 0.47              |
| 2:2:55:VAL:HG21   | 2:2:94:ILE:HG21   | 1.96                     | 0.47              |
| 5:5:104:TYR:CE1   | 5:5:110:PRO:HD3   | 2.50                     | 0.47              |
| 5:5:179:HIS:CB    | 5:5:188:HIS:CD2   | 2.97                     | 0.47              |
| 6:6:6:ILE:HB      | 6:6:13:VAL:HG22   | 1.96                     | 0.47              |
| 8:A:18:ILE:HD12   | 9:B:20:GLN:NE2    | 2.29                     | 0.47              |
| 8:A:220:LYS:HD2   | 8:A:238:ALA:O     | 2.14                     | 0.47              |
| 8:A:252:ASP:OD2   | 23:P:85:LYS:CE    | 2.57                     | 0.47              |
| 9:B:18:LEU:HB2    | 9:B:21:ILE:HD12   | 1.96                     | 0.47              |
| 10:C:50:ARG:NH2   | 10:C:211:LEU:O    | 2.47                     | 0.47              |
| 15:H:97:LEU:HB2   | 15:H:173:ARG:CD   | 2.44                     | 0.47              |
| 16:I:358:LYS:NZ   | 16:I:385:ASP:CA   | 2.77                     | 0.47              |
| 17:J:219:VAL:O    | 17:J:219:VAL:HG12 | 2.15                     | 0.47              |
| 18:K:272:ASP:HB3  | 19:L:306:MET:HE1  | 0.54                     | 0.47              |
| 20:M:72:ASN:HB2   | 20:M:156:LEU:HD21 | 1.95                     | 0.47              |
| 21:N:147:ALA:O    | 21:N:148:SER:HB2  | 2.14                     | 0.47              |
| 22:O:213:LEU:O    | 22:O:217:LEU:HG   | 2.14                     | 0.47              |
| 24:Q:309:ARG:NH2  | 24:Q:345:SER:OG   | 2.44                     | 0.47              |
| 33:Z:294:ILE:HD13 | 33:Z:320:SER:HB2  | 1.97                     | 0.47              |
| 33:Z:469:PRO:CG   | 33:Z:472:LEU:HD12 | 2.44                     | 0.47              |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:CD2  | 2.19                     | 0.47              |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:CB   | 2.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:744:ALA:O    | 33:Z:748:LEU:HG   | 2.14                     | 0.47              |
| 4:4:65:LEU:HD11   | 4:4:69:ARG:HE     | 1.80                     | 0.47              |
| 5:5:128:CYS:SG    | 5:5:140:LEU:HD12  | 2.54                     | 0.47              |
| 5:5:199:LYS:HG2   | 5:5:203:GLU:OE1   | 2.15                     | 0.47              |
| 7:7:33:ARG:NH2    | 7:7:45:ILE:C      | 2.73                     | 0.47              |
| 15:H:96:PRO:HB2   | 16:I:111:GLU:OE2  | 2.14                     | 0.47              |
| 21:N:298:TYR:CD1  | 21:N:768:ILE:HD11 | 2.50                     | 0.47              |
| 21:N:436:ASP:O    | 21:N:439:VAL:HG12 | 2.14                     | 0.47              |
| 22:O:131:SER:HB3  | 22:O:135:ARG:HH12 | 1.77                     | 0.47              |
| 23:P:264:ILE:HG21 | 23:P:280:LEU:HD11 | 1.95                     | 0.47              |
| 25:R:194:VAL:O    | 25:R:197:MET:SD   | 2.73                     | 0.47              |
| 25:R:217:HIS:O    | 25:R:220:ALA:HB3  | 2.15                     | 0.47              |
| 25:R:411:LEU:HD23 | 26:S:464:ARG:HH12 | 1.72                     | 0.47              |
| 26:S:315:LYS:HZ3  | 26:S:345:TYR:HD1  | 1.52                     | 0.47              |
| 28:U:67:PHE:CZ    | 30:W:97:THR:CB    | 2.98                     | 0.47              |
| 28:U:111:LYS:HA   | 28:U:118:PRO:HG3  | 1.95                     | 0.47              |
| 30:W:52:ILE:HG22  | 30:W:61:VAL:HA    | 1.95                     | 0.47              |
| 33:Z:574:TYR:CZ   | 33:Z:584:VAL:CB   | 2.97                     | 0.47              |
| 1:1:-2:LEU:HD12   | 1:1:-2:LEU:C      | 2.39                     | 0.47              |
| 3:3:136:GLN:HB3   | 3:3:168:ARG:HH21  | 1.80                     | 0.47              |
| 10:C:41:SER:CB    | 10:C:184:MET:HE3  | 2.45                     | 0.47              |
| 10:C:65:LYS:HA    | 10:C:67:TYR:CE1   | 2.49                     | 0.47              |
| 11:D:188:VAL:HG21 | 11:D:216:LYS:HE2  | 1.96                     | 0.47              |
| 12:E:45:GLY:HA3   | 12:E:193:LEU:HD13 | 1.96                     | 0.47              |
| 13:F:72:LEU:C     | 13:F:72:LEU:HD12  | 2.39                     | 0.47              |
| 13:F:102:LYS:O    | 13:F:103:LEU:HB3  | 2.14                     | 0.47              |
| 13:F:114:ASP:O    | 13:F:118:LYS:HG3  | 2.14                     | 0.47              |
| 13:F:179:PHE:CE1  | 13:F:192:ALA:HB2  | 2.49                     | 0.47              |
| 17:J:342:ASN:OD1  | 17:J:344:ARG:HB2  | 2.15                     | 0.47              |
| 21:N:584:ARG:HD2  | 21:N:614:ASN:ND2  | 2.29                     | 0.47              |
| 21:N:762:ARG:CG   | 21:N:890:PHE:HE2  | 2.24                     | 0.47              |
| 22:O:62:TYR:HD2   | 22:O:82:LEU:CD1   | 2.03                     | 0.47              |
| 26:S:151:GLU:OE1  | 26:S:154:GLN:CB   | 2.62                     | 0.47              |
| 27:T:115:SER:HB2  | 27:T:180:ILE:HG21 | 1.96                     | 0.47              |
| 33:Z:50:GLU:OE2   | 33:Z:55:ARG:NE    | 2.48                     | 0.47              |
| 1:1:19:ARG:HH21   | 1:1:171:GLY:HA2   | 1.74                     | 0.47              |
| 1:1:175:MET:HB2   | 1:1:186:LEU:HB2   | 1.97                     | 0.47              |
| 5:5:4:LEU:C       | 5:5:4:LEU:HD12    | 2.40                     | 0.47              |
| 5:5:8:PHE:CD1     | 5:5:13:ILE:HG12   | 2.46                     | 0.47              |
| 7:7:131:SER:HB3   | 7:7:134:LEU:CD2   | 2.45                     | 0.47              |
| 8:A:30:TYR:CD1    | 14:G:16:PRO:HB3   | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:B:139:HIS:CE1   | 9:B:145:PHE:CE1   | 3.03                     | 0.47              |
| 11:D:189:GLU:HG3  | 11:D:232:TYR:OH   | 2.14                     | 0.47              |
| 12:E:166:ARG:HB2  | 13:F:60:GLN:CD    | 2.40                     | 0.47              |
| 13:F:146:GLU:OE2  | 13:F:148:GLN:NE2  | 2.45                     | 0.47              |
| 17:J:332:SER:HB2  | 17:J:337:LEU:HD12 | 1.96                     | 0.47              |
| 17:J:376:HIS:CG   | 25:R:235:LEU:HD22 | 2.49                     | 0.47              |
| 20:M:303:ARG:HH12 | 20:M:307:GLU:CB   | 2.25                     | 0.47              |
| 21:N:682:PHE:CE2  | 21:N:702:ALA:HB1  | 2.50                     | 0.47              |
| 22:O:15:ARG:HA    | 30:W:20:ASP:OD1   | 2.13                     | 0.47              |
| 27:T:266:TYR:CD1  | 27:T:267:ALA:N    | 2.82                     | 0.47              |
| 28:U:62:ASN:CG    | 28:U:65:VAL:HG23  | 2.39                     | 0.47              |
| 33:Z:290:GLU:CD   | 33:Z:293:MET:HE3  | 2.39                     | 0.47              |
| 3:3:155:PHE:CD1   | 3:3:189:ARG:HD2   | 2.50                     | 0.47              |
| 4:4:69:ARG:HG2    | 11:D:90:ARG:HD3   | 1.95                     | 0.47              |
| 6:6:38:GLY:O      | 6:6:39:ASP:HB2    | 2.15                     | 0.47              |
| 9:B:67:LEU:CD1    | 9:B:73:ALA:HB2    | 2.43                     | 0.47              |
| 11:D:6:ARG:HH12   | 13:F:123:TYR:HB2  | 1.80                     | 0.47              |
| 12:E:220:SER:HA   | 12:E:231:TYR:CD1  | 2.49                     | 0.47              |
| 14:G:111:PHE:CD1  | 14:G:114:ARG:CZ   | 2.97                     | 0.47              |
| 16:I:278:ILE:HG21 | 16:I:325:ILE:CD1  | 2.44                     | 0.47              |
| 17:J:232:GLU:O    | 17:J:235:VAL:HB   | 2.15                     | 0.47              |
| 18:K:48:TYR:CE2   | 21:N:156:ILE:HD11 | 2.49                     | 0.47              |
| 19:L:82:ARG:CG    | 19:L:86:LYS:HE3   | 2.45                     | 0.47              |
| 19:L:92:GLU:HG2   | 20:M:65:ASN:HD21  | 1.80                     | 0.47              |
| 20:M:74:GLN:O     | 20:M:77:TYR:CD1   | 2.66                     | 0.47              |
| 20:M:129:LEU:CD2  | 20:M:155:ILE:HG13 | 2.45                     | 0.47              |
| 21:N:329:HIS:CE1  | 21:N:363:ALA:HB1  | 2.49                     | 0.47              |
| 21:N:362:TRP:CH2  | 29:V:23:THR:CB    | 2.97                     | 0.47              |
| 23:P:61:LYS:O     | 23:P:65:LEU:HG    | 2.15                     | 0.47              |
| 23:P:143:LEU:HG   | 23:P:147:LYS:HE3  | 1.96                     | 0.47              |
| 23:P:184:MET:HB2  | 23:P:223:LEU:CD1  | 2.38                     | 0.47              |
| 23:P:264:ILE:HG22 | 23:P:280:LEU:HD11 | 1.97                     | 0.47              |
| 23:P:324:GLU:O    | 23:P:325:ASP:CG   | 2.58                     | 0.47              |
| 24:Q:66:VAL:HG11  | 24:Q:107:VAL:HG23 | 1.97                     | 0.47              |
| 24:Q:325:LEU:HD21 | 24:Q:335:PHE:CE2  | 2.49                     | 0.47              |
| 25:R:241:ILE:HG22 | 25:R:242:GLU:CG   | 2.28                     | 0.47              |
| 25:R:316:LEU:CD2  | 25:R:322:LEU:HB3  | 2.43                     | 0.47              |
| 25:R:397:ASN:ND2  | 26:S:450:ASN:O    | 2.48                     | 0.47              |
| 27:T:20:TYR:CE1   | 27:T:71:GLN:HG3   | 2.49                     | 0.47              |
| 28:U:65:VAL:CG1   | 30:W:96:LEU:CD1   | 2.93                     | 0.47              |
| 28:U:92:TRP:CZ2   | 28:U:120:LEU:HD11 | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:W:35:PHE:CD2   | 30:W:182:TYR:CD2  | 3.02                     | 0.47              |
| 30:W:141:ILE:CG2  | 30:W:154:LEU:HD13 | 2.40                     | 0.47              |
| 33:Z:205:LEU:HD23 | 33:Z:236:PHE:CE1  | 2.49                     | 0.47              |
| 33:Z:301:THR:HG22 | 33:Z:307:HIS:ND1  | 2.23                     | 0.47              |
| 33:Z:436:LEU:CD2  | 33:Z:455:ILE:CG1  | 2.92                     | 0.47              |
| 1:1:48:SER:O      | 1:1:52:THR:HG23   | 2.15                     | 0.47              |
| 3:3:17:ASP:C      | 3:3:17:ASP:OD1    | 2.57                     | 0.47              |
| 7:7:33:ARG:HH21   | 7:7:46:SER:N      | 2.09                     | 0.47              |
| 10:C:173:GLN:NE2  | 11:D:52:LEU:HB2   | 2.29                     | 0.47              |
| 12:E:14:THR:HG22  | 12:E:22:PHE:CE2   | 2.50                     | 0.47              |
| 13:F:159:THR:HA   | 13:F:169:LYS:CD   | 2.45                     | 0.47              |
| 16:I:97:GLU:HB2   | 16:I:100:ARG:HH21 | 1.80                     | 0.47              |
| 19:L:163:THR:OG1  | 19:L:265:GLU:HG3  | 2.14                     | 0.47              |
| 21:N:53:ASP:CB    | 21:N:58:ARG:HH21  | 2.27                     | 0.47              |
| 21:N:329:HIS:HB2  | 29:V:182:LYS:NZ   | 1.90                     | 0.47              |
| 24:Q:83:GLU:HA    | 24:Q:86:MET:HG2   | 1.96                     | 0.47              |
| 24:Q:348:CYS:SG   | 24:Q:386:PHE:CD1  | 3.08                     | 0.47              |
| 25:R:259:PHE:HE1  | 25:R:332:GLU:CB   | 2.28                     | 0.47              |
| 33:Z:985:LYS:CD   | 33:Z:991:GLU:H    | 2.28                     | 0.47              |
| 3:3:177:VAL:CG1   | 3:3:190:TYR:CE1   | 2.98                     | 0.47              |
| 6:6:56:VAL:HG12   | 6:6:60:LYS:HE3    | 1.97                     | 0.47              |
| 6:6:91:LYS:O      | 6:6:96:TYR:CD1    | 2.68                     | 0.47              |
| 10:C:15:PRO:HG3   | 15:H:456:LYS:NZ   | 2.29                     | 0.47              |
| 13:F:12:THR:HG22  | 13:F:19:LEU:CD2   | 2.45                     | 0.47              |
| 13:F:74:LEU:C     | 13:F:74:LEU:HD12  | 2.40                     | 0.47              |
| 14:G:111:PHE:HB2  | 14:G:114:ARG:NH2  | 2.30                     | 0.47              |
| 15:H:423:CYS:HA   | 15:H:443:PHE:HE1  | 1.80                     | 0.47              |
| 16:I:384:LYS:HZ3  | 16:I:420:LYS:HZ2  | 0.58                     | 0.47              |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:CB   | 2.44                     | 0.47              |
| 19:L:357:ARG:NH1  | 19:L:386:PHE:HB2  | 2.17                     | 0.47              |
| 21:N:137:PHE:O    | 21:N:141:ILE:HG12 | 2.14                     | 0.47              |
| 21:N:536:ILE:CD1  | 21:N:555:ILE:HG13 | 2.43                     | 0.47              |
| 23:P:298:SER:O    | 23:P:302:LEU:HG   | 2.13                     | 0.47              |
| 26:S:271:ARG:HG2  | 26:S:309:PHE:CE1  | 2.50                     | 0.47              |
| 33:Z:75:ILE:CG2   | 33:Z:121:ILE:HD13 | 2.44                     | 0.47              |
| 1:1:66:TYR:HE2    | 1:1:73:PRO:CA     | 2.27                     | 0.47              |
| 2:2:82:MET:HE3    | 2:2:86:HIS:CE1    | 2.39                     | 0.47              |
| 4:4:95:ARG:CZ     | 5:5:88:TYR:OH     | 2.63                     | 0.47              |
| 4:4:106:TYR:CE2   | 4:4:185:LYS:HB3   | 2.50                     | 0.47              |
| 7:7:17:ASP:HA     | 7:7:187:PHE:HA    | 1.97                     | 0.47              |
| 8:A:237:SER:O     | 8:A:241:ILE:HG13  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:D:102:ASP:OD1  | 11:D:103:PRO:HD2  | 2.13                     | 0.47              |
| 13:F:159:THR:CB   | 13:F:169:LYS:HZ3  | 2.28                     | 0.47              |
| 14:G:164:THR:HA   | 14:G:168:ARG:HD2  | 1.98                     | 0.47              |
| 15:H:334:LEU:CD1  | 20:M:285:ALA:HB2  | 2.44                     | 0.47              |
| 15:H:365:LEU:HA   | 15:H:370:ARG:NH1  | 2.30                     | 0.47              |
| 16:I:78:ASN:O     | 16:I:82:LEU:HG    | 2.15                     | 0.47              |
| 21:N:302:PHE:CE1  | 21:N:306:ASN:ND2  | 2.83                     | 0.47              |
| 23:P:154:ASP:OD1  | 23:P:190:LYS:CE   | 2.62                     | 0.47              |
| 24:Q:382:LEU:CD1  | 25:R:263:ARG:NH1  | 2.77                     | 0.47              |
| 26:S:234:ILE:HG13 | 26:S:257:LEU:HD13 | 1.97                     | 0.47              |
| 31:X:76:VAL:HB    | 31:X:88:ALA:HB3   | 1.96                     | 0.47              |
| 33:Z:65:GLU:HA    | 33:Z:111:LEU:HD21 | 1.96                     | 0.47              |
| 33:Z:160:GLU:OE2  | 33:Z:164:VAL:HG21 | 2.15                     | 0.47              |
| 33:Z:385:PHE:CZ   | 33:Z:389:PHE:HE2  | 1.98                     | 0.47              |
| 33:Z:813:PHE:CD2  | 33:Z:888:LEU:CD2  | 2.97                     | 0.47              |
| 33:Z:833:GLN:NE2  | 33:Z:837:TYR:CZ   | 2.81                     | 0.47              |
| 4:4:34:THR:CG2    | 4:4:181:LYS:HZ2   | 2.28                     | 0.46              |
| 11:D:37:LYS:HD3   | 11:D:147:LEU:CB   | 2.45                     | 0.46              |
| 11:D:193:LYS:CG   | 11:D:197:ARG:CZ   | 2.93                     | 0.46              |
| 16:I:119:ILE:HG23 | 16:I:127:ASP:OD1  | 2.14                     | 0.46              |
| 16:I:245:LEU:CG   | 16:I:247:ILE:HD11 | 2.41                     | 0.46              |
| 17:J:143:PRO:O    | 17:J:204:HIS:ND1  | 2.48                     | 0.46              |
| 21:N:32:VAL:CG2   | 21:N:64:ILE:HG23  | 2.45                     | 0.46              |
| 21:N:368:THR:O    | 21:N:371:LEU:HB2  | 2.15                     | 0.46              |
| 22:O:137:TYR:HB3  | 22:O:141:ASN:HD21 | 1.80                     | 0.46              |
| 22:O:291:ILE:HG23 | 22:O:292:CYS:N    | 2.30                     | 0.46              |
| 23:P:203:ILE:HG23 | 23:P:220:TYR:CE2  | 2.49                     | 0.46              |
| 24:Q:373:VAL:HG12 | 24:Q:377:LEU:CD1  | 2.45                     | 0.46              |
| 28:U:19:LEU:HD11  | 29:V:212:MET:HB2  | 1.96                     | 0.46              |
| 28:U:77:ASN:ND2   | 28:U:81:LYS:HE3   | 2.30                     | 0.46              |
| 33:Z:71:LEU:CD2   | 33:Z:118:VAL:HG13 | 2.45                     | 0.46              |
| 33:Z:376:SER:OG   | 33:Z:379:GLN:HB2  | 2.14                     | 0.46              |
| 33:Z:394:TYR:CG   | 33:Z:859:LYS:NZ   | 2.83                     | 0.46              |
| 33:Z:497:PHE:CG   | 33:Z:505:VAL:HG11 | 2.51                     | 0.46              |
| 2:2:59:ILE:CD1    | 2:2:82:MET:HB3    | 2.42                     | 0.46              |
| 3:3:37:TYR:CE1    | 3:3:59:ARG:HB2    | 2.49                     | 0.46              |
| 3:3:116:ASP:CG    | 3:3:117:LEU:H     | 2.23                     | 0.46              |
| 3:3:133:ALA:O     | 3:3:137:LEU:HG    | 2.16                     | 0.46              |
| 6:6:68:PHE:HZ     | 13:F:67:ASP:CA    | 2.28                     | 0.46              |
| 6:6:68:PHE:HE1    | 13:F:65:LYS:HG2   | 1.79                     | 0.46              |
| 8:A:78:THR:HG22   | 8:A:231:ASP:C     | 2.40                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:335:GLU:OE1  | 20:M:249:PRO:HB2  | 2.15                     | 0.46              |
| 16:I:190:GLN:OE1  | 16:I:190:GLN:N    | 2.46                     | 0.46              |
| 18:K:67:TYR:CD1   | 21:N:572:LEU:HB3  | 2.49                     | 0.46              |
| 21:N:193:ALA:O    | 21:N:197:VAL:HB   | 2.16                     | 0.46              |
| 21:N:230:VAL:HG22 | 21:N:265:ALA:HB2  | 1.97                     | 0.46              |
| 21:N:710:GLY:O    | 21:N:711:ARG:HB2  | 2.15                     | 0.46              |
| 22:O:356:ARG:NH2  | 28:U:234:ASN:OD1  | 2.48                     | 0.46              |
| 22:O:377:VAL:CG2  | 28:U:200:LEU:CD1  | 2.88                     | 0.46              |
| 23:P:140:THR:HG21 | 23:P:163:LEU:HD22 | 1.97                     | 0.46              |
| 24:Q:11:ALA:CB    | 24:Q:27:TYR:CE1   | 2.98                     | 0.46              |
| 24:Q:409:TYR:HB2  | 25:R:399:GLN:HG2  | 1.96                     | 0.46              |
| 25:R:67:CYS:SG    | 25:R:92:ILE:O     | 2.73                     | 0.46              |
| 26:S:425:ARG:CZ   | 27:T:153:MET:O    | 2.63                     | 0.46              |
| 27:T:130:ASP:HB3  | 27:T:135:ASN:HD21 | 1.80                     | 0.46              |
| 33:Z:64:TYR:CE1   | 33:Z:68:LEU:HD21  | 2.50                     | 0.46              |
| 33:Z:217:GLU:O    | 33:Z:221:VAL:HG23 | 2.15                     | 0.46              |
| 33:Z:229:SER:OG   | 33:Z:233:LEU:HG   | 2.15                     | 0.46              |
| 33:Z:393:GLY:O    | 33:Z:394:TYR:HB2  | 2.16                     | 0.46              |
| 33:Z:493:LEU:HD11 | 33:Z:497:PHE:HZ   | 1.55                     | 0.46              |
| 10:C:21:GLN:NE2   | 10:C:129:ARG:HA   | 2.30                     | 0.46              |
| 11:D:74:SER:HG    | 11:D:134:LEU:HB2  | 1.79                     | 0.46              |
| 11:D:214:VAL:HB   | 11:D:222:VAL:CG1  | 2.45                     | 0.46              |
| 14:G:33:GLY:O     | 14:G:166:LYS:HG3  | 2.16                     | 0.46              |
| 14:G:111:PHE:CE2  | 14:G:115:LEU:CD1  | 2.98                     | 0.46              |
| 15:H:278:GLU:CD   | 16:I:262:ARG:HH11 | 2.22                     | 0.46              |
| 15:H:367:ARG:NH1  | 20:M:223:PRO:HB3  | 2.29                     | 0.46              |
| 16:I:290:LYS:NZ   | 16:I:336:PRO:HD3  | 2.30                     | 0.46              |
| 17:J:135:SER:O    | 17:J:136:LEU:HG   | 2.14                     | 0.46              |
| 18:K:212:TYR:OH   | 18:K:320:ARG:HA   | 2.15                     | 0.46              |
| 19:L:331:ASP:OD2  | 20:M:292:ASP:O    | 2.33                     | 0.46              |
| 21:N:85:ALA:O     | 21:N:86:LYS:HB2   | 2.16                     | 0.46              |
| 21:N:117:TYR:OH   | 21:N:202:PHE:HA   | 2.15                     | 0.46              |
| 22:O:41:LEU:HG    | 22:O:58:ARG:HD2   | 1.97                     | 0.46              |
| 22:O:58:ARG:HB2   | 22:O:61:LEU:HD12  | 1.97                     | 0.46              |
| 23:P:315:GLN:OE1  | 23:P:341:LEU:HD13 | 2.15                     | 0.46              |
| 27:T:270:ILE:HD11 | 29:V:288:LEU:CD2  | 2.45                     | 0.46              |
| 28:U:50:ASN:ND2   | 28:U:87:GLU:CD    | 2.73                     | 0.46              |
| 28:U:273:LEU:HD11 | 29:V:298:ALA:CB   | 2.45                     | 0.46              |
| 33:Z:809:MET:CE   | 33:Z:847:ILE:HD11 | 2.45                     | 0.46              |
| 3:3:60:TYR:HD2    | 10:C:96:GLN:HB3   | 1.72                     | 0.46              |
| 15:H:173:ARG:HH21 | 16:I:119:ILE:HG21 | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:76:VAL:HG12  | 33:Z:621:LEU:CD1  | 2.45                     | 0.46              |
| 16:I:246:ARG:HE   | 17:J:274:GLU:HB3  | 1.80                     | 0.46              |
| 17:J:132:PRO:HG3  | 17:J:139:VAL:H    | 1.79                     | 0.46              |
| 18:K:132:LYS:HB3  | 18:K:133:PRO:HD2  | 1.97                     | 0.46              |
| 20:M:354:GLU:HG2  | 20:M:357:ARG:HH22 | 1.80                     | 0.46              |
| 20:M:379:LEU:O    | 20:M:383:THR:HG23 | 2.15                     | 0.46              |
| 21:N:53:ASP:CA    | 21:N:58:ARG:NH2   | 2.60                     | 0.46              |
| 22:O:384:MET:CE   | 28:U:189:ARG:C    | 2.84                     | 0.46              |
| 25:R:354:ALA:HA   | 25:R:364:LEU:CD2  | 2.45                     | 0.46              |
| 27:T:51:TYR:O     | 27:T:54:ASP:HB2   | 2.15                     | 0.46              |
| 31:X:45:PHE:CE2   | 31:X:67:ILE:HD13  | 2.51                     | 0.46              |
| 33:Z:187:SER:CA   | 33:Z:198:GLU:HG2  | 2.44                     | 0.46              |
| 33:Z:207:ILE:HA   | 33:Z:210:TYR:HD2  | 1.80                     | 0.46              |
| 1:1:84:GLU:O      | 1:1:88:GLU:HG3    | 2.16                     | 0.46              |
| 2:2:59:ILE:CD1    | 2:2:86:HIS:CE1    | 2.98                     | 0.46              |
| 3:3:7:THR:CG2     | 3:3:112:ILE:CD1   | 2.93                     | 0.46              |
| 3:3:37:TYR:HE1    | 3:3:59:ARG:CG     | 2.22                     | 0.46              |
| 9:B:18:LEU:HD12   | 9:B:21:ILE:HD12   | 1.98                     | 0.46              |
| 10:C:107:PRO:HB3  | 10:C:143:ARG:HH22 | 1.76                     | 0.46              |
| 13:F:67:ASP:OD2   | 13:F:69:HIS:NE2   | 2.48                     | 0.46              |
| 15:H:329:VAL:HG11 | 16:I:300:ARG:CZ   | 2.45                     | 0.46              |
| 17:J:193:THR:HB   | 17:J:316:PHE:HE2  | 1.80                     | 0.46              |
| 18:K:212:TYR:CD1  | 18:K:321:ALA:HB2  | 2.50                     | 0.46              |
| 19:L:145:ARG:NE   | 19:L:162:GLU:CG   | 2.76                     | 0.46              |
| 21:N:10:LEU:HD22  | 21:N:42:GLU:HG3   | 1.96                     | 0.46              |
| 22:O:185:PHE:CD1  | 22:O:223:LEU:HD13 | 2.50                     | 0.46              |
| 24:Q:141:LEU:HG   | 24:Q:145:HIS:NE2  | 2.30                     | 0.46              |
| 24:Q:315:ASN:OD1  | 24:Q:339:TYR:HE1  | 1.99                     | 0.46              |
| 25:R:167:LYS:HG2  | 25:R:197:MET:HE1  | 1.96                     | 0.46              |
| 25:R:237:THR:C    | 25:R:246:TYR:HE1  | 2.23                     | 0.46              |
| 28:U:111:LYS:HA   | 28:U:118:PRO:CG   | 2.45                     | 0.46              |
| 9:B:48:GLU:CG     | 9:B:200:VAL:HG11  | 2.44                     | 0.46              |
| 11:D:216:LYS:HB3  | 11:D:217:PRO:HD2  | 1.97                     | 0.46              |
| 13:F:3:ARG:NH2    | 15:H:359:ASN:HD21 | 1.98                     | 0.46              |
| 13:F:110:HIS:CE1  | 14:G:85:ARG:HB3   | 2.50                     | 0.46              |
| 16:I:418:GLN:HB3  | 16:I:422:ARG:HH12 | 1.81                     | 0.46              |
| 17:J:59:LYS:HG2   | 17:J:63:ARG:HH12  | 1.80                     | 0.46              |
| 17:J:210:PHE:HE2  | 17:J:212:ARG:HD2  | 1.79                     | 0.46              |
| 19:L:170:MET:HE2  | 19:L:262:ILE:O    | 2.15                     | 0.46              |
| 20:M:160:PRO:HB2  | 20:M:166:ARG:NH2  | 2.28                     | 0.46              |
| 21:N:778:LYS:HZ3  | 21:N:863:SER:H    | 1.63                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:O:106:PHE:CG   | 22:O:106:PHE:O    | 2.68                     | 0.46              |
| 24:Q:382:LEU:CB   | 25:R:263:ARG:HH12 | 2.29                     | 0.46              |
| 25:R:209:ARG:CZ   | 25:R:243:LEU:HD13 | 2.45                     | 0.46              |
| 26:S:283:GLN:O    | 26:S:284:LEU:HB2  | 2.15                     | 0.46              |
| 27:T:115:SER:HB2  | 27:T:180:ILE:CG2  | 2.45                     | 0.46              |
| 28:U:67:PHE:HD2   | 30:W:100:HIS:HE1  | 1.58                     | 0.46              |
| 29:V:188:LEU:C    | 29:V:188:LEU:CD1  | 2.89                     | 0.46              |
| 30:W:89:THR:HG22  | 30:W:93:ILE:HD12  | 1.98                     | 0.46              |
| 33:Z:212:LEU:HD23 | 33:Z:217:GLU:HG2  | 1.97                     | 0.46              |
| 33:Z:440:LEU:HD12 | 33:Z:455:ILE:HD11 | 1.97                     | 0.46              |
| 33:Z:866:VAL:HB   | 33:Z:873:LEU:CD1  | 2.46                     | 0.46              |
| 1:1:112:THR:HG21  | 7:7:27:ARG:HH21   | 1.81                     | 0.46              |
| 5:5:4:LEU:HD12    | 5:5:4:LEU:O       | 2.15                     | 0.46              |
| 5:5:66:HIS:CE1    | 5:5:70:GLU:CD     | 2.94                     | 0.46              |
| 8:A:218:PHE:CD2   | 8:A:223:LEU:HD21  | 2.50                     | 0.46              |
| 11:D:48:ARG:NH1   | 11:D:57:THR:HB    | 2.29                     | 0.46              |
| 13:F:65:LYS:CG    | 13:F:222:PHE:CD2  | 2.95                     | 0.46              |
| 13:F:101:ARG:NH1  | 13:F:104:ALA:H    | 2.14                     | 0.46              |
| 15:H:382:LEU:HD22 | 15:H:408:SER:C    | 2.41                     | 0.46              |
| 16:I:253:ILE:O    | 16:I:253:ILE:HG22 | 2.15                     | 0.46              |
| 16:I:354:ASP:OD1  | 16:I:354:ASP:C    | 2.59                     | 0.46              |
| 17:J:145:SER:OG   | 17:J:201:ALA:N    | 2.49                     | 0.46              |
| 20:M:159:LEU:HB3  | 20:M:160:PRO:CD   | 2.45                     | 0.46              |
| 20:M:197:ILE:C    | 20:M:200:PRO:HD2  | 2.40                     | 0.46              |
| 21:N:232:LEU:HD12 | 21:N:237:LEU:HD11 | 1.97                     | 0.46              |
| 21:N:427:ILE:CD1  | 21:N:450:ILE:HG12 | 2.46                     | 0.46              |
| 21:N:892:PRO:HA   | 21:N:905:LEU:HG   | 1.97                     | 0.46              |
| 23:P:138:ARG:NH1  | 23:P:141:LYS:HD3  | 2.31                     | 0.46              |
| 23:P:395:ARG:HD2  | 24:Q:357:VAL:HB   | 1.96                     | 0.46              |
| 24:Q:165:PHE:CE1  | 24:Q:170:ASP:HB2  | 2.51                     | 0.46              |
| 25:R:73:ASN:HB2   | 25:R:76:GLN:NE2   | 2.31                     | 0.46              |
| 25:R:140:TYR:CD2  | 25:R:141:TYR:CD1  | 3.03                     | 0.46              |
| 25:R:378:ASN:HB3  | 25:R:391:ASN:CG   | 2.40                     | 0.46              |
| 26:S:327:ILE:HG21 | 26:S:349:THR:HG21 | 1.98                     | 0.46              |
| 27:T:89:TYR:CE2   | 27:T:102:LYS:HG3  | 2.51                     | 0.46              |
| 33:Z:61:SER:HA    | 33:Z:111:LEU:HD11 | 1.96                     | 0.46              |
| 33:Z:213:LYS:HA   | 33:Z:240:ASN:HD21 | 1.80                     | 0.46              |
| 7:7:13:ILE:CG2    | 7:7:169:ILE:HG13  | 2.46                     | 0.46              |
| 8:A:91:ARG:HH12   | 8:A:95:LEU:HB2    | 1.79                     | 0.46              |
| 9:B:217:GLU:OE1   | 9:B:222:LEU:HD21  | 2.16                     | 0.46              |
| 9:B:231:LYS:HD3   | 9:B:234:ARG:NH2   | 2.28                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:122:HIS:ND1  | 14:G:128:VAL:HG12 | 2.28                     | 0.46              |
| 16:I:317:ASP:CB   | 16:I:343:ARG:NH2  | 2.69                     | 0.46              |
| 20:M:203:ARG:HD3  | 20:M:206:LYS:HZ2  | 1.80                     | 0.46              |
| 20:M:308:LEU:O    | 20:M:312:LEU:HG   | 2.15                     | 0.46              |
| 21:N:21:LYS:HD3   | 21:N:49:LEU:CD2   | 2.46                     | 0.46              |
| 22:O:117:ASN:OD1  | 22:O:118:GLY:N    | 2.48                     | 0.46              |
| 23:P:141:LYS:HG3  | 23:P:182:GLU:OE2  | 2.16                     | 0.46              |
| 23:P:344:ARG:NH2  | 23:P:347:GLU:OE2  | 2.49                     | 0.46              |
| 24:Q:146:TYR:CD1  | 24:Q:151:TYR:CD1  | 3.03                     | 0.46              |
| 25:R:354:ALA:CB   | 25:R:364:LEU:HD23 | 2.44                     | 0.46              |
| 33:Z:130:GLY:O    | 33:Z:131:LYS:CG   | 2.64                     | 0.46              |
| 1:1:38:HIS:HB3    | 1:1:41:ILE:HB     | 1.98                     | 0.46              |
| 3:3:29:ASN:OD1    | 3:3:174:TRP:HE3   | 1.99                     | 0.46              |
| 4:4:59:ILE:O      | 4:4:63:ILE:HG12   | 2.16                     | 0.46              |
| 7:7:33:ARG:HH21   | 7:7:45:ILE:C      | 2.24                     | 0.46              |
| 7:7:33:ARG:NH2    | 7:7:46:SER:C      | 2.74                     | 0.46              |
| 14:G:51:LYS:HE2   | 14:G:63:ASN:CB    | 2.44                     | 0.46              |
| 15:H:292:ARG:NH1  | 15:H:296:GLU:OE2  | 2.48                     | 0.46              |
| 15:H:326:ASP:C    | 15:H:329:VAL:HG22 | 2.40                     | 0.46              |
| 18:K:210:LEU:HB2  | 18:K:334:LEU:HD11 | 1.98                     | 0.46              |
| 18:K:280:LYS:CE   | 18:K:296:LEU:HD22 | 2.46                     | 0.46              |
| 21:N:443:LEU:HD21 | 21:N:469:VAL:HG22 | 1.97                     | 0.46              |
| 22:O:370:LEU:HD22 | 28:U:207:VAL:HG21 | 1.97                     | 0.46              |
| 24:Q:232:TYR:CB   | 24:Q:272:LEU:HD21 | 2.39                     | 0.46              |
| 27:T:183:SER:HA   | 27:T:186:ARG:CD   | 2.45                     | 0.46              |
| 33:Z:165:TYR:CE1  | 33:Z:190:THR:OG1  | 2.57                     | 0.46              |
| 33:Z:339:PHE:HB3  | 33:Z:341:TYR:CE1  | 2.51                     | 0.46              |
| 33:Z:394:TYR:HB3  | 33:Z:859:LYS:CE   | 2.46                     | 0.46              |
| 1:1:82:PHE:CB     | 1:1:113:ILE:CD1   | 2.94                     | 0.46              |
| 3:3:75:PRO:HD2    | 3:3:104:ASN:ND2   | 2.31                     | 0.46              |
| 7:7:13:ILE:HG21   | 7:7:169:ILE:HG13  | 1.98                     | 0.46              |
| 7:7:178:TYR:OH    | 7:7:210:LYS:NZ    | 2.28                     | 0.46              |
| 8:A:66:PRO:HG2    | 8:A:67:THR:HG23   | 1.98                     | 0.46              |
| 8:A:197:GLU:O     | 8:A:198:SER:OG    | 2.23                     | 0.46              |
| 13:F:85:SER:O     | 13:F:89:ARG:HG3   | 2.15                     | 0.46              |
| 15:H:328:GLU:HG2  | 15:H:331:ARG:HH21 | 1.80                     | 0.46              |
| 17:J:119:SER:HB3  | 17:J:121:MET:HE2  | 1.97                     | 0.46              |
| 18:K:123:LEU:HD12 | 18:K:147:VAL:O    | 2.16                     | 0.46              |
| 20:M:72:ASN:O     | 20:M:77:TYR:CE2   | 2.69                     | 0.46              |
| 21:N:256:GLN:OE1  | 21:N:904:VAL:N    | 2.49                     | 0.46              |
| 21:N:466:LEU:O    | 21:N:469:VAL:HB   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:O:317:THR:O    | 22:O:318:HIS:HB2  | 2.15                     | 0.46              |
| 23:P:131:PHE:CD1  | 23:P:136:ARG:HD2  | 2.50                     | 0.46              |
| 23:P:137:ALA:HB1  | 23:P:179:PHE:CZ   | 2.50                     | 0.46              |
| 23:P:369:LEU:HD12 | 23:P:376:THR:HG23 | 1.97                     | 0.46              |
| 24:Q:141:LEU:O    | 24:Q:145:HIS:CD2  | 2.69                     | 0.46              |
| 24:Q:188:LEU:O    | 24:Q:189:ARG:HB2  | 2.15                     | 0.46              |
| 25:R:102:LEU:HD23 | 25:R:102:LEU:C    | 2.41                     | 0.46              |
| 26:S:286:TYR:OH   | 26:S:323:LEU:HD22 | 2.16                     | 0.46              |
| 28:U:24:ARG:HH22  | 29:V:66:VAL:HG12  | 1.81                     | 0.46              |
| 28:U:293:GLU:HG2  | 29:V:277:LYS:CD   | 2.46                     | 0.46              |
| 33:Z:501:LYS:HG3  | 33:Z:534:PHE:CD2  | 2.50                     | 0.46              |
| 2:2:36:ARG:NE     | 2:2:38:SER:C      | 2.74                     | 0.45              |
| 4:4:174:ASP:CG    | 4:4:176:LYS:NZ    | 2.75                     | 0.45              |
| 5:5:159:ARG:HH11  | 5:5:200:VAL:HG13  | 1.81                     | 0.45              |
| 10:C:106:ILE:HG12 | 10:C:107:PRO:O    | 2.15                     | 0.45              |
| 11:D:10:ILE:HD11  | 12:E:10:ARG:HB3   | 1.99                     | 0.45              |
| 11:D:11:PHE:HA    | 11:D:17:ILE:HD12  | 1.96                     | 0.45              |
| 11:D:193:LYS:HZ2  | 11:D:236:ILE:HG13 | 1.80                     | 0.45              |
| 12:E:68:VAL:HG12  | 12:E:93:ARG:NH2   | 2.31                     | 0.45              |
| 14:G:59:VAL:CG2   | 14:G:60:PRO:HD2   | 2.45                     | 0.45              |
| 15:H:49:LEU:O     | 33:Z:765:MET:CE   | 2.63                     | 0.45              |
| 17:J:337:LEU:N    | 25:R:204:TRP:HE1  | 1.98                     | 0.45              |
| 19:L:118:ILE:HG12 | 19:L:128:ILE:CD1  | 2.46                     | 0.45              |
| 22:O:33:TYR:CE2   | 22:O:34:GLU:OE2   | 2.69                     | 0.45              |
| 22:O:277:ILE:HG22 | 22:O:279:ILE:H    | 1.81                     | 0.45              |
| 26:S:288:THR:CG2  | 26:S:292:TYR:CE2  | 2.99                     | 0.45              |
| 27:T:229:VAL:CG1  | 27:T:230:ASN:N    | 2.80                     | 0.45              |
| 29:V:247:ILE:HD12 | 29:V:250:GLN:HB2  | 1.98                     | 0.45              |
| 31:X:38:ASN:OD1   | 31:X:43:LEU:CD1   | 2.64                     | 0.45              |
| 33:Z:103:TYR:CZ   | 33:Z:137:TYR:CD1  | 3.04                     | 0.45              |
| 33:Z:486:SER:O    | 33:Z:489:ALA:HB3  | 2.16                     | 0.45              |
| 33:Z:884:THR:CB   | 33:Z:904:LEU:HD21 | 2.46                     | 0.45              |
| 9:B:39:ALA:O      | 9:B:40:THR:HG23   | 2.16                     | 0.45              |
| 12:E:157:HIS:HB3  | 12:E:167:TYR:CE1  | 2.51                     | 0.45              |
| 15:H:62:ARG:HH21  | 16:I:92:GLU:HG2   | 1.81                     | 0.45              |
| 15:H:97:LEU:CB    | 15:H:173:ARG:CG   | 2.94                     | 0.45              |
| 15:H:326:ASP:CA   | 15:H:329:VAL:HG22 | 2.45                     | 0.45              |
| 18:K:224:LYS:NZ   | 18:K:236:ARG:NH2  | 2.51                     | 0.45              |
| 18:K:342:SER:O    | 18:K:343:LEU:CB   | 2.62                     | 0.45              |
| 19:L:389:ALA:CA   | 20:M:339:ARG:HE   | 2.29                     | 0.45              |
| 21:N:423:LEU:O    | 21:N:426:ILE:HB   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:664:LEU:CD2  | 21:N:672:ASN:ND2  | 2.80                     | 0.45              |
| 23:P:184:MET:SD   | 23:P:223:LEU:HD12 | 2.56                     | 0.45              |
| 23:P:366:ASN:HD21 | 23:P:373:GLU:CA   | 2.15                     | 0.45              |
| 23:P:375:GLN:O    | 23:P:379:TYR:CD2  | 2.69                     | 0.45              |
| 24:Q:263:LYS:CE   | 24:Q:295:GLY:HA3  | 2.43                     | 0.45              |
| 25:R:214:TYR:HE2  | 25:R:226:GLU:O    | 1.99                     | 0.45              |
| 26:S:443:ILE:HG22 | 26:S:445:THR:CG2  | 2.47                     | 0.45              |
| 26:S:455:GLU:H    | 28:U:274:MET:HE1  | 1.81                     | 0.45              |
| 27:T:89:TYR:HB3   | 27:T:90:PHE:CD1   | 2.51                     | 0.45              |
| 28:U:190:LEU:HD23 | 28:U:190:LEU:C    | 2.41                     | 0.45              |
| 30:W:21:PHE:CE1   | 30:W:25:ARG:NH2   | 2.81                     | 0.45              |
| 31:X:48:PHE:CG    | 31:X:68:LEU:HD11  | 2.51                     | 0.45              |
| 33:Z:65:GLU:N     | 33:Z:111:LEU:HD21 | 2.31                     | 0.45              |
| 33:Z:138:ARG:CZ   | 33:Z:157:LEU:HA   | 2.46                     | 0.45              |
| 33:Z:403:ASN:ND2  | 33:Z:406:TRP:HB2  | 2.31                     | 0.45              |
| 33:Z:457:ILE:HG23 | 33:Z:905:ASN:ND2  | 2.32                     | 0.45              |
| 33:Z:748:LEU:HD11 | 33:Z:782:ILE:O    | 2.15                     | 0.45              |
| 1:1:82:PHE:HB2    | 1:1:113:ILE:CD1   | 2.46                     | 0.45              |
| 8:A:135:ARG:HD3   | 14:G:124:LEU:HD23 | 1.98                     | 0.45              |
| 11:D:146:LYS:HE2  | 11:D:148:TYR:CE2  | 2.51                     | 0.45              |
| 14:G:108:ILE:HD12 | 14:G:146:HIS:HB2  | 1.97                     | 0.45              |
| 15:H:311:ILE:CD1  | 15:H:361:LEU:HD13 | 2.46                     | 0.45              |
| 16:I:380:LEU:O    | 16:I:384:LYS:HG3  | 2.16                     | 0.45              |
| 16:I:416:PHE:O    | 16:I:420:LYS:HG2  | 2.16                     | 0.45              |
| 17:J:170:HIS:NE2  | 25:R:124:ASP:HB3  | 2.32                     | 0.45              |
| 19:L:67:HIS:N     | 19:L:70:TYR:HD2   | 2.14                     | 0.45              |
| 19:L:123:SER:HB3  | 20:M:125:GLN:HE21 | 1.82                     | 0.45              |
| 19:L:166:LEU:HD12 | 19:L:170:MET:HE3  | 1.98                     | 0.45              |
| 21:N:208:ARG:HG2  | 21:N:232:LEU:HD13 | 1.97                     | 0.45              |
| 23:P:94:GLN:OE1   | 23:P:136:ARG:CG   | 2.62                     | 0.45              |
| 24:Q:275:ILE:CG1  | 24:Q:306:TYR:HD2  | 2.28                     | 0.45              |
| 25:R:161:ALA:O    | 25:R:162:ILE:HG23 | 2.17                     | 0.45              |
| 26:S:145:PHE:HD2  | 26:S:152:LEU:HD23 | 1.81                     | 0.45              |
| 28:U:298:ASN:O    | 28:U:302:GLN:HG3  | 2.16                     | 0.45              |
| 33:Z:65:GLU:HA    | 33:Z:111:LEU:CD2  | 2.46                     | 0.45              |
| 33:Z:322:GLU:CG   | 33:Z:464:ASP:OD2  | 2.53                     | 0.45              |
| 33:Z:510:LEU:N    | 33:Z:511:PRO:HD2  | 2.31                     | 0.45              |
| 1:1:173:ILE:HD12  | 1:1:193:TYR:CG    | 2.51                     | 0.45              |
| 2:2:88:PHE:O      | 2:2:91:GLN:NE2    | 2.48                     | 0.45              |
| 3:3:57:MET:CE     | 3:3:89:ARG:NH2    | 2.74                     | 0.45              |
| 4:4:106:TYR:CZ    | 4:4:185:LYS:HA    | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:17:ASP:C      | 5:5:17:ASP:OD1    | 2.59                     | 0.45              |
| 5:5:118:ASP:OD1   | 5:5:118:ASP:O     | 2.33                     | 0.45              |
| 6:6:34:VAL:HG12   | 6:6:196:LEU:CD1   | 2.44                     | 0.45              |
| 8:A:34:ALA:C      | 8:A:35:THR:HG23   | 2.41                     | 0.45              |
| 9:B:184:GLU:HG2   | 9:B:186:GLU:N     | 2.30                     | 0.45              |
| 11:D:37:LYS:HG2   | 11:D:42:VAL:HG23  | 1.97                     | 0.45              |
| 11:D:106:VAL:HB   | 11:D:146:LYS:CE   | 2.47                     | 0.45              |
| 11:D:120:TYR:CG   | 11:D:126:VAL:HG21 | 2.50                     | 0.45              |
| 15:H:340:LEU:HD12 | 15:H:370:ARG:HG3  | 1.95                     | 0.45              |
| 16:I:103:PRO:CB   | 17:J:120:TYR:CZ   | 2.94                     | 0.45              |
| 17:J:167:PRO:HA   | 17:J:174:PHE:CE2  | 2.47                     | 0.45              |
| 18:K:186:GLU:HA   | 18:K:190:LEU:CD1  | 2.43                     | 0.45              |
| 19:L:190:ILE:O    | 19:L:194:ARG:HG3  | 2.16                     | 0.45              |
| 20:M:303:ARG:NH2  | 20:M:307:GLU:OE1  | 2.49                     | 0.45              |
| 23:P:203:ILE:HG13 | 23:P:220:TYR:OH   | 2.08                     | 0.45              |
| 25:R:304:TYR:HD2  | 25:R:305:PHE:CD1  | 2.34                     | 0.45              |
| 26:S:138:MET:O    | 26:S:142:VAL:HG23 | 2.16                     | 0.45              |
| 28:U:76:MET:SD    | 29:V:94:MET:HG3   | 2.56                     | 0.45              |
| 30:W:21:PHE:HB3   | 30:W:22:PRO:HD2   | 1.97                     | 0.45              |
| 33:Z:483:THR:HB   | 33:Z:521:GLU:HG3  | 1.99                     | 0.45              |
| 33:Z:886:VAL:HG13 | 33:Z:893:PHE:CE2  | 2.48                     | 0.45              |
| 4:4:43:MET:HE3    | 4:4:103:ILE:CG1   | 2.46                     | 0.45              |
| 11:D:215:VAL:HG22 | 11:D:221:ILE:HG12 | 1.98                     | 0.45              |
| 19:L:400:PHE:HZ   | 20:M:215:PRO:HD3  | 1.82                     | 0.45              |
| 20:M:203:ARG:HH11 | 20:M:206:LYS:HZ2  | 1.63                     | 0.45              |
| 21:N:63:LEU:HD22  | 21:N:88:ARG:HB3   | 1.99                     | 0.45              |
| 21:N:321:LEU:C    | 21:N:321:LEU:HD12 | 2.41                     | 0.45              |
| 21:N:771:PHE:CE2  | 21:N:773:MET:CG   | 2.99                     | 0.45              |
| 22:O:76:LEU:HD22  | 22:O:124:ASP:N    | 2.31                     | 0.45              |
| 23:P:299:LEU:HD12 | 23:P:302:LEU:HD12 | 1.97                     | 0.45              |
| 23:P:422:LEU:HD12 | 28:U:262:GLN:HE22 | 1.81                     | 0.45              |
| 24:Q:309:ARG:NE   | 24:Q:345:SER:CB   | 2.51                     | 0.45              |
| 27:T:109:TYR:O    | 27:T:113:LEU:HG   | 2.17                     | 0.45              |
| 28:U:191:THR:CG2  | 28:U:195:LYS:HE3  | 2.47                     | 0.45              |
| 33:Z:865:ASP:OD1  | 33:Z:909:ARG:NH2  | 2.42                     | 0.45              |
| 1:1:14:LEU:HD21   | 1:1:100:ALA:HB3   | 0.57                     | 0.45              |
| 3:3:104:ASN:HB3   | 3:3:107:SER:OG    | 2.16                     | 0.45              |
| 6:6:115:SER:OG    | 6:6:128:ARG:HG2   | 2.17                     | 0.45              |
| 8:A:163:TYR:C     | 8:A:164:VAL:CG1   | 2.90                     | 0.45              |
| 10:C:221:ASN:ND2  | 10:C:226:TYR:HE1  | 2.14                     | 0.45              |
| 15:H:174:VAL:HG11 | 15:H:183:ILE:HG21 | 1.85                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:298:ALA:HB2  | 15:H:306:ILE:HD11 | 1.98                     | 0.45              |
| 17:J:115:LEU:HD13 | 17:J:122:LEU:CD2  | 2.46                     | 0.45              |
| 23:P:440:HIS:CE1  | 28:U:209:GLU:CB   | 2.96                     | 0.45              |
| 24:Q:429:LYS:HD2  | 29:V:269:ARG:CZ   | 2.46                     | 0.45              |
| 27:T:29:PRO:HA    | 27:T:32:ILE:HD12  | 1.97                     | 0.45              |
| 27:T:112:ASN:CA   | 27:T:177:PHE:CZ   | 3.00                     | 0.45              |
| 28:U:36:VAL:HB    | 28:U:54:LEU:HD11  | 1.99                     | 0.45              |
| 28:U:138:VAL:CG1  | 28:U:157:LEU:HD11 | 2.47                     | 0.45              |
| 31:X:7:VAL:HG12   | 31:X:8:ILE:HG13   | 1.99                     | 0.45              |
| 33:Z:823:ASN:CG   | 33:Z:856:HIS:ND1  | 2.73                     | 0.45              |
| 5:5:178:TYR:HD2   | 5:5:185:TRP:CE3   | 2.35                     | 0.45              |
| 8:A:43:LEU:C      | 8:A:43:LEU:HD12   | 2.42                     | 0.45              |
| 9:B:96:SER:O      | 9:B:97:TYR:CD1    | 2.70                     | 0.45              |
| 12:E:53:ARG:NH1   | 12:E:209:GLU:OE2  | 2.50                     | 0.45              |
| 14:G:7:TYR:CD1    | 14:G:13:VAL:CG2   | 2.97                     | 0.45              |
| 15:H:171:GLY:O    | 16:I:129:TYR:CZ   | 2.70                     | 0.45              |
| 17:J:162:GLU:HG2  | 17:J:166:LEU:CD1  | 2.46                     | 0.45              |
| 18:K:92:VAL:HA    | 18:K:94:LEU:HG    | 1.99                     | 0.45              |
| 18:K:280:LYS:HZ3  | 18:K:293:GLN:CD   | 2.24                     | 0.45              |
| 19:L:298:ASP:OD1  | 19:L:301:ILE:CD1  | 2.63                     | 0.45              |
| 21:N:207:LEU:CD1  | 21:N:232:LEU:CD2  | 2.94                     | 0.45              |
| 21:N:324:LYS:CG   | 21:N:325:PHE:HD2  | 2.28                     | 0.45              |
| 21:N:330:THR:HG21 | 21:N:739:PHE:CZ   | 2.48                     | 0.45              |
| 21:N:515:ARG:NE   | 21:N:741:TYR:CD2  | 2.85                     | 0.45              |
| 23:P:237:VAL:HG12 | 23:P:267:PHE:CE2  | 2.51                     | 0.45              |
| 25:R:127:GLU:HB3  | 25:R:162:ILE:HD13 | 1.98                     | 0.45              |
| 25:R:128:LEU:HD23 | 25:R:162:ILE:HD11 | 1.99                     | 0.45              |
| 25:R:312:TYR:CE2  | 25:R:317:ILE:HD11 | 2.52                     | 0.45              |
| 25:R:350:LEU:HB2  | 25:R:388:VAL:HG23 | 1.98                     | 0.45              |
| 26:S:456:ASP:HB2  | 26:S:457:PRO:HD3  | 1.98                     | 0.45              |
| 27:T:152:LEU:HD12 | 27:T:157:TYR:HE1  | 1.82                     | 0.45              |
| 33:Z:172:ASP:HB3  | 33:Z:177:THR:OG1  | 2.16                     | 0.45              |
| 33:Z:286:VAL:HG21 | 33:Z:317:GLN:HG2  | 1.98                     | 0.45              |
| 33:Z:321:PHE:CE2  | 33:Z:351:PRO:CG   | 2.79                     | 0.45              |
| 8:A:91:ARG:NH1    | 8:A:95:LEU:HB2    | 2.32                     | 0.45              |
| 8:A:154:ILE:HG23  | 8:A:166:TYR:HB2   | 1.99                     | 0.45              |
| 14:G:68:VAL:CG1   | 14:G:69:VAL:N     | 2.80                     | 0.45              |
| 15:H:97:LEU:C     | 15:H:97:LEU:HD12  | 2.41                     | 0.45              |
| 15:H:168:ILE:HG22 | 15:H:172:MET:HA   | 1.99                     | 0.45              |
| 15:H:284:VAL:CG1  | 20:M:253:GLN:CA   | 2.94                     | 0.45              |
| 19:L:193:LEU:HA   | 19:L:196:VAL:HG22 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:16:ASN:C     | 21:N:17:GLN:HG2   | 2.41                     | 0.45              |
| 22:O:222:LEU:HB3  | 22:O:280:LEU:CD1  | 2.46                     | 0.45              |
| 22:O:243:VAL:HG23 | 22:O:248:TYR:CD2  | 2.52                     | 0.45              |
| 22:O:296:LEU:HD13 | 22:O:312:ASP:HB3  | 1.98                     | 0.45              |
| 25:R:58:GLU:O     | 25:R:144:ILE:HD12 | 2.17                     | 0.45              |
| 25:R:161:ALA:O    | 25:R:162:ILE:CG2  | 2.65                     | 0.45              |
| 27:T:104:LYS:O    | 27:T:108:LEU:HG   | 2.16                     | 0.45              |
| 29:V:154:ASP:CB   | 29:V:156:PHE:CZ   | 2.97                     | 0.45              |
| 33:Z:436:LEU:CD2  | 33:Z:455:ILE:HG12 | 2.46                     | 0.45              |
| 1:1:-8:LYS:CE     | 2:2:117:GLY:HA3   | 2.47                     | 0.45              |
| 1:1:11:GLY:HA3    | 1:1:102:TYR:CE1   | 2.52                     | 0.45              |
| 2:2:8:PHE:CD2     | 2:2:11:GLY:N      | 2.84                     | 0.45              |
| 2:2:63:ILE:O      | 2:2:66:HIS:HB3    | 2.17                     | 0.45              |
| 3:3:63:ASN:O      | 3:3:67:LEU:HG     | 2.16                     | 0.45              |
| 3:3:158:ILE:HG23  | 3:3:159:SER:N     | 2.30                     | 0.45              |
| 4:4:13:ILE:CG2    | 4:4:160:LEU:HD11  | 2.47                     | 0.45              |
| 4:4:26:VAL:CG1    | 4:4:28:LYS:O      | 2.65                     | 0.45              |
| 4:4:106:TYR:OH    | 4:4:185:LYS:HB3   | 2.17                     | 0.45              |
| 6:6:81:ALA:HB2    | 6:6:102:ILE:HD11  | 1.99                     | 0.45              |
| 10:C:4:ARG:NH1    | 12:E:11:GLY:HA2   | 2.32                     | 0.45              |
| 10:C:194:LEU:HD11 | 10:C:238:ILE:HG22 | 1.99                     | 0.45              |
| 15:H:244:LYS:NZ   | 15:H:244:LYS:HB3  | 2.31                     | 0.45              |
| 21:N:668:THR:HG21 | 21:N:783:SER:O    | 2.17                     | 0.45              |
| 24:Q:165:PHE:CZ   | 24:Q:173:SER:CB   | 2.99                     | 0.45              |
| 26:S:315:LYS:HZ3  | 26:S:345:TYR:HE1  | 1.43                     | 0.45              |
| 33:Z:75:ILE:HD13  | 33:Z:121:ILE:HG21 | 1.99                     | 0.45              |
| 33:Z:272:TYR:HE2  | 33:Z:284:LEU:CD1  | 2.27                     | 0.45              |
| 33:Z:506:LEU:HB2  | 33:Z:534:PHE:CZ   | 2.47                     | 0.45              |
| 1:1:57:ASP:CA     | 8:A:106:TYR:HE1   | 2.29                     | 0.45              |
| 6:6:68:PHE:CE2    | 13:F:66:CYS:O     | 2.70                     | 0.45              |
| 15:H:382:LEU:HD23 | 15:H:385:ARG:HH11 | 1.82                     | 0.45              |
| 18:K:67:TYR:CD1   | 21:N:572:LEU:HD22 | 2.52                     | 0.45              |
| 18:K:174:VAL:CG2  | 18:K:177:LEU:HD11 | 2.47                     | 0.45              |
| 18:K:196:ASP:O    | 18:K:200:GLN:HG3  | 2.17                     | 0.45              |
| 18:K:344:ARG:HE   | 18:K:380:GLY:N    | 2.15                     | 0.45              |
| 21:N:31:VAL:CG2   | 21:N:35:LEU:CD1   | 2.94                     | 0.45              |
| 22:O:96:LEU:HD22  | 22:O:137:TYR:CE1  | 2.51                     | 0.45              |
| 22:O:250:TRP:HA   | 22:O:269:LEU:CG   | 2.45                     | 0.45              |
| 24:Q:263:LYS:HE2  | 24:Q:295:GLY:CA   | 2.42                     | 0.45              |
| 25:R:72:VAL:O     | 25:R:72:VAL:HG12  | 2.16                     | 0.45              |
| 26:S:461:PHE:CZ   | 28:U:278:ILE:N    | 2.85                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:205:LEU:HD23 | 33:Z:205:LEU:C    | 2.42                     | 0.45              |
| 33:Z:546:ILE:O    | 33:Z:550:PHE:CD2  | 2.70                     | 0.45              |
| 7:7:52:MET:HE1    | 7:7:53:GLN:HE21   | 1.82                     | 0.44              |
| 9:B:221:LEU:HD11  | 9:B:236:ARG:HD2   | 1.99                     | 0.44              |
| 12:E:51:GLU:HG2   | 12:E:53:ARG:HG3   | 1.99                     | 0.44              |
| 13:F:65:LYS:HG3   | 13:F:222:PHE:HD2  | 1.77                     | 0.44              |
| 13:F:74:LEU:HD22  | 13:F:81:ALA:HB1   | 1.98                     | 0.44              |
| 15:H:282:LYS:N    | 16:I:257:LEU:HG   | 2.32                     | 0.44              |
| 17:J:109:ALA:O    | 17:J:110:SER:HB2  | 2.17                     | 0.44              |
| 22:O:253:GLN:OE1  | 22:O:269:LEU:HG   | 2.17                     | 0.44              |
| 22:O:310:PHE:HE1  | 22:O:348:VAL:HG22 | 1.81                     | 0.44              |
| 25:R:259:PHE:O    | 25:R:259:PHE:CD1  | 2.70                     | 0.44              |
| 25:R:417:TYR:CZ   | 28:U:292:ILE:HG21 | 2.52                     | 0.44              |
| 33:Z:457:ILE:HD11 | 33:Z:902:TYR:CG   | 2.52                     | 0.44              |
| 33:Z:463:HIS:HE1  | 33:Z:497:PHE:HE1  | 1.63                     | 0.44              |
| 33:Z:562:TRP:CE2  | 33:Z:566:LEU:CG   | 2.91                     | 0.44              |
| 33:Z:911:LYS:CB   | 33:Z:962:ARG:HG3  | 2.47                     | 0.44              |
| 8:A:42:SER:HB2    | 8:A:171:THR:CG2   | 2.47                     | 0.44              |
| 9:B:184:GLU:CD    | 9:B:186:GLU:HB2   | 2.41                     | 0.44              |
| 13:F:14:SER:OG    | 13:F:18:ARG:O     | 2.35                     | 0.44              |
| 16:I:257:LEU:HD13 | 16:I:304:ARG:HD3  | 1.99                     | 0.44              |
| 19:L:88:TYR:O     | 19:L:91:THR:HB    | 2.18                     | 0.44              |
| 19:L:361:PHE:CE1  | 19:L:391:ILE:HD12 | 2.47                     | 0.44              |
| 19:L:416:MET:HB3  | 19:L:420:ARG:HH12 | 1.82                     | 0.44              |
| 20:M:358:ALA:O    | 20:M:362:GLN:HG2  | 2.16                     | 0.44              |
| 20:M:397:GLU:O    | 20:M:400:MET:HB2  | 2.18                     | 0.44              |
| 21:N:255:ALA:O    | 21:N:259:PHE:HD2  | 2.00                     | 0.44              |
| 21:N:376:LYS:HA   | 21:N:411:ILE:HG12 | 1.98                     | 0.44              |
| 22:O:373:TRP:CZ3  | 28:U:200:LEU:CD2  | 3.00                     | 0.44              |
| 23:P:176:LYS:NZ   | 23:P:206:LYS:NZ   | 2.64                     | 0.44              |
| 25:R:171:MET:HG3  | 25:R:209:ARG:NH1  | 2.32                     | 0.44              |
| 25:R:249:ILE:HG23 | 25:R:250:ALA:N    | 2.33                     | 0.44              |
| 26:S:147:TRP:CE3  | 26:S:148:ASP:HB2  | 2.51                     | 0.44              |
| 26:S:188:TYR:OH   | 26:S:240:ASP:CB   | 2.66                     | 0.44              |
| 30:W:16:SER:HA    | 30:W:25:ARG:HB3   | 1.99                     | 0.44              |
| 33:Z:59:ASP:O     | 33:Z:60:ASP:HB2   | 2.17                     | 0.44              |
| 33:Z:812:ILE:CG2  | 33:Z:847:ILE:HG22 | 2.47                     | 0.44              |
| 2:2:36:ARG:CZ     | 2:2:38:SER:C      | 2.91                     | 0.44              |
| 3:3:59:ARG:NH2    | 10:C:100:LYS:HA   | 2.32                     | 0.44              |
| 3:3:69:GLU:HG3    | 3:3:71:ARG:H      | 1.82                     | 0.44              |
| 7:7:16:ALA:HB3    | 7:7:34:LEU:HG     | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:31:VAL:HG11   | 7:7:49:ILE:HD12   | 1.99                     | 0.44              |
| 9:B:160:LYS:HB3   | 10:C:58:GLU:HG2   | 1.99                     | 0.44              |
| 9:B:180:ASN:HD22  | 24:Q:168:LEU:HD23 | 1.83                     | 0.44              |
| 10:C:147:GLN:HB3  | 10:C:149:TYR:HE1  | 1.83                     | 0.44              |
| 11:D:37:LYS:HD3   | 11:D:147:LEU:HB3  | 2.00                     | 0.44              |
| 13:F:52:ASN:ND2   | 13:F:54:ASP:O     | 2.51                     | 0.44              |
| 14:G:168:ARG:NE   | 14:G:172:LYS:HZ1  | 2.07                     | 0.44              |
| 14:G:205:ASP:O    | 14:G:206:ASN:OD1  | 2.35                     | 0.44              |
| 15:H:62:ARG:HH12  | 16:I:95:GLN:HB2   | 1.82                     | 0.44              |
| 15:H:149:LEU:HD22 | 15:H:177:ASP:HB3  | 2.00                     | 0.44              |
| 16:I:124:THR:O    | 16:I:125:MET:HB2  | 2.18                     | 0.44              |
| 16:I:264:CYS:C    | 16:I:312:GLN:HE22 | 2.25                     | 0.44              |
| 17:J:377:VAL:CG1  | 17:J:382:PHE:CZ   | 3.01                     | 0.44              |
| 18:K:123:LEU:HD11 | 18:K:147:VAL:HA   | 1.99                     | 0.44              |
| 18:K:237:VAL:CG1  | 18:K:242:PHE:HZ   | 2.31                     | 0.44              |
| 21:N:770:LYS:HE3  | 21:N:917:ILE:CD1  | 2.43                     | 0.44              |
| 22:O:59:LEU:CD2   | 22:O:85:SER:HB2   | 2.47                     | 0.44              |
| 29:V:67:ASP:C     | 29:V:68:VAL:HG13  | 2.43                     | 0.44              |
| 29:V:159:ILE:HD11 | 29:V:188:LEU:HD11 | 1.98                     | 0.44              |
| 30:W:29:GLN:NE2   | 30:W:115:CYS:SG   | 2.90                     | 0.44              |
| 30:W:118:ILE:CD1  | 30:W:153:LEU:HD12 | 2.47                     | 0.44              |
| 33:Z:64:TYR:CD2   | 33:Z:111:LEU:HD11 | 2.25                     | 0.44              |
| 33:Z:623:ARG:HG2  | 33:Z:739:ALA:HB2  | 1.99                     | 0.44              |
| 15:H:152:ILE:O    | 15:H:153:ALA:HB3  | 2.17                     | 0.44              |
| 17:J:193:THR:HG23 | 17:J:355:GLY:H    | 1.81                     | 0.44              |
| 19:L:114:GLU:HB3  | 19:L:137:ARG:CD   | 2.45                     | 0.44              |
| 19:L:193:LEU:CD2  | 19:L:347:VAL:HG21 | 2.47                     | 0.44              |
| 20:M:290:ARG:HH11 | 20:M:294:GLU:HB3  | 1.82                     | 0.44              |
| 21:N:584:ARG:NH1  | 21:N:614:ASN:ND2  | 2.35                     | 0.44              |
| 21:N:641:LEU:HD12 | 21:N:660:LEU:HD23 | 1.98                     | 0.44              |
| 21:N:739:PHE:CD1  | 21:N:743:PHE:O    | 2.70                     | 0.44              |
| 23:P:241:LEU:HD23 | 23:P:264:ILE:HG12 | 2.00                     | 0.44              |
| 25:R:161:ALA:C    | 25:R:162:ILE:HG23 | 2.42                     | 0.44              |
| 25:R:164:THR:CG2  | 25:R:199:GLU:OE1  | 2.65                     | 0.44              |
| 26:S:315:LYS:CE   | 26:S:345:TYR:HE1  | 2.27                     | 0.44              |
| 27:T:53:ASN:H     | 27:T:57:ILE:HB    | 1.83                     | 0.44              |
| 29:V:247:ILE:O    | 29:V:247:ILE:HG13 | 2.16                     | 0.44              |
| 31:X:46:TRP:HE1   | 31:X:132:SER:CA   | 2.30                     | 0.44              |
| 33:Z:339:PHE:HB3  | 33:Z:341:TYR:CZ   | 2.53                     | 0.44              |
| 33:Z:363:ASP:O    | 33:Z:366:LYS:HE2  | 2.16                     | 0.44              |
| 33:Z:752:ILE:O    | 33:Z:756:MET:HG2  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:54:ALA:CB     | 3:3:87:TYR:CE1    | 3.00                     | 0.44              |
| 5:5:111:THR:HG21  | 5:5:113:TYR:CE2   | 2.51                     | 0.44              |
| 17:J:79:VAL:HG22  | 17:J:83:LYS:O     | 2.17                     | 0.44              |
| 17:J:135:SER:O    | 18:K:293:GLN:NE2  | 2.42                     | 0.44              |
| 17:J:167:PRO:HB3  | 17:J:174:PHE:CD2  | 2.44                     | 0.44              |
| 17:J:210:PHE:CE2  | 17:J:212:ARG:CG   | 3.00                     | 0.44              |
| 19:L:189:GLN:HE21 | 19:L:350:PRO:HD2  | 1.69                     | 0.44              |
| 20:M:131:MET:SD   | 20:M:137:PRO:HB3  | 2.57                     | 0.44              |
| 24:Q:38:SER:CB    | 24:Q:88:PHE:CE1   | 2.99                     | 0.44              |
| 24:Q:343:LEU:CD1  | 24:Q:368:LEU:HD11 | 2.36                     | 0.44              |
| 24:Q:373:VAL:HG12 | 24:Q:377:LEU:HD12 | 1.99                     | 0.44              |
| 25:R:197:MET:HB3  | 25:R:198:ILE:H    | 1.55                     | 0.44              |
| 25:R:301:TYR:CD1  | 25:R:305:PHE:CE1  | 3.03                     | 0.44              |
| 27:T:188:GLU:O    | 27:T:192:ASN:ND2  | 2.50                     | 0.44              |
| 29:V:127:LYS:O    | 29:V:131:GLN:HG2  | 2.16                     | 0.44              |
| 30:W:25:ARG:O     | 30:W:29:GLN:HG3   | 2.17                     | 0.44              |
| 33:Z:306:MET:HE3  | 33:Z:310:LEU:CG   | 2.47                     | 0.44              |
| 3:3:52:THR:CG2    | 4:4:84:ARG:CZ     | 2.94                     | 0.44              |
| 6:6:14:LEU:HD22   | 6:6:42:VAL:HG23   | 2.00                     | 0.44              |
| 12:E:52:LYS:HE2   | 12:E:217:ALA:O    | 2.17                     | 0.44              |
| 16:I:97:GLU:HA    | 16:I:100:ARG:HE   | 1.83                     | 0.44              |
| 18:K:209:VAL:CG1  | 18:K:338:ILE:HD12 | 2.48                     | 0.44              |
| 20:M:290:ARG:HD2  | 20:M:294:GLU:C    | 2.42                     | 0.44              |
| 21:N:32:VAL:HG21  | 21:N:64:ILE:HG23  | 2.00                     | 0.44              |
| 21:N:222:TYR:CZ   | 21:N:253:LEU:HD21 | 2.53                     | 0.44              |
| 21:N:329:HIS:O    | 21:N:332:VAL:HG12 | 2.18                     | 0.44              |
| 21:N:697:PHE:CE1  | 21:N:739:PHE:CZ   | 3.05                     | 0.44              |
| 21:N:758:VAL:HG23 | 21:N:874:ILE:HD13 | 1.99                     | 0.44              |
| 22:O:72:LYS:HG2   | 22:O:73:ILE:HG12  | 1.99                     | 0.44              |
| 23:P:272:PRO:O    | 23:P:273:TYR:CE1  | 2.67                     | 0.44              |
| 25:R:105:LYS:HE2  | 25:R:109:LYS:CE   | 2.47                     | 0.44              |
| 25:R:252:TYR:CE2  | 25:R:321:TYR:HD2  | 2.35                     | 0.44              |
| 26:S:156:VAL:HG22 | 26:S:187:ILE:HG23 | 1.99                     | 0.44              |
| 26:S:295:ALA:HA   | 26:S:298:ARG:HE   | 1.81                     | 0.44              |
| 33:Z:56:LEU:HD22  | 33:Z:68:LEU:HD23  | 1.90                     | 0.44              |
| 33:Z:135:LEU:HD21 | 33:Z:195:PHE:HA   | 2.00                     | 0.44              |
| 33:Z:598:ALA:O    | 33:Z:601:VAL:HG22 | 2.17                     | 0.44              |
| 33:Z:911:LYS:HB3  | 33:Z:962:ARG:HG3  | 2.00                     | 0.44              |
| 2:2:36:ARG:NH2    | 2:2:39:PRO:N      | 2.66                     | 0.44              |
| 10:C:4:ARG:HD3    | 12:E:125:GLU:HG3  | 2.00                     | 0.44              |
| 15:H:168:ILE:HG22 | 15:H:172:MET:SD   | 2.58                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:267:THR:O    | 15:H:268:ASP:HB3  | 2.18                     | 0.44              |
| 18:K:423:LYS:HE3  | 18:K:424:PHE:CE2  | 2.48                     | 0.44              |
| 19:L:289:ARG:CD   | 19:L:334:ASP:OD1  | 2.66                     | 0.44              |
| 21:N:123:PHE:CD1  | 21:N:129:ILE:HD13 | 2.53                     | 0.44              |
| 22:O:384:MET:HE1  | 28:U:189:ARG:HB3  | 2.00                     | 0.44              |
| 24:Q:171:LYS:HB2  | 24:Q:172:PRO:HD3  | 1.99                     | 0.44              |
| 24:Q:262:LEU:HD23 | 24:Q:296:ILE:CD1  | 2.47                     | 0.44              |
| 24:Q:278:VAL:O    | 24:Q:282:LEU:HG   | 2.17                     | 0.44              |
| 25:R:55:LYS:HG2   | 25:R:98:LEU:HD13  | 2.00                     | 0.44              |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:CD2  | 2.31                     | 0.44              |
| 25:R:224:PHE:CE2  | 25:R:328:PHE:CE1  | 3.05                     | 0.44              |
| 25:R:335:ARG:CA   | 25:R:371:PHE:CE2  | 3.01                     | 0.44              |
| 27:T:26:LEU:HB3   | 27:T:30:ILE:HD11  | 1.99                     | 0.44              |
| 30:W:65:PHE:HZ    | 30:W:98:LEU:HD23  | 1.83                     | 0.44              |
| 33:Z:53:VAL:CG2   | 33:Z:91:PHE:CD2   | 3.01                     | 0.44              |
| 33:Z:207:ILE:HA   | 33:Z:210:TYR:CD2  | 2.53                     | 0.44              |
| 33:Z:397:ASP:HB2  | 33:Z:425:ILE:HG21 | 1.99                     | 0.44              |
| 33:Z:518:LEU:CD1  | 33:Z:562:TRP:HE3  | 2.28                     | 0.44              |
| 2:2:83:LEU:CD1    | 2:2:100:VAL:HG21  | 2.48                     | 0.44              |
| 2:2:171:SER:OG    | 2:2:172:ASN:N     | 2.49                     | 0.44              |
| 5:5:4:LEU:HD11    | 5:5:15:ALA:HB3    | 2.00                     | 0.44              |
| 6:6:195:ILE:HG22  | 6:6:197:ILE:HG13  | 2.00                     | 0.44              |
| 13:F:43:HIS:CE1   | 13:F:218:LYS:HB3  | 2.53                     | 0.44              |
| 16:I:106:ILE:HD13 | 16:I:160:LEU:CD2  | 2.48                     | 0.44              |
| 16:I:126:PRO:HB2  | 16:I:128:TYR:CE2  | 2.39                     | 0.44              |
| 16:I:137:ASP:H    | 16:I:140:LEU:HD12 | 1.82                     | 0.44              |
| 16:I:257:LEU:HB2  | 16:I:304:ARG:NH2  | 2.33                     | 0.44              |
| 17:J:248:ASP:O    | 17:J:249:GLU:CB   | 2.66                     | 0.44              |
| 18:K:85:GLU:O     | 18:K:89:ILE:HG12  | 2.17                     | 0.44              |
| 19:L:389:ALA:HA   | 20:M:339:ARG:HE   | 1.83                     | 0.44              |
| 21:N:282:TYR:HH   | 21:N:286:LEU:HD13 | 1.73                     | 0.44              |
| 21:N:584:ARG:HH11 | 21:N:614:ASN:HD22 | 0.71                     | 0.44              |
| 23:P:164:GLN:NE2  | 23:P:179:PHE:C    | 2.76                     | 0.44              |
| 23:P:245:TYR:CE2  | 23:P:257:TRP:NE1  | 2.86                     | 0.44              |
| 24:Q:406:ASP:C    | 24:Q:406:ASP:OD1  | 2.61                     | 0.44              |
| 25:R:34:THR:HG22  | 25:R:70:TYR:HB2   | 2.00                     | 0.44              |
| 25:R:258:LEU:HD22 | 25:R:296:LEU:HD12 | 1.99                     | 0.44              |
| 26:S:204:ASP:O    | 26:S:208:ILE:HD12 | 2.17                     | 0.44              |
| 27:T:15:PHE:CZ    | 27:T:67:LEU:CB    | 2.94                     | 0.44              |
| 27:T:245:TYR:O    | 27:T:246:GLU:HB3  | 2.15                     | 0.44              |
| 33:Z:312:TYR:CE1  | 33:Z:348:LEU:CD2  | 2.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:104:ASP:HB3   | 2:2:105:PRO:CD    | 2.45                     | 0.44              |
| 2:2:213:LEU:HB2   | 3:3:192:LYS:HB2   | 2.00                     | 0.44              |
| 4:4:51:ASP:OD1    | 5:5:88:TYR:CE1    | 2.71                     | 0.44              |
| 9:B:196:LEU:O     | 9:B:200:VAL:HG22  | 2.18                     | 0.44              |
| 10:C:49:GLU:HG3   | 10:C:210:ARG:O    | 2.18                     | 0.44              |
| 11:D:146:LYS:HB3  | 11:D:148:TYR:CE2  | 2.52                     | 0.44              |
| 15:H:284:VAL:HG12 | 20:M:253:GLN:CA   | 2.47                     | 0.44              |
| 25:R:62:TYR:CZ    | 25:R:180:PHE:CB   | 2.99                     | 0.44              |
| 25:R:312:TYR:HA   | 25:R:316:LEU:HD12 | 1.98                     | 0.44              |
| 27:T:108:LEU:HD23 | 27:T:174:PHE:CD1  | 2.53                     | 0.44              |
| 27:T:139:ASP:CB   | 27:T:142:LEU:HD12 | 2.46                     | 0.44              |
| 29:V:23:THR:N     | 29:V:167:ASN:HB2  | 2.33                     | 0.44              |
| 30:W:14:GLU:O     | 30:W:18:ASN:ND2   | 2.51                     | 0.44              |
| 30:W:46:GLU:O     | 30:W:47:ASN:ND2   | 2.50                     | 0.44              |
| 33:Z:100:CYS:SG   | 33:Z:137:TYR:OH   | 2.63                     | 0.44              |
| 33:Z:234:PRO:HA   | 33:Z:271:ILE:HG12 | 2.00                     | 0.44              |
| 33:Z:269:TYR:CZ   | 33:Z:293:MET:HB3  | 2.53                     | 0.44              |
| 33:Z:301:THR:C    | 33:Z:307:HIS:HE1  | 2.25                     | 0.44              |
| 33:Z:863:THR:CG2  | 33:Z:911:LYS:HZ2  | 2.14                     | 0.44              |
| 3:3:129:VAL:HG21  | 3:3:138:PHE:CD1   | 2.50                     | 0.43              |
| 6:6:190:GLY:O     | 6:6:191:ASP:HB2   | 2.17                     | 0.43              |
| 17:J:377:VAL:HG11 | 17:J:382:PHE:CZ   | 2.52                     | 0.43              |
| 18:K:95:VAL:HG12  | 19:L:127:TYR:CE1  | 2.53                     | 0.43              |
| 21:N:602:VAL:HG11 | 21:N:625:LEU:HD23 | 2.00                     | 0.43              |
| 21:N:925:ASP:OD1  | 21:N:925:ASP:O    | 2.36                     | 0.43              |
| 24:Q:429:LYS:CB   | 29:V:269:ARG:NH2  | 2.57                     | 0.43              |
| 25:R:31:PHE:CD1   | 25:R:320:LYS:HG2  | 2.53                     | 0.43              |
| 26:S:205:ASN:OD1  | 27:T:44:LEU:HD22  | 2.18                     | 0.43              |
| 33:Z:64:TYR:CE2   | 33:Z:68:LEU:CD1   | 2.88                     | 0.43              |
| 5:5:7:ARG:CZ      | 5:5:110:PRO:HG2   | 2.48                     | 0.43              |
| 6:6:2:THR:N       | 6:6:46:ASN:HD21   | 2.16                     | 0.43              |
| 6:6:10:ASP:OD1    | 6:6:11:PHE:CD1    | 2.60                     | 0.43              |
| 9:B:239:THR:O     | 9:B:243:ILE:HG13  | 2.19                     | 0.43              |
| 11:D:67:ILE:HD11  | 11:D:73:LEU:HB2   | 2.00                     | 0.43              |
| 13:F:7:ASP:HB3    | 13:F:21:GLN:NE2   | 2.34                     | 0.43              |
| 15:H:62:ARG:HD2   | 16:I:96:LEU:CD2   | 2.49                     | 0.43              |
| 15:H:156:VAL:HA   | 15:H:181:TYR:CZ   | 2.53                     | 0.43              |
| 17:J:135:SER:OG   | 18:K:280:LYS:HD3  | 2.17                     | 0.43              |
| 18:K:88:ARG:HH11  | 29:V:149:GLY:HA3  | 1.82                     | 0.43              |
| 19:L:317:ASN:OD1  | 19:L:317:ASN:C    | 2.61                     | 0.43              |
| 20:M:384:ASP:N    | 20:M:386:PHE:CD1  | 2.86                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:109:TYR:CE1  | 21:N:129:ILE:HD12 | 2.50                     | 0.43              |
| 22:O:15:ARG:NH2   | 22:O:73:ILE:CD1   | 2.71                     | 0.43              |
| 22:O:190:TYR:CE2  | 22:O:194:LEU:HD11 | 2.53                     | 0.43              |
| 23:P:350:LEU:HD13 | 23:P:383:LEU:HD12 | 2.00                     | 0.43              |
| 25:R:408:ASP:OD1  | 26:S:464:ARG:NH1  | 2.46                     | 0.43              |
| 27:T:89:TYR:CZ    | 27:T:102:LYS:HB2  | 2.53                     | 0.43              |
| 30:W:21:PHE:CE1   | 30:W:25:ARG:HG3   | 2.53                     | 0.43              |
| 33:Z:301:THR:CG2  | 33:Z:307:HIS:ND1  | 2.81                     | 0.43              |
| 33:Z:415:MET:HG2  | 33:Z:446:GLU:HB2  | 1.99                     | 0.43              |
| 33:Z:766:HIS:CD2  | 33:Z:767:TYR:CD1  | 3.06                     | 0.43              |
| 33:Z:972:SER:OG   | 33:Z:976:HIS:N    | 2.50                     | 0.43              |
| 33:Z:975:SER:C    | 33:Z:977:ILE:HG23 | 2.43                     | 0.43              |
| 1:1:82:PHE:HB2    | 1:1:113:ILE:HD13  | 2.00                     | 0.43              |
| 1:1:175:MET:HE2   | 1:1:188:PHE:CE1   | 2.53                     | 0.43              |
| 7:7:91:VAL:HG12   | 7:7:102:LEU:HD11  | 1.99                     | 0.43              |
| 11:D:203:VAL:O    | 11:D:204:GLN:CB   | 2.66                     | 0.43              |
| 13:F:215:ILE:HG22 | 13:F:223:THR:O    | 2.19                     | 0.43              |
| 15:H:155:PHE:CE2  | 20:M:76:PRO:HB2   | 2.53                     | 0.43              |
| 15:H:282:LYS:HB2  | 16:I:257:LEU:HB3  | 1.99                     | 0.43              |
| 16:I:204:HIS:CB   | 16:I:207:LEU:HB2  | 2.26                     | 0.43              |
| 16:I:207:LEU:CG   | 33:Z:930:GLY:HA2  | 2.48                     | 0.43              |
| 17:J:79:VAL:O     | 17:J:104:VAL:HG21 | 2.17                     | 0.43              |
| 20:M:130:PRO:HD2  | 20:M:154:LEU:CD2  | 2.47                     | 0.43              |
| 21:N:337:GLY:C    | 21:N:373:VAL:HG11 | 2.42                     | 0.43              |
| 22:O:260:VAL:HG12 | 22:O:262:ASP:CG   | 2.43                     | 0.43              |
| 22:O:384:MET:CE   | 28:U:190:LEU:HA   | 2.48                     | 0.43              |
| 23:P:138:ARG:HH11 | 23:P:141:LYS:HD3  | 1.83                     | 0.43              |
| 23:P:265:VAL:HG12 | 23:P:296:GLN:HE21 | 1.83                     | 0.43              |
| 23:P:415:TRP:HD1  | 28:U:265:LEU:HB2  | 1.83                     | 0.43              |
| 25:R:397:ASN:CG   | 26:S:452:TYR:O    | 2.62                     | 0.43              |
| 25:R:422:ARG:NH1  | 26:S:474:GLU:CG   | 2.81                     | 0.43              |
| 29:V:41:GLY:HA2   | 29:V:49:VAL:CG2   | 2.48                     | 0.43              |
| 30:W:178:PRO:O    | 30:W:179:ARG:HB2  | 2.17                     | 0.43              |
| 1:1:114:PRO:CG    | 1:1:118:SER:HB2   | 2.45                     | 0.43              |
| 3:3:-2:ASN:HA     | 3:3:21:GLY:H      | 1.83                     | 0.43              |
| 6:6:91:LYS:HB2    | 6:6:96:TYR:CE1    | 2.47                     | 0.43              |
| 7:7:187:PHE:CE2   | 7:7:204:LEU:CD1   | 3.02                     | 0.43              |
| 8:A:148:GLU:CD    | 8:A:230:LYS:HG3   | 2.44                     | 0.43              |
| 9:B:48:GLU:HB3    | 9:B:50:LYS:HE3    | 1.99                     | 0.43              |
| 11:D:34:VAL:HG12  | 11:D:163:THR:HG1  | 1.81                     | 0.43              |
| 14:G:111:PHE:HB2  | 14:G:114:ARG:HH21 | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:99:VAL:O     | 15:H:173:ARG:CD   | 2.65                     | 0.43              |
| 17:J:71:TYR:HE1   | 18:K:118:TYR:HE2  | 1.66                     | 0.43              |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:HG22 | 1.93                     | 0.43              |
| 18:K:131:LEU:HA   | 18:K:135:MET:SD   | 2.58                     | 0.43              |
| 19:L:67:HIS:HD2   | 19:L:68:ARG:HG3   | 1.82                     | 0.43              |
| 21:N:641:LEU:HD13 | 21:N:660:LEU:HD23 | 1.99                     | 0.43              |
| 25:R:338:TYR:CE1  | 25:R:377:LEU:HD13 | 2.53                     | 0.43              |
| 25:R:421:VAL:O    | 25:R:422:ARG:CB   | 2.66                     | 0.43              |
| 31:X:37:PRO:HB3   | 31:X:46:TRP:CE3   | 2.53                     | 0.43              |
| 33:Z:100:CYS:O    | 33:Z:103:TYR:HB3  | 2.18                     | 0.43              |
| 33:Z:301:THR:HG22 | 33:Z:307:HIS:NE2  | 2.26                     | 0.43              |
| 33:Z:375:ASP:C    | 33:Z:375:ASP:OD1  | 2.62                     | 0.43              |
| 33:Z:762:GLY:HA2  | 33:Z:765:MET:CE   | 2.49                     | 0.43              |
| 1:1:83:LYS:HZ2    | 1:1:118:SER:CA    | 2.15                     | 0.43              |
| 6:6:141:LEU:CD1   | 6:6:145:VAL:CG2   | 2.95                     | 0.43              |
| 9:B:205:ASN:O     | 9:B:209:ILE:HG13  | 2.18                     | 0.43              |
| 10:C:144:TYR:CB   | 10:C:147:GLN:NE2  | 2.79                     | 0.43              |
| 10:C:162:ALA:CB   | 10:C:176:LEU:HD21 | 2.47                     | 0.43              |
| 15:H:317:ALA:HB2  | 15:H:360:THR:HB   | 2.00                     | 0.43              |
| 16:I:128:TYR:HD2  | 16:I:154:MET:HG3  | 1.81                     | 0.43              |
| 19:L:85:GLU:HG3   | 20:M:58:MET:CE    | 2.48                     | 0.43              |
| 19:L:353:ASN:HB2  | 19:L:356:GLY:H    | 1.84                     | 0.43              |
| 20:M:179:THR:OG1  | 20:M:182:ASP:CG   | 2.61                     | 0.43              |
| 20:M:258:GLU:O    | 20:M:262:LEU:HG   | 2.18                     | 0.43              |
| 20:M:263:VAL:HG21 | 20:M:304:THR:HG23 | 1.99                     | 0.43              |
| 21:N:525:ASN:ND2  | 21:N:554:THR:HG23 | 2.33                     | 0.43              |
| 23:P:129:LYS:O    | 23:P:130:ILE:HB   | 2.19                     | 0.43              |
| 26:S:258:GLU:C    | 26:S:259:TYR:CD1  | 2.97                     | 0.43              |
| 33:Z:383:SER:HA   | 33:Z:849:ARG:NH1  | 2.33                     | 0.43              |
| 33:Z:518:LEU:HD11 | 33:Z:562:TRP:CD2  | 2.54                     | 0.43              |
| 2:2:160:GLN:HG3   | 2:2:164:TRP:CD1   | 2.53                     | 0.43              |
| 2:2:163:ILE:HG23  | 2:2:170:GLY:HA2   | 2.01                     | 0.43              |
| 4:4:153:THR:HG21  | 4:4:182:ILE:HD13  | 2.00                     | 0.43              |
| 6:6:112:ALA:HB1   | 6:6:114:TYR:CE1   | 2.53                     | 0.43              |
| 10:C:66:LEU:HD12  | 10:C:212:GLU:HG2  | 1.99                     | 0.43              |
| 14:G:59:VAL:HG23  | 14:G:60:PRO:HD2   | 1.99                     | 0.43              |
| 15:H:147:ILE:HG23 | 15:H:181:TYR:HD2  | 1.83                     | 0.43              |
| 15:H:168:ILE:HG21 | 15:H:172:MET:O    | 2.18                     | 0.43              |
| 15:H:328:GLU:HA   | 15:H:331:ARG:CZ   | 2.49                     | 0.43              |
| 21:N:67:LYS:HG3   | 21:N:97:PHE:CE1   | 2.53                     | 0.43              |
| 22:O:4:ASN:HB2    | 22:O:39:PHE:CD1   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:P:302:LEU:HD11 | 23:P:314:VAL:HG11 | 2.01                     | 0.43              |
| 24:Q:369:ASP:OD1  | 24:Q:369:ASP:C    | 2.59                     | 0.43              |
| 25:R:237:THR:HG22 | 25:R:275:GLU:CD   | 2.43                     | 0.43              |
| 26:S:227:ASN:HB2  | 26:S:263:ASP:OD2  | 2.18                     | 0.43              |
| 27:T:89:TYR:CE1   | 27:T:102:LYS:CD   | 2.97                     | 0.43              |
| 28:U:13:LEU:HD11  | 29:V:36:LYS:CG    | 2.45                     | 0.43              |
| 31:X:37:PRO:O     | 31:X:38:ASN:CB    | 2.67                     | 0.43              |
| 33:Z:368:VAL:HG12 | 33:Z:369:PHE:N    | 2.32                     | 0.43              |
| 1:1:11:GLY:HA2    | 1:1:102:TYR:CE1   | 2.53                     | 0.43              |
| 1:1:54:ALA:HB1    | 2:2:88:PHE:CE1    | 2.53                     | 0.43              |
| 7:7:180:ASP:OD1   | 7:7:182:ARG:HB2   | 2.18                     | 0.43              |
| 12:E:208:MET:SD   | 12:E:210:GLU:O    | 2.77                     | 0.43              |
| 13:F:54:ASP:HB3   | 13:F:57:SER:H     | 1.83                     | 0.43              |
| 18:K:127:ASP:CG   | 18:K:128:ARG:H    | 2.27                     | 0.43              |
| 18:K:411:TYR:O    | 18:K:415:VAL:HG22 | 2.18                     | 0.43              |
| 19:L:166:LEU:HD22 | 19:L:168:TYR:CZ   | 2.54                     | 0.43              |
| 19:L:336:ALA:O    | 19:L:342:ARG:NH1  | 2.47                     | 0.43              |
| 20:M:195:GLU:HG3  | 20:M:199:LEU:HD12 | 2.01                     | 0.43              |
| 21:N:58:ARG:HG3   | 21:N:59:GLU:N     | 2.34                     | 0.43              |
| 22:O:228:TYR:OH   | 22:O:294:MET:HE1  | 2.17                     | 0.43              |
| 24:Q:355:GLU:CG   | 24:Q:397:LEU:HG   | 2.47                     | 0.43              |
| 26:S:180:ASN:OD1  | 26:S:182:LYS:HG3  | 2.18                     | 0.43              |
| 28:U:173:HIS:CE1  | 29:V:150:LYS:HB2  | 2.54                     | 0.43              |
| 29:V:135:ARG:CD   | 29:V:157:ARG:NH1  | 2.80                     | 0.43              |
| 29:V:153:ILE:O    | 29:V:154:ASP:OD1  | 2.37                     | 0.43              |
| 31:X:61:LEU:HD22  | 31:X:97:TYR:CD2   | 2.53                     | 0.43              |
| 33:Z:64:TYR:HB3   | 33:Z:111:LEU:HD11 | 2.01                     | 0.43              |
| 33:Z:103:TYR:CE1  | 33:Z:116:ALA:HB2  | 2.47                     | 0.43              |
| 33:Z:312:TYR:CZ   | 33:Z:348:LEU:CD2  | 3.02                     | 0.43              |
| 33:Z:394:TYR:CB   | 33:Z:859:LYS:NZ   | 2.81                     | 0.43              |
| 33:Z:958:ASN:N    | 33:Z:961:GLU:OE2  | 2.45                     | 0.43              |
| 7:7:8:TYR:CZ      | 7:7:11:GLY:CA     | 3.01                     | 0.43              |
| 7:7:133:THR:HG21  | 7:7:148:ARG:HG2   | 2.01                     | 0.43              |
| 9:B:160:LYS:HE3   | 10:C:56:LEU:HD23  | 2.00                     | 0.43              |
| 15:H:351:VAL:HG12 | 15:H:353:PHE:CD1  | 2.51                     | 0.43              |
| 19:L:218:VAL:HB   | 19:L:324:ILE:HG12 | 2.00                     | 0.43              |
| 20:M:368:MET:HG3  | 20:M:369:THR:O    | 2.18                     | 0.43              |
| 21:N:602:VAL:HG12 | 21:N:625:LEU:CD2  | 2.48                     | 0.43              |
| 21:N:627:ILE:HG23 | 21:N:717:LEU:HD21 | 2.01                     | 0.43              |
| 25:R:241:ILE:HG22 | 25:R:242:GLU:N    | 2.34                     | 0.43              |
| 26:S:321:GLN:O    | 26:S:324:MET:HG2  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:157:TYR:CD1  | 27:T:185:ILE:HG23 | 2.54                     | 0.43              |
| 28:U:46:ILE:HG23  | 28:U:90:ILE:HD12  | 2.00                     | 0.43              |
| 28:U:290:ASP:OD2  | 29:V:281:SER:HA   | 2.19                     | 0.43              |
| 30:W:8:LEU:HD11   | 30:W:113:PHE:HE2  | 1.84                     | 0.43              |
| 33:Z:410:THR:CG2  | 33:Z:414:GLY:HA3  | 2.49                     | 0.43              |
| 33:Z:443:ASP:CG   | 33:Z:447:VAL:CG1  | 2.48                     | 0.43              |
| 33:Z:805:LEU:HD22 | 33:Z:841:GLU:OE1  | 2.14                     | 0.43              |
| 33:Z:968:ASP:OD2  | 33:Z:983:LEU:HD21 | 2.19                     | 0.43              |
| 3:3:100:VAL:CG2   | 3:3:115:PHE:CE1   | 3.01                     | 0.43              |
| 11:D:159:TRP:CZ3  | 12:E:59:LEU:CD1   | 2.97                     | 0.43              |
| 12:E:182:GLU:OE1  | 12:E:203:ILE:HG12 | 2.19                     | 0.43              |
| 13:F:6:TYR:HB2    | 13:F:20:PHE:HD2   | 1.84                     | 0.43              |
| 16:I:164:ALA:O    | 16:I:165:ASP:CB   | 2.62                     | 0.43              |
| 16:I:395:MET:SD   | 16:I:420:LYS:HE2  | 2.58                     | 0.43              |
| 19:L:278:ILE:HG22 | 19:L:280:MET:HG3  | 2.00                     | 0.43              |
| 20:M:81:ASN:HB2   | 20:M:163:PHE:CE1  | 2.53                     | 0.43              |
| 21:N:302:PHE:CZ   | 21:N:757:THR:CB   | 3.01                     | 0.43              |
| 22:O:255:LEU:HD23 | 22:O:255:LEU:O    | 2.18                     | 0.43              |
| 23:P:237:VAL:HG11 | 23:P:267:PHE:CE2  | 2.53                     | 0.43              |
| 23:P:263:HIS:ND1  | 23:P:325:ASP:OD1  | 2.51                     | 0.43              |
| 26:S:443:ILE:HG22 | 26:S:445:THR:HG23 | 2.00                     | 0.43              |
| 27:T:199:PHE:CD1  | 27:T:199:PHE:C    | 2.97                     | 0.43              |
| 28:U:286:ILE:HG21 | 29:V:261:LEU:HD23 | 2.00                     | 0.43              |
| 29:V:145:GLN:CG   | 29:V:148:LYS:HE3  | 2.31                     | 0.43              |
| 31:X:104:LYS:NZ   | 31:X:107:GLY:C    | 2.76                     | 0.43              |
| 33:Z:519:PRO:HD3  | 33:Z:556:ILE:HG23 | 1.99                     | 0.43              |
| 33:Z:893:PHE:HB3  | 33:Z:894:MET:H    | 1.53                     | 0.43              |
| 1:1:141:ASN:CB    | 1:1:154:PHE:HE1   | 2.27                     | 0.43              |
| 1:1:177:VAL:HG12  | 1:1:179:THR:CG2   | 2.44                     | 0.43              |
| 5:5:32:LYS:O      | 5:5:33:ARG:HG2    | 2.18                     | 0.43              |
| 5:5:199:LYS:HG2   | 5:5:203:GLU:CD    | 2.44                     | 0.43              |
| 7:7:92:MET:SD     | 7:7:106:ILE:HD12  | 2.59                     | 0.43              |
| 7:7:193:ASP:OD1   | 7:7:195:ASN:N     | 2.43                     | 0.43              |
| 11:D:60:THR:HG22  | 11:D:61:PRO:O     | 2.18                     | 0.43              |
| 12:E:67:ILE:HG22  | 12:E:228:PHE:HZ   | 1.83                     | 0.43              |
| 12:E:166:ARG:HB2  | 13:F:60:GLN:NE2   | 2.34                     | 0.43              |
| 13:F:128:TYR:HB3  | 13:F:130:VAL:HG12 | 2.00                     | 0.43              |
| 13:F:145:LEU:HD23 | 13:F:146:GLU:N    | 2.33                     | 0.43              |
| 15:H:49:LEU:O     | 33:Z:765:MET:HE1  | 2.19                     | 0.43              |
| 15:H:291:VAL:O    | 15:H:295:PHE:HD1  | 2.02                     | 0.43              |
| 16:I:285:ASP:OD1  | 16:I:286:ALA:N    | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:320:GLY:HA2  | 16:I:323:LYS:HZ3  | 1.84                     | 0.43              |
| 19:L:113:SER:HG   | 19:L:116:LYS:HB2  | 1.84                     | 0.43              |
| 20:M:330:VAL:O    | 20:M:330:VAL:HG13 | 2.19                     | 0.43              |
| 21:N:145:LEU:CB   | 21:N:173:LYS:NZ   | 2.79                     | 0.43              |
| 22:O:40:GLN:HB2   | 22:O:58:ARG:HE    | 1.81                     | 0.43              |
| 22:O:260:VAL:CG1  | 22:O:262:ASP:CG   | 2.92                     | 0.43              |
| 23:P:72:TRP:CD2   | 23:P:104:LEU:HD23 | 2.53                     | 0.43              |
| 24:Q:167:LYS:HG3  | 24:Q:168:LEU:HG   | 2.01                     | 0.43              |
| 24:Q:412:ALA:O    | 24:Q:416:VAL:HG23 | 2.18                     | 0.43              |
| 26:S:425:ARG:NH1  | 27:T:155:GLY:HA2  | 2.29                     | 0.43              |
| 26:S:455:GLU:H    | 28:U:274:MET:CE   | 2.32                     | 0.43              |
| 28:U:121:LEU:HD11 | 28:U:134:THR:CG2  | 2.48                     | 0.43              |
| 28:U:175:LEU:HD21 | 29:V:213:LEU:HB2  | 1.99                     | 0.43              |
| 31:X:122:TYR:O    | 31:X:126:ILE:HG12 | 2.19                     | 0.43              |
| 33:Z:401:VAL:HG22 | 33:Z:439:TYR:HE2  | 1.84                     | 0.43              |
| 2:2:6:VAL:CG1     | 2:2:13:VAL:HB     | 2.49                     | 0.42              |
| 3:3:7:THR:HG21    | 3:3:125:LYS:HB3   | 2.01                     | 0.42              |
| 4:4:142:LEU:HD12  | 4:4:146:HIS:ND1   | 2.33                     | 0.42              |
| 4:4:167:LEU:O     | 4:4:171:MET:HB3   | 2.19                     | 0.42              |
| 11:D:11:PHE:CE2   | 12:E:26:TYR:C     | 2.98                     | 0.42              |
| 12:E:165:TYR:CE2  | 20:M:434:ALA:HB2  | 2.53                     | 0.42              |
| 13:F:86:ASN:HA    | 13:F:89:ARG:NH2   | 2.34                     | 0.42              |
| 15:H:402:ILE:HG13 | 15:H:440:GLU:HG2  | 1.99                     | 0.42              |
| 17:J:199:ALA:CB   | 17:J:210:PHE:CE1  | 3.01                     | 0.42              |
| 20:M:396:VAL:O    | 20:M:400:MET:HG2  | 2.18                     | 0.42              |
| 21:N:344:THR:O    | 21:N:344:THR:HG22 | 2.18                     | 0.42              |
| 23:P:212:LYS:HD3  | 23:P:247:THR:CG2  | 2.46                     | 0.42              |
| 23:P:266:TYR:CE1  | 23:P:322:LEU:HA   | 2.54                     | 0.42              |
| 23:P:315:GLN:O    | 23:P:319:GLU:HG3  | 2.19                     | 0.42              |
| 24:Q:148:LYS:O    | 24:Q:149:LYS:CB   | 2.66                     | 0.42              |
| 25:R:356:ALA:HA   | 32:Y:89:GLN:CD    | 2.44                     | 0.42              |
| 26:S:428:ARG:CA   | 27:T:195:LEU:HD22 | 2.42                     | 0.42              |
| 29:V:93:ASP:O     | 29:V:96:LYS:HB3   | 2.19                     | 0.42              |
| 33:Z:103:TYR:CE2  | 33:Z:137:TYR:CE1  | 3.07                     | 0.42              |
| 33:Z:410:THR:HG22 | 33:Z:414:GLY:HA3  | 1.99                     | 0.42              |
| 33:Z:744:ALA:CA   | 33:Z:783:VAL:HG22 | 2.48                     | 0.42              |
| 33:Z:886:VAL:HA   | 33:Z:893:PHE:CZ   | 2.50                     | 0.42              |
| 2:2:87:LEU:HD23   | 2:2:94:ILE:HB     | 2.00                     | 0.42              |
| 3:3:63:ASN:CB     | 10:C:96:GLN:NE2   | 2.82                     | 0.42              |
| 5:5:35:ILE:HG21   | 5:5:56:GLU:HB2    | 2.01                     | 0.42              |
| 6:6:36:ASP:OD1    | 6:6:38:GLY:N      | 2.51                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:21:PRO:HB3    | 9:B:23:TYR:CE1    | 2.54                     | 0.42              |
| 15:H:102:CYS:HB2  | 15:H:105:ILE:CD1  | 2.27                     | 0.42              |
| 15:H:156:VAL:CG2  | 15:H:181:TYR:CZ   | 2.83                     | 0.42              |
| 15:H:285:GLY:H    | 15:H:331:ARG:NH1  | 2.15                     | 0.42              |
| 15:H:311:ILE:HD12 | 15:H:361:LEU:HD13 | 2.00                     | 0.42              |
| 19:L:149:ASP:CB   | 19:L:152:THR:HB   | 2.48                     | 0.42              |
| 19:L:290:ARG:CZ   | 19:L:293:GLU:HA   | 2.49                     | 0.42              |
| 21:N:303:LEU:HD13 | 21:N:342:GLY:HA3  | 2.01                     | 0.42              |
| 21:N:515:ARG:HH22 | 21:N:738:GLN:CD   | 2.25                     | 0.42              |
| 21:N:596:LEU:CD2  | 21:N:717:LEU:HD13 | 2.42                     | 0.42              |
| 21:N:669:GLU:O    | 21:N:670:LYS:HB2  | 2.19                     | 0.42              |
| 22:O:43:GLU:OE2   | 22:O:72:LYS:NZ    | 2.53                     | 0.42              |
| 22:O:223:LEU:HD23 | 22:O:280:LEU:HB2  | 2.01                     | 0.42              |
| 23:P:281:ILE:HD11 | 23:P:297:GLU:HG3  | 2.00                     | 0.42              |
| 26:S:201:ILE:HD13 | 26:S:205:ASN:HD22 | 1.84                     | 0.42              |
| 33:Z:542:ILE:HG21 | 33:Z:573:LEU:HD11 | 2.01                     | 0.42              |
| 33:Z:584:VAL:O    | 33:Z:588:ILE:HG13 | 2.19                     | 0.42              |
| 1:1:66:TYR:HE2    | 1:1:73:PRO:HA     | 1.85                     | 0.42              |
| 2:2:197:GLU:O     | 3:3:142:GLU:OE2   | 2.37                     | 0.42              |
| 5:5:34:VAL:HG11   | 5:5:42:LEU:HD22   | 2.00                     | 0.42              |
| 6:6:171:VAL:O     | 6:6:175:VAL:HG23  | 2.20                     | 0.42              |
| 8:A:18:ILE:HD12   | 9:B:20:GLN:HE22   | 1.84                     | 0.42              |
| 9:B:2:THR:HB      | 14:G:127:SER:OG   | 2.19                     | 0.42              |
| 9:B:43:VAL:HG11   | 9:B:137:ALA:CB    | 2.41                     | 0.42              |
| 10:C:18:ARG:NH2   | 11:D:29:ARG:HH22  | 2.11                     | 0.42              |
| 10:C:50:ARG:HH12  | 10:C:232:PRO:HG3  | 1.85                     | 0.42              |
| 12:E:56:SER:OG    | 12:E:59:LEU:HB2   | 2.19                     | 0.42              |
| 15:H:49:LEU:C     | 33:Z:765:MET:HE1  | 2.45                     | 0.42              |
| 15:H:210:ASP:HA   | 15:H:388:ILE:HG12 | 2.00                     | 0.42              |
| 16:I:172:LYS:HD3  | 17:J:231:ARG:HH12 | 1.84                     | 0.42              |
| 17:J:349:LYS:NZ   | 17:J:383:GLU:HB2  | 2.35                     | 0.42              |
| 18:K:346:ARG:CG   | 18:K:349:ARG:HH22 | 2.25                     | 0.42              |
| 21:N:162:ARG:HD3  | 21:N:165:ILE:HG13 | 1.97                     | 0.42              |
| 21:N:221:ASP:HA   | 21:N:894:ARG:NH1  | 2.34                     | 0.42              |
| 21:N:489:MET:HE3  | 21:N:493:GLY:HA2  | 2.00                     | 0.42              |
| 22:O:365:LYS:HB3  | 22:O:369:ARG:HH12 | 1.83                     | 0.42              |
| 24:Q:190:ASN:HD21 | 24:Q:193:LYS:HE3  | 1.85                     | 0.42              |
| 24:Q:245:SER:O    | 24:Q:249:LEU:HG   | 2.18                     | 0.42              |
| 24:Q:373:VAL:O    | 24:Q:377:LEU:HG   | 2.19                     | 0.42              |
| 1:1:36:ARG:HD3    | 1:1:42:TRP:CZ2    | 2.54                     | 0.42              |
| 3:3:7:THR:HG23    | 3:3:112:ILE:HD13  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:18:ILE:HB     | 9:B:20:GLN:NE2    | 2.33                     | 0.42              |
| 9:B:43:VAL:HG21   | 9:B:146:SER:O     | 2.19                     | 0.42              |
| 10:C:13:PHE:CD1   | 10:C:19:LEU:HD21  | 2.54                     | 0.42              |
| 11:D:19:GLN:CD    | 11:D:128:PRO:HD2  | 2.43                     | 0.42              |
| 13:F:7:ASP:O      | 13:F:21:GLN:NE2   | 2.52                     | 0.42              |
| 15:H:284:VAL:CG2  | 20:M:254:MET:CA   | 2.79                     | 0.42              |
| 15:H:423:CYS:HA   | 15:H:443:PHE:CE1  | 2.54                     | 0.42              |
| 16:I:128:TYR:CE2  | 16:I:154:MET:HG3  | 2.53                     | 0.42              |
| 17:J:301:ASP:O    | 17:J:304:LEU:HB2  | 2.19                     | 0.42              |
| 18:K:197:LEU:HD23 | 18:K:200:GLN:OE1  | 2.20                     | 0.42              |
| 19:L:125:PRO:HB2  | 19:L:127:TYR:HE2  | 1.72                     | 0.42              |
| 19:L:141:LYS:O    | 19:L:144:VAL:HG23 | 2.18                     | 0.42              |
| 20:M:75:LEU:HD22  | 20:M:77:TYR:O     | 2.19                     | 0.42              |
| 20:M:401:ILE:HG12 | 20:M:404:ARG:NH2  | 2.35                     | 0.42              |
| 21:N:4:THR:HG21   | 26:S:215:MET:SD   | 2.60                     | 0.42              |
| 21:N:525:ASN:HA   | 21:N:528:ARG:HD3  | 2.01                     | 0.42              |
| 21:N:745:LEU:O    | 21:N:748:PHE:CD1  | 2.73                     | 0.42              |
| 23:P:95:TYR:CE2   | 23:P:96:MET:CE    | 3.00                     | 0.42              |
| 26:S:223:LEU:O    | 26:S:224:LYS:HD3  | 2.19                     | 0.42              |
| 26:S:461:PHE:HA   | 28:U:281:LEU:HD11 | 2.01                     | 0.42              |
| 33:Z:112:LYS:HA   | 33:Z:115:LEU:HD12 | 2.01                     | 0.42              |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:HD2  | 1.76                     | 0.42              |
| 1:1:63:LEU:HD22   | 1:1:73:PRO:HG3    | 2.01                     | 0.42              |
| 2:2:55:VAL:HG21   | 2:2:94:ILE:CG2    | 2.49                     | 0.42              |
| 2:2:97:TYR:CZ     | 2:2:115:ALA:CB    | 3.02                     | 0.42              |
| 3:3:37:TYR:OH     | 3:3:55:ASN:O      | 2.35                     | 0.42              |
| 3:3:42:LEU:HD22   | 3:3:78:PHE:HZ     | 1.83                     | 0.42              |
| 8:A:52:VAL:CG1    | 8:A:203:VAL:HG22  | 2.49                     | 0.42              |
| 8:A:87:ILE:O      | 8:A:87:ILE:CG2    | 2.67                     | 0.42              |
| 13:F:101:ARG:HG2  | 13:F:103:LEU:N    | 2.19                     | 0.42              |
| 14:G:175:LEU:O    | 14:G:179:VAL:HG23 | 2.19                     | 0.42              |
| 16:I:384:LYS:CE   | 16:I:420:LYS:HZ2  | 2.24                     | 0.42              |
| 20:M:221:TYR:O    | 20:M:349:PHE:HD1  | 2.03                     | 0.42              |
| 21:N:106:ILE:O    | 21:N:110:VAL:HG23 | 2.19                     | 0.42              |
| 21:N:207:LEU:CD1  | 21:N:232:LEU:HD23 | 2.49                     | 0.42              |
| 21:N:653:ARG:HG2  | 21:N:657:MET:HE3  | 2.02                     | 0.42              |
| 21:N:770:LYS:CD   | 21:N:917:ILE:HG21 | 2.50                     | 0.42              |
| 22:O:280:LEU:CD2  | 22:O:280:LEU:C    | 2.89                     | 0.42              |
| 23:P:303:PHE:CZ   | 23:P:345:VAL:HG22 | 2.46                     | 0.42              |
| 23:P:326:ASP:OD1  | 23:P:327:LEU:HG   | 2.20                     | 0.42              |
| 23:P:422:LEU:CD1  | 28:U:262:GLN:NE2  | 2.82                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:52:ASN:HD21  | 24:Q:92:LYS:NZ    | 2.18                     | 0.42              |
| 26:S:436:ILE:HG23 | 27:T:197:TYR:CD2  | 2.55                     | 0.42              |
| 28:U:12:PRO:HD2   | 28:U:167:GLU:OE2  | 2.19                     | 0.42              |
| 33:Z:354:PRO:O    | 33:Z:357:ILE:CG1  | 2.66                     | 0.42              |
| 8:A:83:VAL:HG11   | 8:A:90:ALA:HA     | 2.01                     | 0.42              |
| 8:A:123:ASN:HB3   | 9:B:84:VAL:HG22   | 2.01                     | 0.42              |
| 9:B:75:TYR:HB3    | 9:B:134:LEU:CD2   | 2.49                     | 0.42              |
| 12:E:46:VAL:HG11  | 12:E:145:ALA:CB   | 2.47                     | 0.42              |
| 12:E:50:VAL:HG22  | 12:E:67:ILE:CD1   | 2.45                     | 0.42              |
| 15:H:56:LEU:HD21  | 33:Z:768:GLY:HA2  | 2.01                     | 0.42              |
| 16:I:211:MET:HE1  | 33:Z:930:GLY:O    | 2.20                     | 0.42              |
| 17:J:349:LYS:HZ3  | 17:J:383:GLU:CB   | 2.32                     | 0.42              |
| 18:K:280:LYS:NZ   | 18:K:293:GLN:OE1  | 2.50                     | 0.42              |
| 20:M:338:LEU:HD21 | 20:M:346:LYS:HZ1  | 1.84                     | 0.42              |
| 21:N:211:PHE:O    | 21:N:215:MET:HG2  | 2.18                     | 0.42              |
| 22:O:16:MET:HB2   | 30:W:19:GLY:C     | 2.45                     | 0.42              |
| 22:O:46:THR:CG2   | 22:O:50:ASP:OD2   | 2.68                     | 0.42              |
| 22:O:58:ARG:CB    | 22:O:61:LEU:HD12  | 2.49                     | 0.42              |
| 23:P:154:ASP:OD1  | 23:P:190:LYS:HD3  | 2.20                     | 0.42              |
| 24:Q:151:TYR:CD2  | 24:Q:188:LEU:HD21 | 2.55                     | 0.42              |
| 26:S:162:VAL:HG12 | 26:S:167:LEU:HD22 | 2.00                     | 0.42              |
| 26:S:343:LEU:CG   | 26:S:347:HIS:HE1  | 2.30                     | 0.42              |
| 29:V:88:GLN:NE2   | 29:V:89:ALA:HB2   | 2.34                     | 0.42              |
| 33:Z:89:LEU:CD1   | 33:Z:125:THR:CG2  | 2.97                     | 0.42              |
| 1:1:55:ILE:HD12   | 1:1:95:ALA:HB2    | 2.00                     | 0.42              |
| 2:2:29:LYS:HZ3    | 2:2:195:VAL:HA    | 1.84                     | 0.42              |
| 5:5:135:PHE:CE2   | 5:5:163:ALA:CB    | 2.83                     | 0.42              |
| 6:6:48:PHE:CE2    | 6:6:50:ALA:CB     | 2.95                     | 0.42              |
| 9:B:122:THR:OG1   | 9:B:129:PRO:HG3   | 2.19                     | 0.42              |
| 10:C:72:LYS:HG2   | 10:C:225:VAL:HG11 | 2.01                     | 0.42              |
| 12:E:180:GLN:HA   | 12:E:183:LEU:HD12 | 2.02                     | 0.42              |
| 15:H:101:ARG:NH2  | 15:H:150:LYS:HG3  | 2.35                     | 0.42              |
| 15:H:396:MET:CE   | 15:H:438:ALA:HB3  | 1.94                     | 0.42              |
| 16:I:207:LEU:CD2  | 33:Z:930:GLY:HA2  | 2.49                     | 0.42              |
| 16:I:395:MET:HG3  | 16:I:420:LYS:CD   | 2.44                     | 0.42              |
| 17:J:183:LYS:O    | 17:J:276:LEU:HD13 | 2.20                     | 0.42              |
| 18:K:220:THR:HG22 | 18:K:224:LYS:HE3  | 2.01                     | 0.42              |
| 18:K:385:ALA:HA   | 19:L:340:PRO:HD2  | 2.01                     | 0.42              |
| 19:L:221:TYR:OH   | 19:L:348:GLU:HB3  | 2.20                     | 0.42              |
| 21:N:45:ASP:O     | 21:N:48:ALA:HB3   | 2.19                     | 0.42              |
| 22:O:138:LEU:HG   | 22:O:146:ALA:HB1  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:9:GLU:CG     | 24:Q:13:ARG:HH12  | 2.32                     | 0.42              |
| 25:R:31:PHE:CE1   | 25:R:35:GLN:HG3   | 2.54                     | 0.42              |
| 25:R:392:ARG:HG3  | 25:R:394:ASP:O    | 2.20                     | 0.42              |
| 25:R:411:LEU:HD22 | 26:S:464:ARG:NH1  | 2.21                     | 0.42              |
| 27:T:183:SER:O    | 27:T:186:ARG:HG2  | 2.19                     | 0.42              |
| 28:U:195:LYS:HB3  | 29:V:233:LYS:HD3  | 2.02                     | 0.42              |
| 28:U:278:ILE:HA   | 28:U:281:LEU:HD12 | 2.01                     | 0.42              |
| 31:X:79:LYS:HE3   | 31:X:98:PHE:CD2   | 2.51                     | 0.42              |
| 32:Y:80:GLU:CD    | 32:Y:83:ARG:NH2   | 2.54                     | 0.42              |
| 33:Z:497:PHE:CD2  | 33:Z:505:VAL:CB   | 3.02                     | 0.42              |
| 33:Z:532:HIS:CD2  | 33:Z:572:ILE:HD13 | 2.54                     | 0.42              |
| 1:1:6:VAL:HG13    | 1:1:142:PHE:CD1   | 2.54                     | 0.42              |
| 3:3:36:HIS:HB3    | 3:3:41:PHE:CD2    | 2.55                     | 0.42              |
| 5:5:57:THR:HG21   | 6:6:82:ARG:NH1    | 2.35                     | 0.42              |
| 6:6:175:VAL:HG13  | 6:6:179:PHE:HE2   | 1.84                     | 0.42              |
| 7:7:70:ASN:N      | 7:7:71:PRO:HD3    | 2.33                     | 0.42              |
| 8:A:54:ILE:CD1    | 8:A:207:ILE:HG13  | 2.49                     | 0.42              |
| 13:F:65:LYS:CA    | 13:F:222:PHE:CE2  | 3.02                     | 0.42              |
| 14:G:111:PHE:CG   | 14:G:114:ARG:NH2  | 2.85                     | 0.42              |
| 16:I:320:GLY:HA2  | 16:I:323:LYS:NZ   | 2.34                     | 0.42              |
| 17:J:377:VAL:CG1  | 17:J:378:THR:N    | 2.82                     | 0.42              |
| 17:J:378:THR:C    | 17:J:382:PHE:HD2  | 2.26                     | 0.42              |
| 18:K:156:SER:HB3  | 18:K:253:MET:SD   | 2.60                     | 0.42              |
| 19:L:163:THR:OG1  | 19:L:265:GLU:CD   | 2.63                     | 0.42              |
| 19:L:169:ASN:ND2  | 19:L:262:ILE:HD13 | 2.34                     | 0.42              |
| 21:N:405:LEU:CD1  | 21:N:446:ALA:HB2  | 2.49                     | 0.42              |
| 25:R:73:ASN:N     | 25:R:76:GLN:HE21  | 2.17                     | 0.42              |
| 27:T:157:TYR:HB3  | 27:T:189:ILE:HD11 | 2.02                     | 0.42              |
| 28:U:62:ASN:OD1   | 28:U:64:ASP:N     | 2.46                     | 0.42              |
| 28:U:173:HIS:ND1  | 29:V:150:LYS:HA   | 2.35                     | 0.42              |
| 29:V:140:VAL:HG11 | 29:V:156:PHE:HE2  | 1.83                     | 0.42              |
| 31:X:62:ASP:OD1   | 31:X:62:ASP:C     | 2.62                     | 0.42              |
| 31:X:100:TRP:CZ3  | 31:X:102:GLN:CA   | 2.92                     | 0.42              |
| 33:Z:357:ILE:HD11 | 33:Z:980:VAL:HG21 | 2.01                     | 0.42              |
| 33:Z:408:TYR:CE1  | 33:Z:411:LYS:NZ   | 2.88                     | 0.42              |
| 1:1:57:ASP:HB3    | 8:A:106:TYR:OH    | 2.19                     | 0.42              |
| 4:4:28:LYS:HE2    | 4:4:31:ASP:HB2    | 2.01                     | 0.42              |
| 4:4:181:LYS:HE2   | 4:4:190:GLN:HG2   | 2.01                     | 0.42              |
| 7:7:116:ASP:OD1   | 7:7:116:ASP:C     | 2.62                     | 0.42              |
| 8:A:63:LEU:HD21   | 14:G:176:GLU:HA   | 2.02                     | 0.42              |
| 9:B:239:THR:CG2   | 9:B:240:SER:N     | 2.83                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:D:19:GLN:OE1   | 11:D:128:PRO:HD3  | 2.20                     | 0.42              |
| 12:E:15:PHE:HZ    | 13:F:126:ARG:NH2  | 2.13                     | 0.42              |
| 15:H:379:LEU:HD13 | 15:H:413:ASN:CG   | 2.44                     | 0.42              |
| 18:K:241:GLU:CA   | 19:L:303:ARG:NH1  | 2.72                     | 0.42              |
| 19:L:93:ASN:O     | 19:L:96:LYS:HB2   | 2.20                     | 0.42              |
| 19:L:178:ILE:HD11 | 19:L:230:LEU:O    | 2.20                     | 0.42              |
| 21:N:229:VAL:HG11 | 21:N:238:ALA:HB2  | 2.02                     | 0.42              |
| 21:N:302:PHE:HD1  | 21:N:871:MET:HG3  | 1.83                     | 0.42              |
| 21:N:324:LYS:HD2  | 21:N:325:PHE:CE2  | 2.55                     | 0.42              |
| 23:P:369:LEU:CD1  | 23:P:376:THR:HG23 | 2.49                     | 0.42              |
| 25:R:171:MET:HG3  | 25:R:209:ARG:HH11 | 1.84                     | 0.42              |
| 25:R:334:ARG:HH11 | 25:R:363:PHE:HZ   | 1.60                     | 0.42              |
| 26:S:258:GLU:O    | 26:S:259:TYR:CG   | 2.73                     | 0.42              |
| 27:T:112:ASN:HA   | 27:T:177:PHE:CZ   | 2.55                     | 0.42              |
| 27:T:158:GLN:OE1  | 27:T:210:PHE:HE1  | 2.03                     | 0.42              |
| 27:T:254:ASP:HB2  | 27:T:257:THR:OG1  | 2.19                     | 0.42              |
| 28:U:8:VAL:CG1    | 28:U:10:ILE:HD11  | 2.50                     | 0.42              |
| 29:V:48:GLU:CD    | 29:V:111:HIS:HD1  | 2.28                     | 0.42              |
| 31:X:45:PHE:CZ    | 31:X:67:ILE:HD13  | 2.55                     | 0.42              |
| 33:Z:483:THR:HG22 | 33:Z:521:GLU:HG3  | 2.02                     | 0.42              |
| 1:1:175:MET:HE2   | 1:1:188:PHE:CD1   | 2.55                     | 0.42              |
| 2:2:1:THR:HG21    | 2:2:33:LYS:HE3    | 2.02                     | 0.42              |
| 2:2:7:LYS:O       | 2:2:146:LEU:CD2   | 2.63                     | 0.42              |
| 4:4:13:ILE:CG2    | 4:4:160:LEU:CD1   | 2.97                     | 0.42              |
| 4:4:65:LEU:O      | 4:4:69:ARG:HG3    | 2.19                     | 0.42              |
| 6:6:193:LEU:HD21  | 6:6:195:ILE:HD11  | 2.02                     | 0.42              |
| 7:7:145:PRO:CA    | 7:7:148:ARG:HH21  | 2.32                     | 0.42              |
| 13:F:65:LYS:CE    | 13:F:222:PHE:HD2  | 2.25                     | 0.42              |
| 13:F:211:LEU:HD12 | 13:F:234:ILE:HD11 | 2.01                     | 0.42              |
| 15:H:247:LEU:HB2  | 15:H:371:ILE:HG21 | 2.02                     | 0.42              |
| 16:I:172:LYS:HE2  | 17:J:278:GLN:HB2  | 2.01                     | 0.42              |
| 17:J:84:VAL:HG23  | 17:J:98:VAL:CG1   | 2.49                     | 0.42              |
| 18:K:140:HIS:ND1  | 18:K:143:SER:N    | 2.68                     | 0.42              |
| 18:K:187:ALA:O    | 18:K:313:LYS:NZ   | 2.53                     | 0.42              |
| 19:L:149:ASP:OD2  | 19:L:152:THR:CB   | 2.68                     | 0.42              |
| 19:L:224:PRO:O    | 20:M:342:ARG:NH1  | 2.37                     | 0.42              |
| 21:N:21:LYS:HD3   | 21:N:49:LEU:HD22  | 2.02                     | 0.42              |
| 21:N:338:PHE:HZ   | 21:N:736:PHE:HE1  | 1.67                     | 0.42              |
| 21:N:645:THR:HG22 | 21:N:656:ALA:HB1  | 2.02                     | 0.42              |
| 22:O:250:TRP:CG   | 22:O:269:LEU:HD23 | 2.53                     | 0.42              |
| 24:Q:165:PHE:HE1  | 24:Q:170:ASP:HB2  | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:118:GLN:O    | 25:R:122:GLU:HG3  | 2.20                     | 0.42              |
| 25:R:225:LYS:O    | 25:R:228:ALA:HB3  | 2.19                     | 0.42              |
| 31:X:49:GLU:HG2   | 31:X:65:SER:OG    | 2.20                     | 0.42              |
| 31:X:79:LYS:HD3   | 31:X:98:PHE:HE2   | 1.84                     | 0.42              |
| 33:Z:823:ASN:O    | 33:Z:827:LEU:HD12 | 2.20                     | 0.42              |
| 1:1:3:ILE:HD12    | 1:1:44:CYS:HB2    | 2.02                     | 0.41              |
| 3:3:60:TYR:CD2    | 10:C:96:GLN:CB    | 2.83                     | 0.41              |
| 6:6:91:LYS:HD2    | 6:6:96:TYR:OH     | 2.08                     | 0.41              |
| 8:A:54:ILE:HD12   | 8:A:206:ALA:HB3   | 2.01                     | 0.41              |
| 9:B:249:ALA:CB    | 24:Q:94:VAL:HG12  | 2.50                     | 0.41              |
| 10:C:2:GLY:HA2    | 13:F:123:TYR:CZ   | 2.55                     | 0.41              |
| 12:E:184:LEU:HA   | 13:F:56:LEU:HD11  | 2.02                     | 0.41              |
| 12:E:223:THR:HB   | 12:E:226:ASP:OD1  | 2.20                     | 0.41              |
| 19:L:282:GLU:OE2  | 20:M:306:LEU:CD1  | 2.67                     | 0.41              |
| 19:L:383:SER:HB3  | 19:L:386:PHE:HD2  | 1.85                     | 0.41              |
| 20:M:283:LEU:O    | 20:M:283:LEU:HG   | 2.19                     | 0.41              |
| 20:M:424:ALA:O    | 20:M:425:ARG:CB   | 2.64                     | 0.41              |
| 21:N:414:GLY:HA3  | 21:N:728:LYS:HE2  | 2.02                     | 0.41              |
| 21:N:739:PHE:HD1  | 21:N:743:PHE:O    | 2.02                     | 0.41              |
| 22:O:15:ARG:C     | 30:W:20:ASP:OD1   | 2.63                     | 0.41              |
| 22:O:41:LEU:HG    | 22:O:58:ARG:CG    | 2.50                     | 0.41              |
| 22:O:133:ILE:HG23 | 22:O:134:ALA:N    | 2.34                     | 0.41              |
| 22:O:166:ARG:HG3  | 22:O:167:ILE:N    | 2.35                     | 0.41              |
| 24:Q:141:LEU:CG   | 24:Q:145:HIS:CD2  | 2.99                     | 0.41              |
| 24:Q:146:TYR:HD1  | 24:Q:184:VAL:HG22 | 1.84                     | 0.41              |
| 24:Q:353:PRO:C    | 24:Q:354:PHE:HD1  | 2.26                     | 0.41              |
| 24:Q:419:LEU:CD2  | 28:U:289:ASP:OD2  | 2.68                     | 0.41              |
| 28:U:65:VAL:CG1   | 30:W:96:LEU:HD11  | 2.49                     | 0.41              |
| 29:V:51:GLY:HA2   | 29:V:71:MET:HG3   | 2.02                     | 0.41              |
| 29:V:186:GLN:HG2  | 29:V:190:HIS:HD2  | 1.85                     | 0.41              |
| 33:Z:591:ILE:HG22 | 33:Z:593:HIS:HD2  | 1.85                     | 0.41              |
| 33:Z:827:LEU:HD13 | 33:Z:855:LEU:HD22 | 2.02                     | 0.41              |
| 3:3:63:ASN:HB3    | 10:C:96:GLN:NE2   | 2.35                     | 0.41              |
| 3:3:100:VAL:CG2   | 3:3:115:PHE:HE1   | 2.33                     | 0.41              |
| 5:5:54:PHE:HB2    | 6:6:85:GLN:HE22   | 1.85                     | 0.41              |
| 13:F:11:VAL:HG22  | 13:F:120:THR:O    | 2.20                     | 0.41              |
| 13:F:72:LEU:HD23  | 13:F:88:LEU:HD23  | 2.01                     | 0.41              |
| 15:H:147:ILE:HG13 | 15:H:183:ILE:CD1  | 2.50                     | 0.41              |
| 15:H:168:ILE:HD12 | 15:H:187:LEU:CD1  | 2.42                     | 0.41              |
| 15:H:379:LEU:HD23 | 15:H:415:THR:HG22 | 1.95                     | 0.41              |
| 16:I:245:LEU:HG   | 16:I:247:ILE:CD1  | 2.43                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:L:163:THR:HG21 | 19:L:264:ARG:NH2  | 2.34                     | 0.41              |
| 19:L:361:PHE:CE2  | 19:L:391:ILE:HD12 | 2.51                     | 0.41              |
| 20:M:148:VAL:HG22 | 20:M:155:ILE:CG1  | 2.34                     | 0.41              |
| 21:N:293:LEU:HD22 | 21:N:379:LEU:CD1  | 2.27                     | 0.41              |
| 21:N:315:ASN:CG   | 21:N:318:LYS:NZ   | 2.74                     | 0.41              |
| 22:O:321:LYS:O    | 22:O:325:GLU:HG3  | 2.20                     | 0.41              |
| 23:P:131:PHE:CB   | 23:P:136:ARG:NH1  | 2.80                     | 0.41              |
| 24:Q:38:SER:OG    | 24:Q:39:SER:N     | 2.45                     | 0.41              |
| 24:Q:120:LYS:O    | 24:Q:123:GLU:HB2  | 2.20                     | 0.41              |
| 25:R:73:ASN:N     | 25:R:76:GLN:NE2   | 2.68                     | 0.41              |
| 25:R:131:ALA:O    | 25:R:135:ILE:HG13 | 2.20                     | 0.41              |
| 25:R:237:THR:O    | 25:R:246:TYR:CE1  | 2.72                     | 0.41              |
| 25:R:298:ALA:O    | 25:R:299:SER:HB3  | 2.20                     | 0.41              |
| 25:R:367:ASP:OD1  | 25:R:370:LYS:HD2  | 2.19                     | 0.41              |
| 27:T:92:ASN:O     | 27:T:130:ASP:OD1  | 2.38                     | 0.41              |
| 28:U:189:ARG:CZ   | 29:V:296:LEU:HD22 | 2.50                     | 0.41              |
| 29:V:202:ASP:OD1  | 29:V:203:TYR:N    | 2.53                     | 0.41              |
| 30:W:2:VAL:HG23   | 30:W:4:GLU:HG3    | 2.02                     | 0.41              |
| 30:W:37:PHE:CE2   | 30:W:69:PHE:HB3   | 2.55                     | 0.41              |
| 30:W:129:ALA:O    | 30:W:161:VAL:HG23 | 2.20                     | 0.41              |
| 31:X:91:PHE:O     | 31:X:96:ARG:NE    | 2.42                     | 0.41              |
| 33:Z:303:ASP:N    | 33:Z:307:HIS:NE2  | 2.67                     | 0.41              |
| 33:Z:392:LEU:HD11 | 33:Z:427:GLN:OE1  | 2.20                     | 0.41              |
| 33:Z:497:PHE:HB2  | 33:Z:533:VAL:CG2  | 2.46                     | 0.41              |
| 5:5:159:ARG:NH1   | 5:5:200:VAL:HG13  | 2.35                     | 0.41              |
| 7:7:137:GLY:O     | 7:7:140:ALA:HB3   | 2.19                     | 0.41              |
| 10:C:4:ARG:NH1    | 12:E:125:GLU:HG3  | 2.36                     | 0.41              |
| 10:C:86:ILE:O     | 10:C:90:THR:HG23  | 2.20                     | 0.41              |
| 13:F:37:GLY:HA2   | 13:F:46:LEU:HD23  | 2.02                     | 0.41              |
| 13:F:101:ARG:HH11 | 13:F:104:ALA:H    | 1.68                     | 0.41              |
| 13:F:194:VAL:O    | 13:F:197:ILE:HG22 | 2.20                     | 0.41              |
| 14:G:61:GLN:HG2   | 14:G:214:GLU:OE1  | 2.20                     | 0.41              |
| 14:G:168:ARG:HH21 | 14:G:172:LYS:HZ1  | 1.68                     | 0.41              |
| 15:H:206:VAL:CG2  | 15:H:261:ARG:NE   | 2.64                     | 0.41              |
| 15:H:278:GLU:CD   | 16:I:262:ARG:HD2  | 2.46                     | 0.41              |
| 17:J:166:LEU:O    | 17:J:174:PHE:CE1  | 2.74                     | 0.41              |
| 17:J:280:ASP:CG   | 17:J:286:LYS:HZ3  | 2.28                     | 0.41              |
| 19:L:282:GLU:CD   | 20:M:306:LEU:HD13 | 2.45                     | 0.41              |
| 20:M:152:SER:O    | 20:M:154:LEU:HG   | 2.20                     | 0.41              |
| 20:M:200:PRO:HB2  | 20:M:319:ASP:OD2  | 2.20                     | 0.41              |
| 22:O:15:ARG:NH1   | 22:O:72:LYS:HG2   | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:O:23:HIS:CG    | 22:O:24:PRO:HD2   | 2.55                     | 0.41              |
| 23:P:425:HIS:CG   | 28:U:228:LYS:HZ1  | 2.38                     | 0.41              |
| 24:Q:343:LEU:O    | 24:Q:347:LEU:HG   | 2.20                     | 0.41              |
| 25:R:37:LYS:HG3   | 25:R:38:VAL:HG23  | 2.01                     | 0.41              |
| 25:R:158:LEU:HD21 | 25:R:197:MET:CE   | 2.48                     | 0.41              |
| 31:X:48:PHE:HE1   | 31:X:128:VAL:HG11 | 1.85                     | 0.41              |
| 3:3:-2:ASN:ND2    | 3:3:48:ALA:HB2    | 2.36                     | 0.41              |
| 3:3:65:TYR:CD2    | 3:3:73:ILE:HG22   | 2.54                     | 0.41              |
| 6:6:43:MET:HG3    | 6:6:102:ILE:CG2   | 2.41                     | 0.41              |
| 8:A:137:LEU:HD21  | 14:G:124:LEU:HD11 | 2.03                     | 0.41              |
| 10:C:208:TYR:HB3  | 10:C:239:LEU:HD12 | 2.00                     | 0.41              |
| 10:C:244:ILE:O    | 10:C:244:ILE:HG22 | 2.21                     | 0.41              |
| 11:D:127:ARG:HD2  | 11:D:127:ARG:O    | 2.19                     | 0.41              |
| 13:F:14:SER:HB2   | 13:F:15:PRO:HD2   | 2.02                     | 0.41              |
| 13:F:101:ARG:NH2  | 13:F:103:LEU:CD1  | 2.82                     | 0.41              |
| 15:H:331:ARG:HD2  | 20:M:252:VAL:HG11 | 2.01                     | 0.41              |
| 17:J:177:LEU:CD2  | 17:J:179:ILE:HB   | 2.51                     | 0.41              |
| 18:K:234:PHE:CE2  | 18:K:236:ARG:HB2  | 2.56                     | 0.41              |
| 19:L:284:ASP:HB2  | 20:M:295:LYS:HE3  | 2.03                     | 0.41              |
| 20:M:196:ALA:CA   | 20:M:345:ARG:HH21 | 2.32                     | 0.41              |
| 21:N:406:TYR:CE1  | 21:N:448:LEU:HD13 | 2.56                     | 0.41              |
| 22:O:383:LYS:NZ   | 27:T:252:GLU:HG3  | 2.34                     | 0.41              |
| 24:Q:104:PHE:CD2  | 24:Q:114:GLN:CD   | 2.98                     | 0.41              |
| 25:R:266:LEU:C    | 25:R:270:VAL:HG22 | 2.44                     | 0.41              |
| 26:S:323:LEU:HD21 | 26:S:383:LEU:HD23 | 2.02                     | 0.41              |
| 27:T:57:ILE:CG2   | 27:T:58:THR:N     | 2.83                     | 0.41              |
| 28:U:67:PHE:CE1   | 30:W:97:THR:CG2   | 3.04                     | 0.41              |
| 33:Z:103:TYR:CE2  | 33:Z:137:TYR:HE1  | 2.38                     | 0.41              |
| 33:Z:153:TYR:CZ   | 33:Z:157:LEU:HD22 | 2.55                     | 0.41              |
| 33:Z:483:THR:CB   | 33:Z:521:GLU:HG3  | 2.51                     | 0.41              |
| 33:Z:562:TRP:CE2  | 33:Z:566:LEU:CD2  | 2.91                     | 0.41              |
| 2:2:43:CYS:SG     | 2:2:100:VAL:HG22  | 2.61                     | 0.41              |
| 4:4:55:PHE:O      | 4:4:59:ILE:HG12   | 2.21                     | 0.41              |
| 6:6:14:LEU:CD2    | 6:6:42:VAL:HG23   | 2.50                     | 0.41              |
| 7:7:5:SER:OG      | 7:7:119:LEU:HD11  | 2.20                     | 0.41              |
| 10:C:177:GLN:HE22 | 11:D:52:LEU:HB3   | 1.84                     | 0.41              |
| 10:C:222:ASP:C    | 10:C:222:ASP:OD1  | 2.64                     | 0.41              |
| 11:D:16:HIS:HB2   | 11:D:21:GLU:OE2   | 2.20                     | 0.41              |
| 12:E:35:SER:HG    | 12:E:53:ARG:HE    | 1.63                     | 0.41              |
| 15:H:61:ALA:O     | 15:H:65:GLU:HG3   | 2.21                     | 0.41              |
| 15:H:62:ARG:CD    | 16:I:96:LEU:HD21  | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:172:LYS:NZ   | 17:J:234:PHE:CE2  | 2.89                     | 0.41              |
| 17:J:91:GLU:HB3   | 17:J:94:TYR:OH    | 2.20                     | 0.41              |
| 21:N:386:MET:C    | 21:N:390:LEU:HG   | 2.43                     | 0.41              |
| 21:N:903:VAL:C    | 21:N:904:VAL:HG23 | 2.46                     | 0.41              |
| 23:P:72:TRP:CE3   | 23:P:104:LEU:CD2  | 3.03                     | 0.41              |
| 23:P:130:ILE:O    | 23:P:130:ILE:CG2  | 2.65                     | 0.41              |
| 24:Q:88:PHE:CE2   | 24:Q:89:ALA:CB    | 3.04                     | 0.41              |
| 24:Q:348:CYS:SG   | 24:Q:380:MET:HG3  | 2.60                     | 0.41              |
| 25:R:243:LEU:O    | 25:R:244:THR:HB   | 2.20                     | 0.41              |
| 27:T:28:PRO:O     | 27:T:31:LYS:HB2   | 2.20                     | 0.41              |
| 28:U:288:PHE:CE2  | 28:U:292:ILE:HD11 | 2.56                     | 0.41              |
| 30:W:21:PHE:HZ    | 30:W:25:ARG:HH12  | 1.58                     | 0.41              |
| 31:X:31:GLY:HA2   | 31:X:53:THR:HG23  | 2.02                     | 0.41              |
| 33:Z:452:LEU:HD22 | 33:Z:477:TYR:CD2  | 2.56                     | 0.41              |
| 33:Z:971:ILE:HG22 | 33:Z:972:SER:O    | 2.20                     | 0.41              |
| 4:4:117:GLN:NE2   | 4:4:130:GLY:HA3   | 2.34                     | 0.41              |
| 6:6:19:ARG:HE     | 6:6:190:GLY:HA3   | 1.85                     | 0.41              |
| 6:6:56:VAL:O      | 6:6:60:LYS:HG3    | 2.20                     | 0.41              |
| 11:D:48:ARG:HH12  | 11:D:57:THR:CB    | 2.30                     | 0.41              |
| 11:D:174:PHE:CZ   | 11:D:197:ARG:HB3  | 2.56                     | 0.41              |
| 13:F:159:THR:C    | 13:F:169:LYS:HD3  | 2.45                     | 0.41              |
| 15:H:284:VAL:C    | 15:H:286:GLU:H    | 2.28                     | 0.41              |
| 16:I:104:LEU:HD21 | 16:I:149:LEU:N    | 2.36                     | 0.41              |
| 16:I:128:TYR:CD2  | 16:I:154:MET:CG   | 3.01                     | 0.41              |
| 16:I:371:LEU:HA   | 16:I:411:VAL:H    | 1.86                     | 0.41              |
| 17:J:349:LYS:HZ3  | 17:J:383:GLU:HB2  | 1.86                     | 0.41              |
| 18:K:425:ASP:OD1  | 18:K:428:LYS:NZ   | 2.52                     | 0.41              |
| 20:M:278:ILE:HB   | 20:M:323:VAL:HG22 | 2.02                     | 0.41              |
| 21:N:205:SER:O    | 21:N:209:LYS:HG3  | 2.20                     | 0.41              |
| 21:N:340:HIS:HB3  | 21:N:374:ILE:HG12 | 2.03                     | 0.41              |
| 21:N:692:GLU:O    | 21:N:696:LYS:HG3  | 2.20                     | 0.41              |
| 21:N:892:PRO:CA   | 21:N:905:LEU:HG   | 2.51                     | 0.41              |
| 22:O:225:ASP:HA   | 22:O:287:LEU:HD21 | 2.02                     | 0.41              |
| 22:O:266:PHE:CE1  | 22:O:284:GLU:OE1  | 2.73                     | 0.41              |
| 22:O:310:PHE:CD2  | 22:O:346:GLU:HA   | 2.56                     | 0.41              |
| 23:P:119:ILE:HD13 | 23:P:143:LEU:HB2  | 2.02                     | 0.41              |
| 24:Q:88:PHE:CD2   | 24:Q:89:ALA:CB    | 3.04                     | 0.41              |
| 25:R:140:TYR:CD2  | 25:R:141:TYR:CE1  | 3.08                     | 0.41              |
| 26:S:437:ASN:CG   | 27:T:199:PHE:CZ   | 2.99                     | 0.41              |
| 28:U:277:TYR:OH   | 29:V:295:VAL:HG12 | 2.19                     | 0.41              |
| 33:Z:436:LEU:CD2  | 33:Z:455:ILE:HG13 | 2.49                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:17:ASP:OD1    | 2:2:17:ASP:C      | 2.64                     | 0.41              |
| 5:5:162:LEU:HD23  | 5:5:200:VAL:HG11  | 2.03                     | 0.41              |
| 9:B:58:SER:HA     | 9:B:61:LEU:HD12   | 2.03                     | 0.41              |
| 10:C:50:ARG:HH21  | 10:C:209:ASP:HA   | 1.86                     | 0.41              |
| 11:D:27:VAL:HG21  | 11:D:132:SER:OG   | 2.20                     | 0.41              |
| 11:D:151:GLU:HB2  | 11:D:152:PRO:HD2  | 2.02                     | 0.41              |
| 11:D:214:VAL:HB   | 11:D:222:VAL:HG13 | 2.03                     | 0.41              |
| 15:H:308:PHE:CD1  | 15:H:351:VAL:CG1  | 3.03                     | 0.41              |
| 17:J:213:VAL:HG11 | 17:J:233:LEU:CD2  | 2.51                     | 0.41              |
| 21:N:87:ASP:OD1   | 21:N:88:ARG:HG2   | 2.20                     | 0.41              |
| 21:N:379:LEU:O    | 21:N:380:LEU:HD23 | 2.21                     | 0.41              |
| 22:O:116:ASN:HB3  | 22:O:127:LEU:CG   | 2.50                     | 0.41              |
| 25:R:224:PHE:CE2  | 25:R:328:PHE:CZ   | 3.08                     | 0.41              |
| 25:R:264:THR:HA   | 25:R:267:LYS:HE2  | 2.02                     | 0.41              |
| 25:R:304:TYR:HD2  | 25:R:305:PHE:HD1  | 1.69                     | 0.41              |
| 26:S:164:ILE:HB   | 26:S:165:PRO:CD   | 2.51                     | 0.41              |
| 28:U:172:GLU:O    | 28:U:176:ARG:HG3  | 2.20                     | 0.41              |
| 29:V:186:GLN:C    | 29:V:190:HIS:HD2  | 2.29                     | 0.41              |
| 30:W:162:ASN:OD1  | 30:W:162:ASN:C    | 2.63                     | 0.41              |
| 33:Z:763:HIS:CD2  | 33:Z:766:HIS:CE1  | 3.07                     | 0.41              |
| 33:Z:888:LEU:CB   | 33:Z:901:PHE:HE1  | 2.19                     | 0.41              |
| 2:2:3:ILE:HG13    | 2:2:99:ILE:CD1    | 2.50                     | 0.41              |
| 7:7:112:GLN:HG2   | 7:7:114:ASN:H     | 1.86                     | 0.41              |
| 8:A:64:LEU:CD1    | 14:G:157:TRP:HD1  | 2.33                     | 0.41              |
| 8:A:91:ARG:HG2    | 14:G:156:TYR:OH   | 2.21                     | 0.41              |
| 8:A:91:ARG:NH2    | 14:G:113:ASP:OD2  | 2.45                     | 0.41              |
| 9:B:211:LEU:CD2   | 9:B:238:LEU:HD12  | 2.47                     | 0.41              |
| 12:E:86:ARG:HH12  | 12:E:90:GLU:CB    | 2.21                     | 0.41              |
| 15:H:161:GLU:HA   | 15:H:184:GLU:OE1  | 2.21                     | 0.41              |
| 15:H:218:ILE:O    | 15:H:222:ARG:HG3  | 2.21                     | 0.41              |
| 16:I:214:LYS:NZ   | 16:I:318:ASP:O    | 2.37                     | 0.41              |
| 17:J:28:GLN:HG3   | 26:S:225:HIS:CE1  | 2.56                     | 0.41              |
| 17:J:183:LYS:HD2  | 17:J:308:GLY:O    | 2.21                     | 0.41              |
| 19:L:163:THR:OG1  | 19:L:265:GLU:CG   | 2.69                     | 0.41              |
| 19:L:283:VAL:HA   | 19:L:286:ILE:HG12 | 2.02                     | 0.41              |
| 20:M:220:MET:HE2  | 20:M:324:LEU:HB3  | 2.02                     | 0.41              |
| 21:N:270:LEU:O    | 21:N:274:VAL:HG23 | 2.20                     | 0.41              |
| 21:N:535:LEU:O    | 21:N:539:MET:HG3  | 2.21                     | 0.41              |
| 21:N:771:PHE:HD2  | 21:N:772:GLN:O    | 2.04                     | 0.41              |
| 22:O:102:LEU:O    | 22:O:103:LYS:CG   | 2.68                     | 0.41              |
| 22:O:211:GLN:HE22 | 22:O:248:TYR:HE2  | 1.69                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:15:PHE:HZ    | 27:T:67:LEU:HB3   | 1.77                     | 0.41              |
| 28:U:32:ARG:NE    | 28:U:94:HIS:HE1   | 2.14                     | 0.41              |
| 28:U:66:TRP:CE3   | 28:U:66:TRP:C     | 2.99                     | 0.41              |
| 28:U:77:ASN:HD21  | 28:U:81:LYS:HE3   | 1.85                     | 0.41              |
| 29:V:258:GLU:CD   | 29:V:287:THR:HG21 | 2.46                     | 0.41              |
| 32:Y:83:ARG:HB2   | 32:Y:86:ARG:NH2   | 2.35                     | 0.41              |
| 33:Z:415:MET:HB3  | 33:Z:446:GLU:CB   | 2.47                     | 0.41              |
| 33:Z:857:LEU:HD21 | 33:Z:908:ILE:CD1  | 2.47                     | 0.41              |
| 1:1:-8:LYS:HD3    | 2:2:116:HIS:O     | 2.20                     | 0.41              |
| 1:1:87:TYR:HA     | 1:1:116:GLY:O     | 2.21                     | 0.41              |
| 2:2:38:SER:HB2    | 2:2:39:PRO:HD2    | 2.02                     | 0.41              |
| 4:4:13:ILE:HG21   | 4:4:160:LEU:CD1   | 2.50                     | 0.41              |
| 4:4:65:LEU:HD11   | 4:4:69:ARG:NE     | 2.36                     | 0.41              |
| 6:6:21:ILE:C      | 6:6:27:ASN:ND2    | 2.79                     | 0.41              |
| 7:7:153:ARG:HG3   | 7:7:155:SER:OG    | 2.20                     | 0.41              |
| 7:7:180:ASP:OD1   | 7:7:182:ARG:N     | 2.41                     | 0.41              |
| 8:A:54:ILE:HD12   | 8:A:206:ALA:HB1   | 2.03                     | 0.41              |
| 8:A:174:LYS:HG3   | 8:A:214:LEU:HD23  | 2.03                     | 0.41              |
| 10:C:13:PHE:HZ    | 11:D:127:ARG:HH12 | 1.58                     | 0.41              |
| 11:D:106:VAL:HB   | 11:D:146:LYS:HZ3  | 1.86                     | 0.41              |
| 12:E:15:PHE:CZ    | 13:F:126:ARG:CZ   | 3.04                     | 0.41              |
| 12:E:125:GLU:H    | 13:F:124:GLY:HA3  | 1.85                     | 0.41              |
| 13:F:105:VAL:HG22 | 13:F:145:LEU:CB   | 2.45                     | 0.41              |
| 15:H:168:ILE:CD1  | 15:H:187:LEU:HD12 | 2.41                     | 0.41              |
| 15:H:285:GLY:C    | 15:H:287:GLY:H    | 2.20                     | 0.41              |
| 16:I:136:VAL:HG11 | 16:I:159:VAL:CG1  | 2.50                     | 0.41              |
| 16:I:233:ALA:O    | 16:I:236:VAL:HG12 | 2.20                     | 0.41              |
| 16:I:336:PRO:HA   | 16:I:339:ILE:HD12 | 2.02                     | 0.41              |
| 17:J:305:LEU:HB3  | 17:J:313:LYS:HZ1  | 1.86                     | 0.41              |
| 18:K:71:GLU:O     | 18:K:75:LEU:HG    | 2.20                     | 0.41              |
| 19:L:159:LEU:HD12 | 19:L:159:LEU:C    | 2.46                     | 0.41              |
| 19:L:383:SER:HB3  | 19:L:386:PHE:CD2  | 2.55                     | 0.41              |
| 20:M:281:ASP:O    | 20:M:282:GLU:HB2  | 2.20                     | 0.41              |
| 20:M:290:ARG:NH1  | 20:M:294:GLU:HB3  | 2.35                     | 0.41              |
| 20:M:376:TRP:CD2  | 20:M:377:GLN:N    | 2.89                     | 0.41              |
| 21:N:43:LEU:HD11  | 21:N:69:TYR:CZ    | 2.56                     | 0.41              |
| 21:N:346:ASN:O    | 21:N:350:LYS:HG3  | 2.20                     | 0.41              |
| 21:N:572:LEU:O    | 21:N:576:VAL:HG23 | 2.21                     | 0.41              |
| 21:N:664:LEU:HD21 | 21:N:672:ASN:ND2  | 2.36                     | 0.41              |
| 21:N:697:PHE:CZ   | 21:N:701:VAL:HG21 | 2.56                     | 0.41              |
| 22:O:189:TYR:CE1  | 22:O:193:LEU:HD11 | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:O:304:ASN:HD22 | 28:U:261:LEU:HA   | 1.86                     | 0.41              |
| 22:O:374:ASN:OD1  | 28:U:200:LEU:HB3  | 2.21                     | 0.41              |
| 23:P:233:GLU:CD   | 23:P:236:GLU:HB2  | 2.46                     | 0.41              |
| 23:P:392:LYS:HE2  | 24:Q:354:PHE:CE2  | 2.56                     | 0.41              |
| 23:P:431:HIS:HE1  | 28:U:137:TYR:HE1  | 1.67                     | 0.41              |
| 25:R:316:LEU:HD11 | 25:R:329:PHE:CZ   | 2.52                     | 0.41              |
| 26:S:343:LEU:HB3  | 26:S:344:PRO:CD   | 2.49                     | 0.41              |
| 28:U:48:VAL:HG22  | 28:U:90:ILE:HD11  | 2.02                     | 0.41              |
| 29:V:156:PHE:CD1  | 29:V:198:SER:HA   | 2.55                     | 0.41              |
| 30:W:8:LEU:HD21   | 30:W:33:VAL:HG22  | 2.03                     | 0.41              |
| 30:W:20:ASP:CB    | 30:W:25:ARG:CZ    | 2.92                     | 0.41              |
| 31:X:75:TRP:HE1   | 31:X:122:TYR:HA   | 1.86                     | 0.41              |
| 33:Z:71:LEU:CD2   | 33:Z:118:VAL:HG11 | 2.48                     | 0.41              |
| 33:Z:187:SER:CA   | 33:Z:201:LEU:HD12 | 2.51                     | 0.41              |
| 33:Z:246:CYS:SG   | 33:Z:271:ILE:HG22 | 2.50                     | 0.41              |
| 33:Z:295:ARG:HE   | 33:Z:325:GLY:C    | 2.28                     | 0.41              |
| 33:Z:383:SER:CA   | 33:Z:849:ARG:NH1  | 2.84                     | 0.41              |
| 33:Z:449:ALA:HB1  | 33:Z:485:ILE:HG23 | 2.03                     | 0.41              |
| 33:Z:761:PHE:HD2  | 33:Z:780:MET:HE1  | 1.83                     | 0.41              |
| 7:7:157:ILE:HB    | 7:7:158:PRO:HD3   | 2.03                     | 0.41              |
| 9:B:184:GLU:CG    | 9:B:185:LEU:N     | 2.84                     | 0.41              |
| 12:E:229:LYS:O    | 12:E:231:TYR:CD1  | 2.74                     | 0.41              |
| 15:H:147:ILE:CD1  | 15:H:181:TYR:HB3  | 2.43                     | 0.41              |
| 15:H:249:TYR:CD1  | 15:H:249:TYR:C    | 2.99                     | 0.41              |
| 15:H:400:ARG:HH22 | 33:Z:366:LYS:HD2  | 1.85                     | 0.41              |
| 16:I:135:PHE:C    | 16:I:136:VAL:HG13 | 2.47                     | 0.41              |
| 18:K:220:THR:CG2  | 18:K:224:LYS:HE3  | 2.51                     | 0.41              |
| 20:M:195:GLU:CA   | 20:M:199:LEU:HD12 | 2.39                     | 0.41              |
| 21:N:9:LEU:HD22   | 21:N:27:SER:HB2   | 2.03                     | 0.41              |
| 21:N:23:TYR:HE2   | 27:T:41:ILE:HG23  | 1.86                     | 0.41              |
| 21:N:482:ALA:HB1  | 21:N:517:LEU:CD2  | 2.50                     | 0.41              |
| 21:N:508:THR:CG2  | 21:N:510:HIS:H    | 2.32                     | 0.41              |
| 22:O:71:ASP:O     | 30:W:18:ASN:CB    | 2.64                     | 0.41              |
| 22:O:223:LEU:HD22 | 22:O:279:ILE:HB   | 2.02                     | 0.41              |
| 23:P:239:GLN:HG2  | 23:P:276:LEU:HD11 | 2.03                     | 0.41              |
| 24:Q:215:VAL:O    | 24:Q:218:LEU:HB2  | 2.21                     | 0.41              |
| 24:Q:331:THR:CG2  | 24:Q:335:PHE:CZ   | 3.04                     | 0.41              |
| 25:R:77:SER:C     | 25:R:92:ILE:HG22  | 2.46                     | 0.41              |
| 25:R:158:LEU:O    | 25:R:161:ALA:HB2  | 2.21                     | 0.41              |
| 25:R:237:THR:CG2  | 25:R:275:GLU:OE1  | 2.68                     | 0.41              |
| 26:S:201:ILE:HD13 | 26:S:205:ASN:ND2  | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:S:461:PHE:CE1  | 28:U:278:ILE:HA   | 2.55                     | 0.41              |
| 26:S:461:PHE:CG   | 28:U:277:TYR:HB3  | 2.56                     | 0.41              |
| 27:T:229:VAL:CG1  | 27:T:230:ASN:H    | 2.34                     | 0.41              |
| 28:U:65:VAL:HG21  | 30:W:92:GLN:OE1   | 2.21                     | 0.41              |
| 30:W:59:PRO:HG2   | 30:W:89:THR:CG2   | 2.51                     | 0.41              |
| 33:Z:308:LYS:NZ   | 33:Z:919:GLU:OE1  | 2.54                     | 0.41              |
| 33:Z:493:LEU:HD21 | 33:Z:497:PHE:HE2  | 1.85                     | 0.41              |
| 5:5:128:CYS:SG    | 5:5:140:LEU:CD1   | 3.09                     | 0.40              |
| 9:B:94:HIS:CD2    | 9:B:98:LYS:NZ     | 2.89                     | 0.40              |
| 9:B:190:HIS:CE1   | 24:Q:94:VAL:HG21  | 2.54                     | 0.40              |
| 11:D:138:PHE:CE1  | 11:D:215:VAL:HG12 | 2.55                     | 0.40              |
| 13:F:43:HIS:CE1   | 13:F:218:LYS:CB   | 3.04                     | 0.40              |
| 13:F:138:ASP:C    | 13:F:138:ASP:OD1  | 2.63                     | 0.40              |
| 17:J:64:LEU:HD21  | 18:K:121:ARG:NE   | 2.36                     | 0.40              |
| 17:J:219:VAL:HB   | 18:K:281:ARG:HB3  | 2.02                     | 0.40              |
| 17:J:277:ASN:ND2  | 17:J:309:ARG:NH2  | 2.67                     | 0.40              |
| 21:N:130:ASP:OD2  | 21:N:133:LEU:HG   | 2.21                     | 0.40              |
| 21:N:207:LEU:HD13 | 21:N:232:LEU:HD23 | 2.02                     | 0.40              |
| 21:N:300:ASN:O    | 21:N:304:LEU:HG   | 2.20                     | 0.40              |
| 22:O:228:TYR:HA   | 22:O:290:LYS:CE   | 2.48                     | 0.40              |
| 23:P:178:GLN:HA   | 23:P:181:LEU:HD12 | 2.01                     | 0.40              |
| 24:Q:36:SER:H     | 24:Q:46:VAL:HG23  | 1.86                     | 0.40              |
| 24:Q:51:ARG:HG2   | 24:Q:85:MET:SD    | 2.61                     | 0.40              |
| 24:Q:198:LEU:CD2  | 24:Q:225:LEU:HD12 | 2.52                     | 0.40              |
| 25:R:63:TYR:HE2   | 25:R:94:PHE:CA    | 2.10                     | 0.40              |
| 25:R:309:LEU:HD13 | 32:Y:79:ALA:HB2   | 2.03                     | 0.40              |
| 26:S:159:ASN:HB3  | 26:S:183:LEU:HD11 | 2.03                     | 0.40              |
| 26:S:295:ALA:HA   | 26:S:298:ARG:HH21 | 1.85                     | 0.40              |
| 28:U:270:ASN:O    | 28:U:274:MET:HG3  | 2.20                     | 0.40              |
| 33:Z:327:GLN:HE22 | 33:Z:346:LEU:HD11 | 1.84                     | 0.40              |
| 8:A:135:ARG:HH11  | 14:G:124:LEU:CD2  | 2.34                     | 0.40              |
| 8:A:170:ALA:HB2   | 8:A:178:ILE:HG21  | 2.01                     | 0.40              |
| 9:B:146:SER:HB2   | 9:B:148:TYR:CE2   | 2.56                     | 0.40              |
| 11:D:70:HIS:CE1   | 11:D:97:ARG:NH2   | 2.87                     | 0.40              |
| 13:F:7:ASP:HB3    | 13:F:21:GLN:HE22  | 1.86                     | 0.40              |
| 14:G:136:ILE:HG12 | 14:G:149:MET:SD   | 2.62                     | 0.40              |
| 15:H:200:VAL:HG13 | 15:H:270:THR:HG23 | 2.03                     | 0.40              |
| 15:H:327:ASN:O    | 15:H:331:ARG:HG3  | 2.21                     | 0.40              |
| 17:J:249:GLU:O    | 17:J:249:GLU:CG   | 2.62                     | 0.40              |
| 18:K:89:ILE:HD13  | 29:V:148:LYS:HB3  | 2.03                     | 0.40              |
| 18:K:210:LEU:CB   | 18:K:334:LEU:HD11 | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:M:197:ILE:HB   | 20:M:322:LYS:HE2  | 1.98                     | 0.40              |
| 21:N:761:ILE:HD13 | 21:N:768:ILE:HG12 | 2.04                     | 0.40              |
| 22:O:99:LEU:HD11  | 22:O:132:GLU:CG   | 2.46                     | 0.40              |
| 22:O:217:LEU:HD13 | 22:O:238:ILE:HG21 | 2.03                     | 0.40              |
| 23:P:98:GLN:OE1   | 23:P:139:VAL:HG23 | 2.22                     | 0.40              |
| 23:P:141:LYS:HE3  | 23:P:182:GLU:OE2  | 2.22                     | 0.40              |
| 23:P:353:ILE:HG22 | 23:P:402:PHE:CZ   | 2.57                     | 0.40              |
| 24:Q:51:ARG:CZ    | 24:Q:55:GLU:OE2   | 2.69                     | 0.40              |
| 26:S:475:TYR:HE1  | 28:U:291:LEU:O    | 1.98                     | 0.40              |
| 27:T:26:LEU:O     | 27:T:30:ILE:HG13  | 2.21                     | 0.40              |
| 27:T:158:GLN:OE1  | 27:T:210:PHE:CE1  | 2.74                     | 0.40              |
| 28:U:69:ASP:OD1   | 28:U:69:ASP:C     | 2.64                     | 0.40              |
| 30:W:168:THR:O    | 30:W:169:SER:OG   | 2.34                     | 0.40              |
| 33:Z:57:LYS:HG2   | 33:Z:98:ASP:OD2   | 2.21                     | 0.40              |
| 33:Z:501:LYS:HD3  | 33:Z:537:THR:HG21 | 2.02                     | 0.40              |
| 2:2:86:HIS:O      | 2:2:90:TYR:HD2    | 2.04                     | 0.40              |
| 7:7:187:PHE:CD2   | 7:7:204:LEU:HB2   | 2.56                     | 0.40              |
| 12:E:165:TYR:CG   | 12:E:167:TYR:OH   | 2.73                     | 0.40              |
| 14:G:118:TYR:CE2  | 14:G:131:PHE:HZ   | 2.39                     | 0.40              |
| 16:I:200:LEU:C    | 33:Z:931:GLN:HG2  | 2.47                     | 0.40              |
| 17:J:208:CYS:SG   | 17:J:244:ILE:HG12 | 2.60                     | 0.40              |
| 17:J:346:VAL:HG12 | 17:J:350:MET:HE2  | 2.04                     | 0.40              |
| 21:N:240:GLN:O    | 21:N:244:LYS:HG2  | 2.21                     | 0.40              |
| 21:N:529:GLN:HB3  | 21:N:530:GLU:OE1  | 2.21                     | 0.40              |
| 22:O:269:LEU:C    | 22:O:269:LEU:CD2  | 2.93                     | 0.40              |
| 24:Q:302:VAL:HG13 | 24:Q:314:PHE:CD1  | 2.55                     | 0.40              |
| 25:R:271:ILE:HB   | 25:R:293:THR:HG21 | 2.03                     | 0.40              |
| 25:R:381:ILE:O    | 25:R:381:ILE:HG13 | 2.21                     | 0.40              |
| 26:S:234:ILE:HG22 | 26:S:238:LEU:CD1  | 2.50                     | 0.40              |
| 26:S:323:LEU:HD23 | 26:S:383:LEU:HD23 | 2.03                     | 0.40              |
| 31:X:9:LYS:HE2    | 31:X:34:GLU:OE2   | 2.22                     | 0.40              |
| 33:Z:278:LEU:HD22 | 33:Z:297:VAL:CG2  | 2.51                     | 0.40              |
| 1:1:12:VAL:HG22   | 1:1:14:LEU:CD1    | 2.50                     | 0.40              |
| 3:3:158:ILE:CG2   | 3:3:159:SER:N     | 2.85                     | 0.40              |
| 4:4:15:ALA:HB1    | 4:4:178:VAL:HG21  | 2.03                     | 0.40              |
| 4:4:168:GLU:OE2   | 4:4:177:GLY:N     | 2.54                     | 0.40              |
| 6:6:138:MET:HB3   | 6:6:139:PRO:HD3   | 2.03                     | 0.40              |
| 8:A:54:ILE:HD13   | 8:A:207:ILE:CG1   | 2.52                     | 0.40              |
| 8:A:54:ILE:CD1    | 8:A:206:ALA:HB3   | 2.51                     | 0.40              |
| 13:F:120:THR:OG1  | 14:G:129:ARG:NH1  | 2.44                     | 0.40              |
| 14:G:243:GLN:O    | 14:G:243:GLN:HG3  | 2.20                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:H:147:ILE:CG1  | 15:H:183:ILE:HD11 | 2.51                     | 0.40              |
| 15:H:182:ASN:ND2  | 15:H:184:GLU:OE2  | 2.49                     | 0.40              |
| 15:H:455:LYS:O    | 15:H:456:LYS:HB2  | 2.22                     | 0.40              |
| 16:I:204:HIS:HB3  | 16:I:207:LEU:CG   | 2.51                     | 0.40              |
| 18:K:105:GLN:HG3  | 18:K:106:ASN:ND2  | 2.37                     | 0.40              |
| 18:K:112:SER:HB2  | 18:K:116:MET:O    | 2.22                     | 0.40              |
| 18:K:132:LYS:N    | 18:K:135:MET:SD   | 2.94                     | 0.40              |
| 21:N:337:GLY:O    | 21:N:373:VAL:CG1  | 2.69                     | 0.40              |
| 21:N:529:GLN:NE2  | 21:N:558:ALA:O    | 2.51                     | 0.40              |
| 21:N:729:SER:O    | 21:N:733:LEU:HG   | 2.22                     | 0.40              |
| 22:O:62:TYR:CE2   | 22:O:82:LEU:HD22  | 2.57                     | 0.40              |
| 22:O:131:SER:CB   | 22:O:135:ARG:HH12 | 2.34                     | 0.40              |
| 22:O:301:PHE:HZ   | 28:U:234:ASN:HA   | 1.84                     | 0.40              |
| 24:Q:122:ILE:O    | 24:Q:126:LYS:HG3  | 2.22                     | 0.40              |
| 24:Q:220:LEU:O    | 24:Q:224:ILE:HG13 | 2.21                     | 0.40              |
| 25:R:211:LYS:HZ1  | 25:R:234:SER:HA   | 1.83                     | 0.40              |
| 25:R:249:ILE:CG2  | 25:R:250:ALA:N    | 2.84                     | 0.40              |
| 26:S:285:ASP:OD2  | 26:S:288:THR:OG1  | 2.36                     | 0.40              |
| 27:T:27:LEU:HB2   | 27:T:28:PRO:HD3   | 2.03                     | 0.40              |
| 29:V:161:THR:HB   | 29:V:162:GLY:H    | 1.65                     | 0.40              |
| 31:X:117:LYS:HG2  | 31:X:118:ASP:H    | 1.86                     | 0.40              |
| 33:Z:187:SER:C    | 33:Z:201:LEU:HD12 | 2.43                     | 0.40              |
| 33:Z:574:TYR:OH   | 33:Z:584:VAL:HG13 | 2.19                     | 0.40              |
| 33:Z:812:ILE:HG22 | 33:Z:847:ILE:HG22 | 2.03                     | 0.40              |
| 33:Z:900:LEU:HB3  | 33:Z:903:MET:HE2  | 2.03                     | 0.40              |
| 2:2:8:PHE:HZ      | 2:2:11:GLY:HA3    | 1.68                     | 0.40              |
| 4:4:26:VAL:HG12   | 4:4:28:LYS:C      | 2.46                     | 0.40              |
| 7:7:52:MET:C      | 7:7:52:MET:SD     | 3.04                     | 0.40              |
| 8:A:91:ARG:NH2    | 14:G:113:ASP:CG   | 2.79                     | 0.40              |
| 8:A:92:ASN:ND2    | 14:G:117:GLN:HE22 | 2.19                     | 0.40              |
| 8:A:164:VAL:CB    | 9:B:61:LEU:CD2    | 2.94                     | 0.40              |
| 9:B:123:GLN:NE2   | 10:C:86:ILE:HG13  | 2.35                     | 0.40              |
| 15:H:98:GLN:HE21  | 15:H:194:SER:HB3  | 1.85                     | 0.40              |
| 16:I:432:LEU:N    | 16:I:433:GLU:OE1  | 2.54                     | 0.40              |
| 17:J:170:HIS:HB2  | 17:J:173:LEU:HD12 | 2.04                     | 0.40              |
| 19:L:280:MET:HE3  | 19:L:325:MET:HG2  | 2.02                     | 0.40              |
| 20:M:376:TRP:CG   | 20:M:377:GLN:N    | 2.89                     | 0.40              |
| 24:Q:4:PRO:CB     | 24:Q:50:ARG:HH11  | 2.31                     | 0.40              |
| 24:Q:422:VAL:HG11 | 29:V:265:GLU:CD   | 2.46                     | 0.40              |
| 25:R:209:ARG:NE   | 25:R:243:LEU:CD2  | 2.75                     | 0.40              |
| 25:R:258:LEU:HD11 | 25:R:288:SER:CA   | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:S:176:LEU:HD22 | 26:S:228:GLU:H    | 1.87                     | 0.40              |
| 26:S:428:ARG:HG3  | 27:T:195:LEU:HD22 | 2.03                     | 0.40              |
| 33:Z:108:ASP:HA   | 33:Z:109:PRO:HD3  | 1.92                     | 0.40              |
| 33:Z:138:ARG:NH1  | 33:Z:157:LEU:HA   | 2.37                     | 0.40              |
| 33:Z:329:ILE:HG23 | 33:Z:330:ILE:N    | 2.37                     | 0.40              |
| 33:Z:371:SER:O    | 33:Z:372:ALA:HB3  | 2.17                     | 0.40              |
| 33:Z:866:VAL:CB   | 33:Z:873:LEU:HG   | 2.43                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 1     | 203/215 (94%) | 188 (93%) | 11 (5%) | 4 (2%)   | 6           | 31  |
| 2   | 2     | 221/261 (85%) | 211 (96%) | 10 (4%) | 0        | 100         | 100 |
| 3   | 3     | 202/205 (98%) | 184 (91%) | 15 (7%) | 3 (2%)   | 8           | 40  |
| 4   | 4     | 196/198 (99%) | 180 (92%) | 13 (7%) | 3 (2%)   | 8           | 40  |
| 5   | 5     | 210/287 (73%) | 197 (94%) | 10 (5%) | 3 (1%)   | 9           | 40  |
| 6   | 6     | 220/241 (91%) | 205 (93%) | 11 (5%) | 4 (2%)   | 6           | 34  |
| 7   | 7     | 231/266 (87%) | 212 (92%) | 17 (7%) | 2 (1%)   | 14          | 51  |
| 8   | A     | 241/252 (96%) | 226 (94%) | 12 (5%) | 3 (1%)   | 10          | 44  |
| 9   | B     | 248/250 (99%) | 233 (94%) | 12 (5%) | 3 (1%)   | 10          | 44  |
| 10  | C     | 243/258 (94%) | 229 (94%) | 11 (4%) | 3 (1%)   | 10          | 44  |
| 11  | D     | 240/254 (94%) | 224 (93%) | 14 (6%) | 2 (1%)   | 16          | 54  |
| 12  | E     | 241/260 (93%) | 223 (92%) | 14 (6%) | 4 (2%)   | 7           | 36  |
| 13  | F     | 231/234 (99%) | 214 (93%) | 12 (5%) | 5 (2%)   | 5           | 29  |
| 14  | G     | 243/288 (84%) | 226 (93%) | 13 (5%) | 4 (2%)   | 7           | 38  |

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| Mol | Chain | Analysed          | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|----------|----------|-------------|-----|
| 15  | H     | 353/467 (76%)     | 305 (86%)  | 27 (8%)  | 21 (6%)  | 1           | 13  |
| 16  | I     | 358/437 (82%)     | 318 (89%)  | 29 (8%)  | 11 (3%)  | 3           | 22  |
| 17  | J     | 369/405 (91%)     | 334 (90%)  | 26 (7%)  | 9 (2%)   | 4           | 27  |
| 18  | K     | 377/428 (88%)     | 338 (90%)  | 32 (8%)  | 7 (2%)   | 6           | 32  |
| 19  | L     | 359/437 (82%)     | 318 (89%)  | 36 (10%) | 5 (1%)   | 9           | 40  |
| 20  | M     | 363/434 (84%)     | 323 (89%)  | 29 (8%)  | 11 (3%)  | 3           | 22  |
| 21  | N     | 843/945 (89%)     | 786 (93%)  | 49 (6%)  | 8 (1%)   | 14          | 51  |
| 22  | O     | 385/393 (98%)     | 340 (88%)  | 31 (8%)  | 14 (4%)  | 2           | 20  |
| 23  | P     | 413/445 (93%)     | 382 (92%)  | 19 (5%)  | 12 (3%)  | 3           | 23  |
| 24  | Q     | 429/434 (99%)     | 395 (92%)  | 23 (5%)  | 11 (3%)  | 4           | 25  |
| 25  | R     | 398/429 (93%)     | 354 (89%)  | 32 (8%)  | 12 (3%)  | 3           | 22  |
| 26  | S     | 351/523 (67%)     | 312 (89%)  | 29 (8%)  | 10 (3%)  | 4           | 24  |
| 27  | T     | 270/274 (98%)     | 240 (89%)  | 18 (7%)  | 12 (4%)  | 2           | 17  |
| 28  | U     | 245/338 (72%)     | 237 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 67  |
| 29  | V     | 239/306 (78%)     | 222 (93%)  | 10 (4%)  | 7 (3%)   | 3           | 23  |
| 30  | W     | 195/268 (73%)     | 171 (88%)  | 14 (7%)  | 10 (5%)  | 1           | 15  |
| 31  | X     | 125/156 (80%)     | 106 (85%)  | 14 (11%) | 5 (4%)   | 2           | 18  |
| 32  | Y     | 17/89 (19%)       | 17 (100%)  | 0        | 0        | 100         | 100 |
| 33  | Z     | 807/993 (81%)     | 722 (90%)  | 52 (6%)  | 33 (4%)  | 2           | 18  |
| All | All   | 10066/11670 (86%) | 9172 (91%) | 652 (6%) | 242 (2%) | 7           | 27  |

All (242) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | A     | 168 | ALA  |
| 11  | D     | 204 | GLN  |
| 13  | F     | 41  | ASN  |
| 15  | H     | 183 | ILE  |
| 15  | H     | 185 | LEU  |
| 15  | H     | 188 | PRO  |
| 15  | H     | 303 | ALA  |
| 15  | H     | 396 | MET  |
| 16  | I     | 125 | MET  |
| 16  | I     | 130 | VAL  |
| 17  | J     | 134 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | J     | 249 | GLU  |
| 19  | L     | 253 | ASP  |
| 20  | M     | 256 | ILE  |
| 20  | M     | 339 | ARG  |
| 21  | N     | 17  | GLN  |
| 22  | O     | 15  | ARG  |
| 22  | O     | 228 | TYR  |
| 23  | P     | 53  | ALA  |
| 23  | P     | 130 | ILE  |
| 23  | P     | 232 | ARG  |
| 23  | P     | 321 | VAL  |
| 23  | P     | 333 | ALA  |
| 24  | Q     | 354 | PHE  |
| 24  | Q     | 356 | CYS  |
| 25  | R     | 197 | MET  |
| 25  | R     | 244 | THR  |
| 25  | R     | 271 | ILE  |
| 26  | S     | 151 | GLU  |
| 27  | T     | 48  | ASN  |
| 27  | T     | 94  | HIS  |
| 27  | T     | 243 | ALA  |
| 27  | T     | 246 | GLU  |
| 27  | T     | 250 | MET  |
| 27  | T     | 254 | ASP  |
| 28  | U     | 43  | SER  |
| 29  | V     | 163 | ALA  |
| 30  | W     | 179 | ARG  |
| 31  | X     | 78  | ILE  |
| 33  | Z     | 60  | ASP  |
| 33  | Z     | 259 | PRO  |
| 33  | Z     | 318 | LYS  |
| 33  | Z     | 372 | ALA  |
| 33  | Z     | 464 | ASP  |
| 33  | Z     | 482 | ASP  |
| 1   | 1     | 19  | ARG  |
| 3   | 3     | 31  | PHE  |
| 3   | 3     | 93  | PRO  |
| 4   | 4     | 175 | PHE  |
| 5   | 5     | 145 | LYS  |
| 11  | D     | 218 | ASP  |
| 12  | E     | 53  | ARG  |
| 13  | F     | 202 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | G     | 184 | GLU  |
| 15  | H     | 104 | LYS  |
| 15  | H     | 167 | ASP  |
| 15  | H     | 189 | PRO  |
| 15  | H     | 323 | ALA  |
| 15  | H     | 370 | ARG  |
| 16  | I     | 135 | PHE  |
| 16  | I     | 162 | ASP  |
| 16  | I     | 298 | GLY  |
| 17  | J     | 207 | ASP  |
| 17  | J     | 225 | GLU  |
| 18  | K     | 248 | GLY  |
| 18  | K     | 397 | LYS  |
| 20  | M     | 385 | GLU  |
| 20  | M     | 423 | GLN  |
| 20  | M     | 431 | SER  |
| 21  | N     | 614 | ASN  |
| 21  | N     | 721 | ASP  |
| 22  | O     | 82  | LEU  |
| 23  | P     | 85  | LYS  |
| 23  | P     | 170 | SER  |
| 23  | P     | 289 | ASN  |
| 23  | P     | 290 | LEU  |
| 25  | R     | 92  | ILE  |
| 25  | R     | 162 | ILE  |
| 25  | R     | 241 | ILE  |
| 26  | S     | 144 | LEU  |
| 26  | S     | 204 | ASP  |
| 26  | S     | 452 | TYR  |
| 27  | T     | 117 | ASN  |
| 29  | V     | 181 | ASN  |
| 30  | W     | 47  | ASN  |
| 30  | W     | 136 | ASN  |
| 30  | W     | 190 | ILE  |
| 31  | X     | 38  | ASN  |
| 31  | X     | 116 | ALA  |
| 33  | Z     | 80  | SER  |
| 33  | Z     | 82  | MET  |
| 33  | Z     | 110 | ASN  |
| 33  | Z     | 132 | HIS  |
| 33  | Z     | 442 | VAL  |
| 33  | Z     | 466 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | Z     | 609 | THR  |
| 1   | 1     | 92  | ASN  |
| 4   | 4     | 111 | ASN  |
| 6   | 6     | 10  | ASP  |
| 6   | 6     | 157 | GLY  |
| 6   | 6     | 211 | LYS  |
| 7   | 7     | 221 | GLY  |
| 9   | B     | 3   | ASP  |
| 9   | B     | 102 | GLY  |
| 9   | B     | 215 | GLY  |
| 10  | C     | 220 | ALA  |
| 10  | C     | 225 | VAL  |
| 12  | E     | 122 | ARG  |
| 12  | E     | 216 | ASN  |
| 14  | G     | 71  | ARG  |
| 15  | H     | 164 | SER  |
| 15  | H     | 325 | GLY  |
| 16  | I     | 228 | GLY  |
| 16  | I     | 320 | GLY  |
| 17  | J     | 194 | GLY  |
| 17  | J     | 317 | PRO  |
| 18  | K     | 343 | LEU  |
| 18  | K     | 427 | TYR  |
| 20  | M     | 167 | VAL  |
| 20  | M     | 227 | GLY  |
| 20  | M     | 282 | GLU  |
| 21  | N     | 742 | TRP  |
| 21  | N     | 769 | PRO  |
| 21  | N     | 781 | ALA  |
| 22  | O     | 107 | GLN  |
| 22  | O     | 142 | ASP  |
| 22  | O     | 247 | ASN  |
| 22  | O     | 304 | ASN  |
| 23  | P     | 231 | LYS  |
| 24  | Q     | 37  | GLN  |
| 24  | Q     | 48  | ASP  |
| 24  | Q     | 149 | LYS  |
| 24  | Q     | 399 | VAL  |
| 25  | R     | 37  | LYS  |
| 26  | S     | 199 | GLU  |
| 26  | S     | 284 | LEU  |
| 27  | T     | 90  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | V     | 194 | ARG  |
| 30  | W     | 101 | ARG  |
| 33  | Z     | 184 | SER  |
| 33  | Z     | 228 | GLU  |
| 33  | Z     | 338 | HIS  |
| 33  | Z     | 443 | ASP  |
| 33  | Z     | 524 | ALA  |
| 33  | Z     | 920 | GLY  |
| 33  | Z     | 974 | THR  |
| 1   | 1     | -7  | LYS  |
| 1   | 1     | 145 | ASN  |
| 3   | 3     | 148 | ASN  |
| 5   | 5     | 118 | ASP  |
| 8   | A     | 13  | ASP  |
| 8   | A     | 198 | SER  |
| 13  | F     | 222 | PHE  |
| 14  | G     | 186 | LEU  |
| 15  | H     | 172 | MET  |
| 15  | H     | 191 | ILE  |
| 18  | K     | 278 | ALA  |
| 21  | N     | 86  | LYS  |
| 22  | O     | 302 | VAL  |
| 22  | O     | 358 | ILE  |
| 22  | O     | 360 | GLY  |
| 24  | Q     | 38  | SER  |
| 24  | Q     | 42  | ALA  |
| 25  | R     | 326 | ALA  |
| 26  | S     | 146 | LEU  |
| 26  | S     | 303 | ASN  |
| 27  | T     | 244 | ASP  |
| 29  | V     | 72  | PRO  |
| 29  | V     | 78  | VAL  |
| 30  | W     | 57  | ALA  |
| 30  | W     | 149 | GLN  |
| 30  | W     | 164 | PRO  |
| 30  | W     | 169 | SER  |
| 33  | Z     | 76  | LYS  |
| 33  | Z     | 142 | ASP  |
| 33  | Z     | 893 | PHE  |
| 5   | 5     | 173 | GLY  |
| 6   | 6     | 40  | ASN  |
| 13  | F     | 69  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | G     | 70  | ASP  |
| 15  | H     | 107 | LYS  |
| 15  | H     | 143 | ALA  |
| 15  | H     | 170 | GLU  |
| 15  | H     | 357 | ARG  |
| 16  | I     | 165 | ASP  |
| 16  | I     | 341 | PRO  |
| 17  | J     | 258 | VAL  |
| 18  | K     | 160 | VAL  |
| 18  | K     | 424 | PHE  |
| 19  | L     | 164 | ASP  |
| 20  | M     | 425 | ARG  |
| 22  | O     | 203 | THR  |
| 24  | Q     | 89  | ALA  |
| 24  | Q     | 273 | ASN  |
| 25  | R     | 39  | SER  |
| 25  | R     | 182 | ASN  |
| 25  | R     | 222 | ARG  |
| 26  | S     | 174 | ARG  |
| 26  | S     | 375 | ASP  |
| 27  | T     | 73  | PHE  |
| 27  | T     | 172 | SER  |
| 29  | V     | 161 | THR  |
| 31  | X     | 28  | PRO  |
| 33  | Z     | 75  | ILE  |
| 33  | Z     | 287 | ARG  |
| 33  | Z     | 957 | LEU  |
| 7   | 7     | 30  | GLY  |
| 10  | C     | 52  | VAL  |
| 12  | E     | 190 | SER  |
| 13  | F     | 103 | LEU  |
| 15  | H     | 105 | ILE  |
| 15  | H     | 161 | GLU  |
| 16  | I     | 205 | PRO  |
| 17  | J     | 126 | LEU  |
| 19  | L     | 175 | GLN  |
| 19  | L     | 183 | ILE  |
| 24  | Q     | 131 | VAL  |
| 25  | R     | 198 | ILE  |
| 27  | T     | 167 | GLY  |
| 31  | X     | 37  | PRO  |
| 33  | Z     | 183 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | Z     | 919 | GLU  |
| 33  | Z     | 929 | VAL  |
| 33  | Z     | 930 | GLY  |
| 21  | N     | 353 | LEU  |
| 23  | P     | 396 | PRO  |
| 30  | W     | 189 | PRO  |
| 33  | Z     | 469 | PRO  |
| 22  | O     | 353 | VAL  |
| 15  | H     | 243 | PRO  |
| 19  | L     | 287 | GLY  |
| 20  | M     | 252 | VAL  |
| 20  | M     | 350 | PRO  |
| 22  | O     | 164 | PRO  |
| 29  | V     | 247 | ILE  |
| 33  | Z     | 578 | GLY  |
| 4   | 4     | 149 | PRO  |
| 17  | J     | 281 | GLY  |
| 22  | O     | 238 | ILE  |
| 23  | P     | 211 | PRO  |
| 16  | I     | 428 | VAL  |
| 33  | Z     | 462 | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | 1     | 169/178 (95%)  | 169 (100%) | 0        | 100         | 100 |
| 2   | 2     | 182/214 (85%)  | 182 (100%) | 0        | 100         | 100 |
| 3   | 3     | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 4   | 4     | 175/175 (100%) | 175 (100%) | 0        | 100         | 100 |
| 5   | 5     | 169/235 (72%)  | 169 (100%) | 0        | 100         | 100 |
| 6   | 6     | 185/201 (92%)  | 185 (100%) | 0        | 100         | 100 |
| 7   | 7     | 199/224 (89%)  | 199 (100%) | 0        | 100         | 100 |
| 8   | A     | 207/210 (99%)  | 207 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 9   | B     | 209/209 (100%)   | 209 (100%)  | 0        | 100         | 100 |
| 10  | C     | 204/216 (94%)    | 204 (100%)  | 0        | 100         | 100 |
| 11  | D     | 214/226 (95%)    | 214 (100%)  | 0        | 100         | 100 |
| 12  | E     | 199/215 (93%)    | 199 (100%)  | 0        | 100         | 100 |
| 13  | F     | 192/193 (100%)   | 192 (100%)  | 0        | 100         | 100 |
| 14  | G     | 201/239 (84%)    | 201 (100%)  | 0        | 100         | 100 |
| 15  | H     | 303/399 (76%)    | 300 (99%)   | 3 (1%)   | 68          | 78  |
| 16  | I     | 319/385 (83%)    | 318 (100%)  | 1 (0%)   | 86          | 86  |
| 17  | J     | 325/352 (92%)    | 325 (100%)  | 0        | 100         | 100 |
| 18  | K     | 334/374 (89%)    | 334 (100%)  | 0        | 100         | 100 |
| 19  | L     | 308/377 (82%)    | 308 (100%)  | 0        | 100         | 100 |
| 20  | M     | 315/375 (84%)    | 315 (100%)  | 0        | 100         | 100 |
| 21  | N     | 713/797 (90%)    | 713 (100%)  | 0        | 100         | 100 |
| 22  | O     | 363/368 (99%)    | 363 (100%)  | 0        | 100         | 100 |
| 23  | P     | 388/415 (94%)    | 386 (100%)  | 2 (0%)   | 81          | 83  |
| 24  | Q     | 388/391 (99%)    | 388 (100%)  | 0        | 100         | 100 |
| 25  | R     | 351/379 (93%)    | 351 (100%)  | 0        | 100         | 100 |
| 26  | S     | 330/489 (68%)    | 330 (100%)  | 0        | 100         | 100 |
| 27  | T     | 254/256 (99%)    | 254 (100%)  | 0        | 100         | 100 |
| 28  | U     | 234/308 (76%)    | 233 (100%)  | 1 (0%)   | 84          | 84  |
| 29  | V     | 217/268 (81%)    | 217 (100%)  | 0        | 100         | 100 |
| 30  | W     | 171/230 (74%)    | 171 (100%)  | 0        | 100         | 100 |
| 31  | X     | 116/144 (81%)    | 116 (100%)  | 0        | 100         | 100 |
| 32  | Y     | 18/81 (22%)      | 18 (100%)   | 0        | 100         | 100 |
| 33  | Z     | 692/850 (81%)    | 692 (100%)  | 0        | 100         | 100 |
| All | All   | 8816/10146 (87%) | 8809 (100%) | 7 (0%)   | 87          | 89  |

All (7) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | H     | 107 | LYS  |
| 15  | H     | 164 | SER  |
| 15  | H     | 280 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | I     | 257 | LEU  |
| 23  | P     | 31  | ASP  |
| 23  | P     | 33  | ASN  |
| 28  | U     | 61  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (193) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 69  | GLN  |
| 1   | 1     | 157 | HIS  |
| 2   | 2     | 160 | GLN  |
| 2   | 2     | 189 | ASN  |
| 3   | 3     | 104 | ASN  |
| 3   | 3     | 160 | GLN  |
| 4   | 4     | 40  | HIS  |
| 4   | 4     | 85  | GLN  |
| 4   | 4     | 98  | GLN  |
| 4   | 4     | 100 | ASN  |
| 4   | 4     | 145 | HIS  |
| 4   | 4     | 146 | HIS  |
| 4   | 4     | 165 | GLN  |
| 5   | 5     | 62  | GLN  |
| 5   | 5     | 66  | HIS  |
| 5   | 5     | 190 | ASN  |
| 6   | 6     | 46  | ASN  |
| 6   | 6     | 70  | HIS  |
| 6   | 6     | 71  | ASN  |
| 7   | 7     | 53  | GLN  |
| 7   | 7     | 70  | ASN  |
| 7   | 7     | 112 | GLN  |
| 7   | 7     | 114 | ASN  |
| 8   | A     | 36  | ASN  |
| 8   | A     | 84  | ASN  |
| 8   | A     | 92  | ASN  |
| 8   | A     | 130 | GLN  |
| 9   | B     | 20  | GLN  |
| 9   | B     | 94  | HIS  |
| 9   | B     | 123 | GLN  |
| 9   | B     | 180 | ASN  |
| 9   | B     | 218 | ASN  |
| 10  | C     | 21  | GLN  |
| 10  | C     | 31  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C     | 96  | GLN  |
| 10  | C     | 125 | HIS  |
| 10  | C     | 177 | GLN  |
| 11  | D     | 19  | GLN  |
| 11  | D     | 55  | GLN  |
| 11  | D     | 118 | GLN  |
| 11  | D     | 122 | GLN  |
| 12  | E     | 108 | ASN  |
| 12  | E     | 114 | GLN  |
| 12  | E     | 180 | GLN  |
| 12  | E     | 188 | HIS  |
| 13  | F     | 21  | GLN  |
| 13  | F     | 60  | GLN  |
| 13  | F     | 91  | GLN  |
| 13  | F     | 210 | ASN  |
| 14  | G     | 11  | ASN  |
| 14  | G     | 89  | ASN  |
| 14  | G     | 194 | GLN  |
| 15  | H     | 98  | GLN  |
| 15  | H     | 339 | GLN  |
| 15  | H     | 348 | ASN  |
| 15  | H     | 359 | ASN  |
| 16  | I     | 102 | ASN  |
| 16  | I     | 295 | ASN  |
| 16  | I     | 312 | GLN  |
| 17  | J     | 111 | GLN  |
| 17  | J     | 156 | GLN  |
| 17  | J     | 220 | GLN  |
| 17  | J     | 240 | HIS  |
| 17  | J     | 278 | GLN  |
| 17  | J     | 331 | HIS  |
| 17  | J     | 336 | ASN  |
| 18  | K     | 74  | HIS  |
| 18  | K     | 98  | GLN  |
| 18  | K     | 106 | ASN  |
| 18  | K     | 182 | GLN  |
| 18  | K     | 238 | ASN  |
| 18  | K     | 414 | GLN  |
| 19  | L     | 67  | HIS  |
| 19  | L     | 99  | GLN  |
| 19  | L     | 133 | ASN  |
| 19  | L     | 189 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | L     | 302 | GLN  |
| 19  | L     | 311 | GLN  |
| 20  | M     | 65  | ASN  |
| 20  | M     | 74  | GLN  |
| 20  | M     | 81  | ASN  |
| 20  | M     | 125 | GLN  |
| 20  | M     | 250 | GLN  |
| 20  | M     | 253 | GLN  |
| 20  | M     | 311 | GLN  |
| 20  | M     | 423 | GLN  |
| 21  | N     | 29  | ASN  |
| 21  | N     | 96  | GLN  |
| 21  | N     | 116 | GLN  |
| 21  | N     | 122 | GLN  |
| 21  | N     | 176 | GLN  |
| 21  | N     | 249 | ASN  |
| 21  | N     | 268 | GLN  |
| 21  | N     | 300 | ASN  |
| 21  | N     | 306 | ASN  |
| 21  | N     | 308 | ASN  |
| 21  | N     | 529 | GLN  |
| 21  | N     | 614 | ASN  |
| 21  | N     | 877 | GLN  |
| 21  | N     | 878 | GLN  |
| 21  | N     | 900 | ASN  |
| 22  | O     | 4   | ASN  |
| 22  | O     | 28  | GLN  |
| 22  | O     | 75  | GLN  |
| 22  | O     | 105 | GLN  |
| 22  | O     | 211 | GLN  |
| 22  | O     | 229 | ASN  |
| 22  | O     | 235 | HIS  |
| 22  | O     | 236 | HIS  |
| 22  | O     | 289 | GLN  |
| 22  | O     | 318 | HIS  |
| 23  | P     | 38  | GLN  |
| 23  | P     | 48  | GLN  |
| 23  | P     | 86  | HIS  |
| 23  | P     | 164 | GLN  |
| 23  | P     | 277 | GLN  |
| 23  | P     | 289 | ASN  |
| 23  | P     | 296 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | P     | 342 | GLN  |
| 23  | P     | 366 | ASN  |
| 23  | P     | 401 | ASN  |
| 23  | P     | 425 | HIS  |
| 23  | P     | 431 | HIS  |
| 24  | Q     | 52  | ASN  |
| 24  | Q     | 150 | GLN  |
| 24  | Q     | 252 | HIS  |
| 24  | Q     | 405 | GLN  |
| 25  | R     | 42  | GLN  |
| 25  | R     | 73  | ASN  |
| 25  | R     | 76  | GLN  |
| 25  | R     | 130 | GLN  |
| 25  | R     | 287 | GLN  |
| 25  | R     | 325 | HIS  |
| 25  | R     | 340 | GLN  |
| 25  | R     | 378 | ASN  |
| 25  | R     | 397 | ASN  |
| 26  | S     | 302 | HIS  |
| 26  | S     | 311 | GLN  |
| 26  | S     | 314 | ASN  |
| 26  | S     | 317 | HIS  |
| 26  | S     | 334 | HIS  |
| 26  | S     | 339 | GLN  |
| 26  | S     | 378 | GLN  |
| 26  | S     | 417 | GLN  |
| 26  | S     | 472 | HIS  |
| 27  | T     | 132 | HIS  |
| 27  | T     | 135 | ASN  |
| 27  | T     | 158 | GLN  |
| 27  | T     | 192 | ASN  |
| 27  | T     | 213 | ASN  |
| 27  | T     | 255 | GLN  |
| 27  | T     | 272 | ASN  |
| 28  | U     | 21  | HIS  |
| 28  | U     | 77  | ASN  |
| 28  | U     | 84  | ASN  |
| 28  | U     | 94  | HIS  |
| 28  | U     | 127 | GLN  |
| 28  | U     | 230 | GLN  |
| 28  | U     | 262 | GLN  |
| 28  | U     | 280 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | U     | 297 | GLN  |
| 29  | V     | 97  | GLN  |
| 29  | V     | 109 | HIS  |
| 29  | V     | 131 | GLN  |
| 29  | V     | 190 | HIS  |
| 29  | V     | 291 | ASN  |
| 30  | W     | 12  | ASN  |
| 30  | W     | 47  | ASN  |
| 30  | W     | 80  | GLN  |
| 30  | W     | 95  | GLN  |
| 30  | W     | 106 | GLN  |
| 31  | X     | 38  | ASN  |
| 31  | X     | 105 | ASN  |
| 31  | X     | 108 | ASN  |
| 32  | Y     | 89  | GLN  |
| 33  | Z     | 132 | HIS  |
| 33  | Z     | 240 | ASN  |
| 33  | Z     | 275 | GLN  |
| 33  | Z     | 317 | GLN  |
| 33  | Z     | 327 | GLN  |
| 33  | Z     | 338 | HIS  |
| 33  | Z     | 379 | GLN  |
| 33  | Z     | 387 | ASN  |
| 33  | Z     | 577 | GLN  |
| 33  | Z     | 593 | HIS  |
| 33  | Z     | 766 | HIS  |
| 33  | Z     | 769 | ASN  |
| 33  | Z     | 789 | GLN  |
| 33  | Z     | 810 | ASN  |
| 33  | Z     | 833 | GLN  |
| 33  | Z     | 897 | HIS  |
| 33  | Z     | 899 | GLN  |
| 33  | Z     | 926 | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 17  | J     | 2                |
| 16  | I     | 1                |
| 18  | K     | 1                |
| 19  | L     | 1                |
| 20  | M     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | J     | 218:LEU   | C      | 219:VAL   | N      | 3.94         |
| 1     | I     | 252:LEU   | C      | 253:ILE   | N      | 3.24         |
| 1     | K     | 242:PHE   | C      | 243:VAL   | N      | 2.17         |
| 1     | J     | 224:GLY   | C      | 225:GLU   | N      | 1.73         |
| 1     | L     | 257:GLY   | C      | 258:GLU   | N      | 1.14         |
| 1     | M     | 251:LEU   | C      | 252:VAL   | N      | 0.84         |

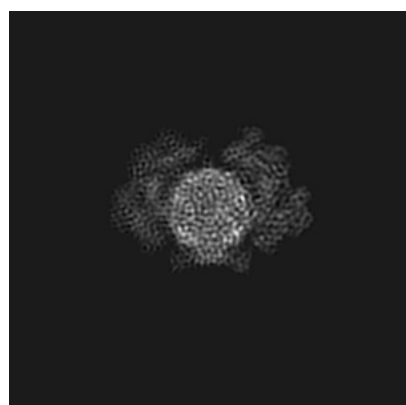
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2594. These allow visual inspection of the internal detail of the map and identification of artifacts.

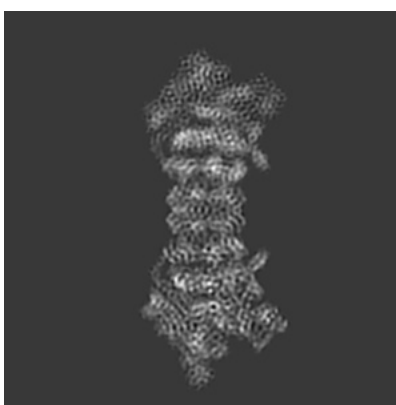
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

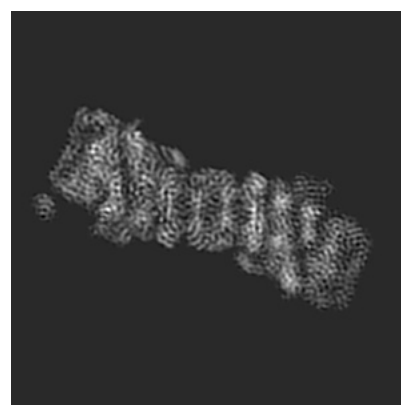
#### 6.1.1 Primary map



X



Y

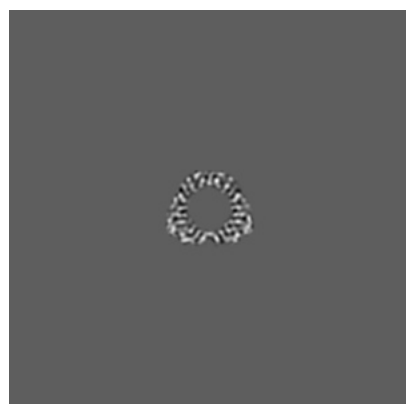


Z

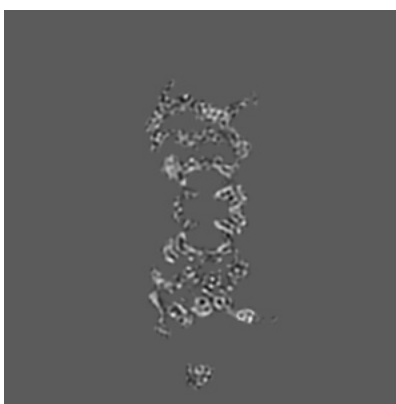
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 140



Y Index: 140



Z Index: 140

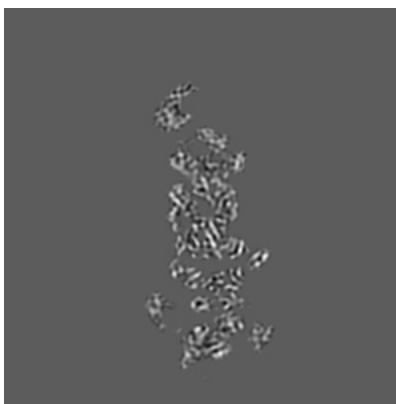
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 72



Y Index: 154

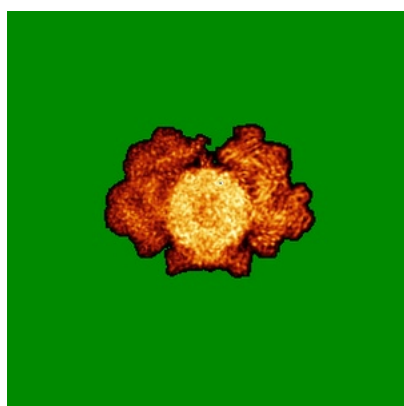


Z Index: 139

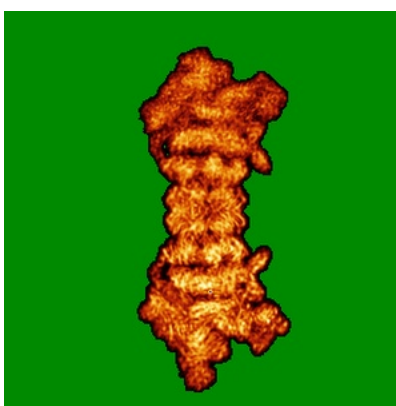
The images above show the largest variance slices of the map in three orthogonal directions.

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

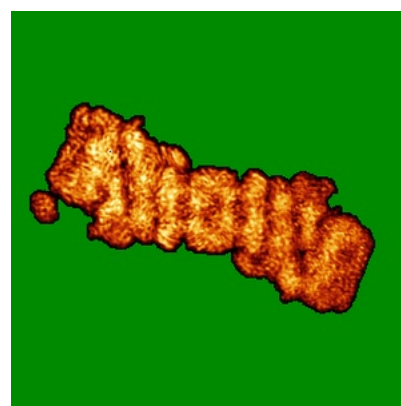
### 6.4.1 Primary map



X



Y

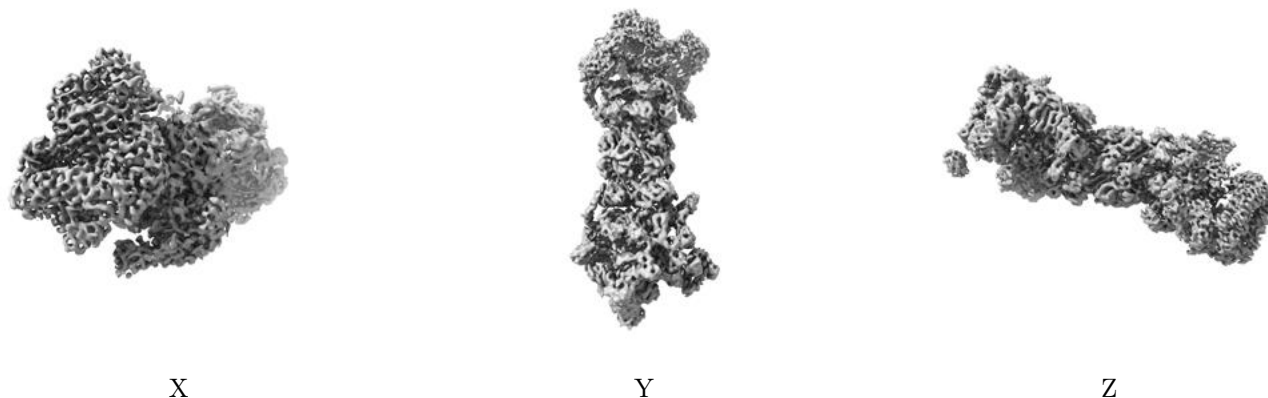


Z

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 0.74. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

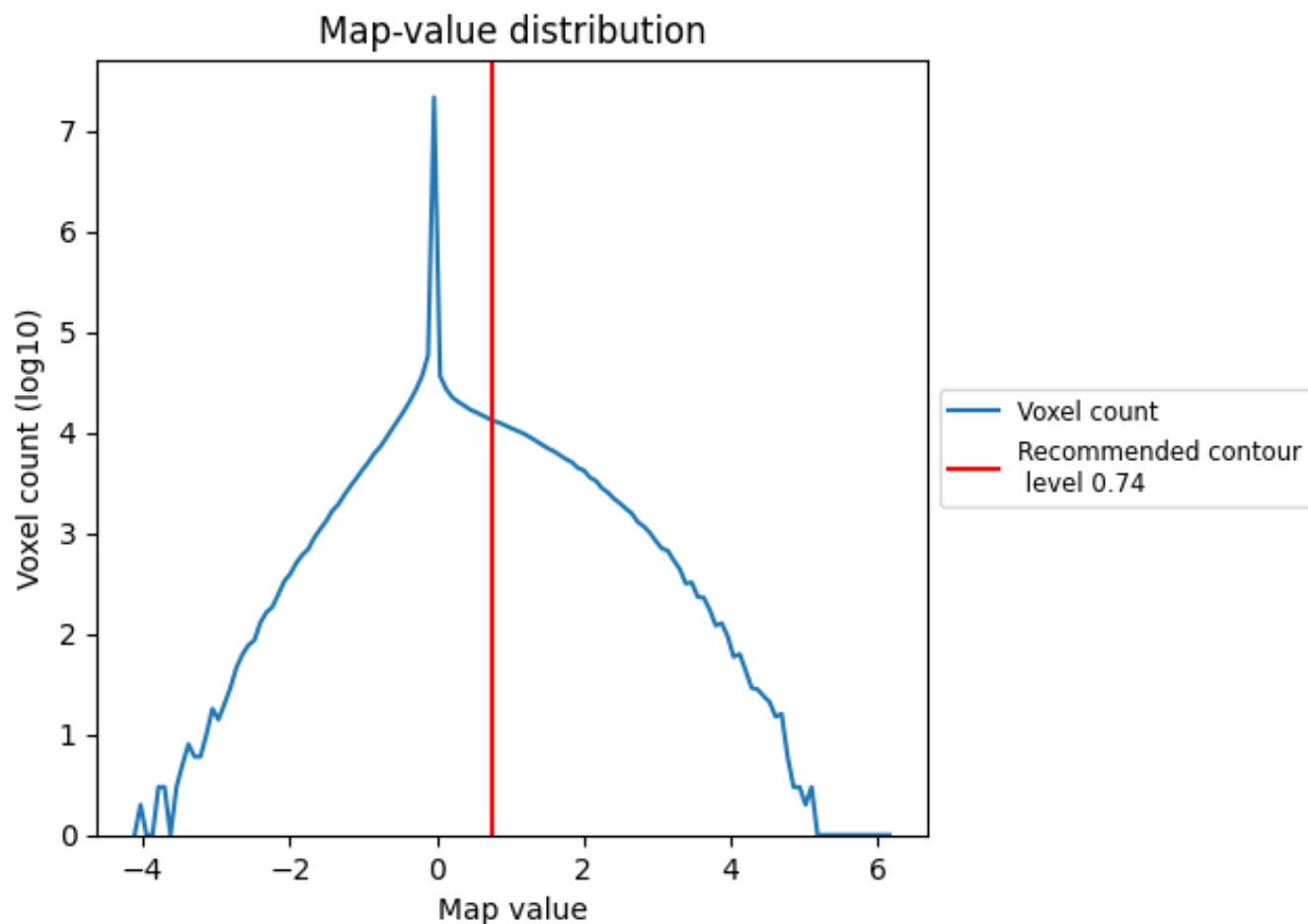
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

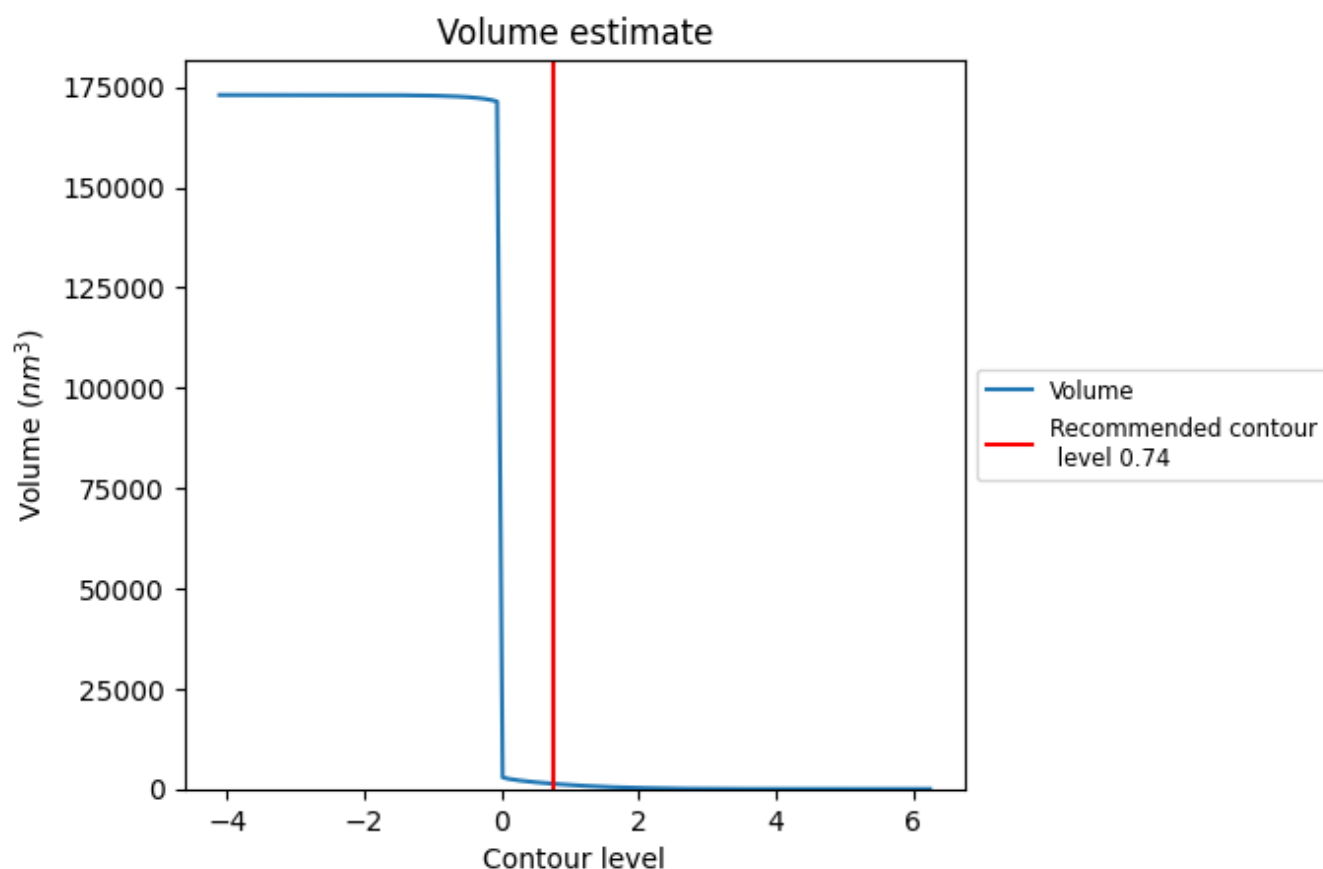
This section contains the results of statistical analysis of the map.

### 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.

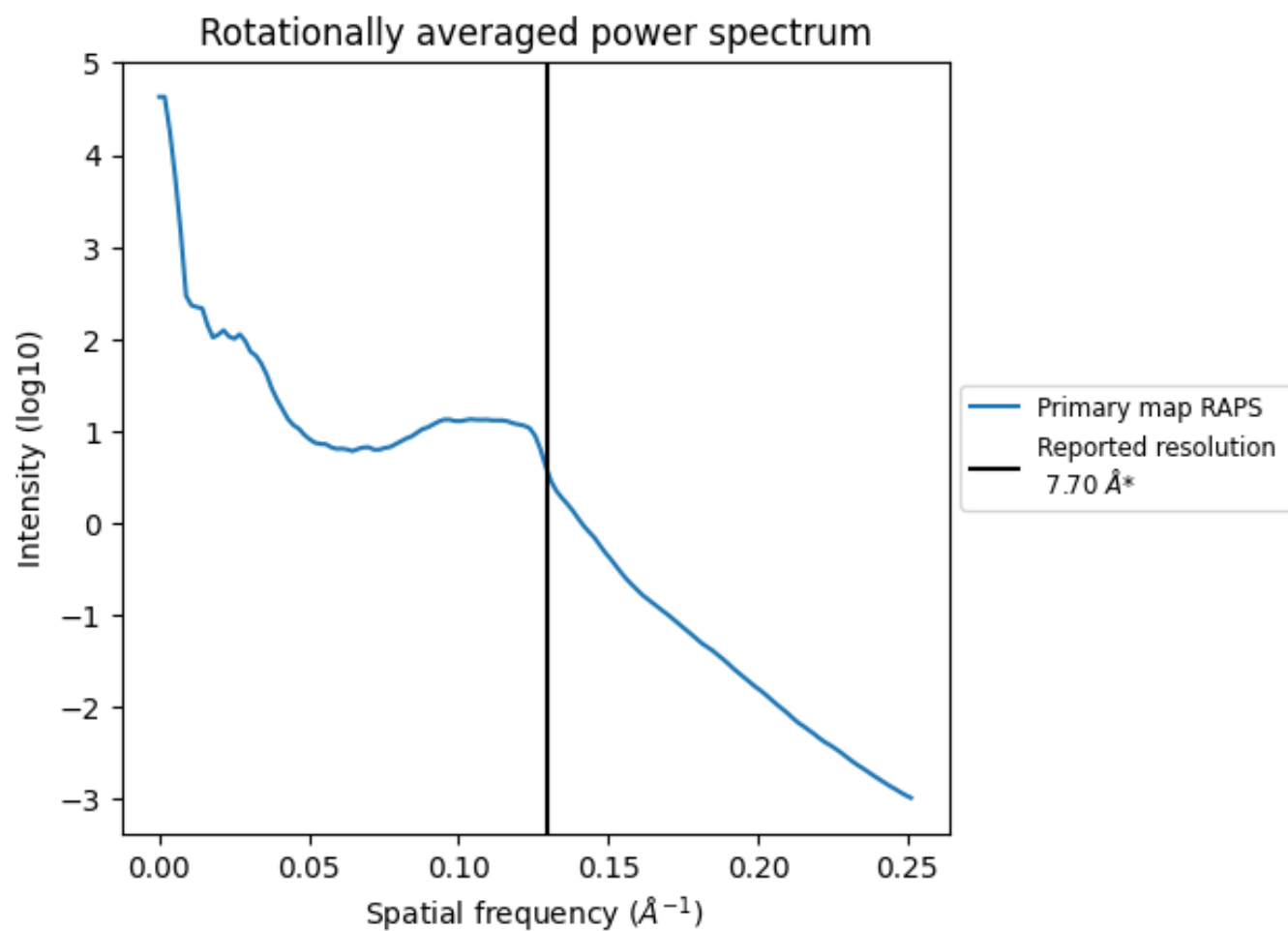
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1311 nm<sup>3</sup>; this corresponds to an approximate mass of 1184 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.130 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

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

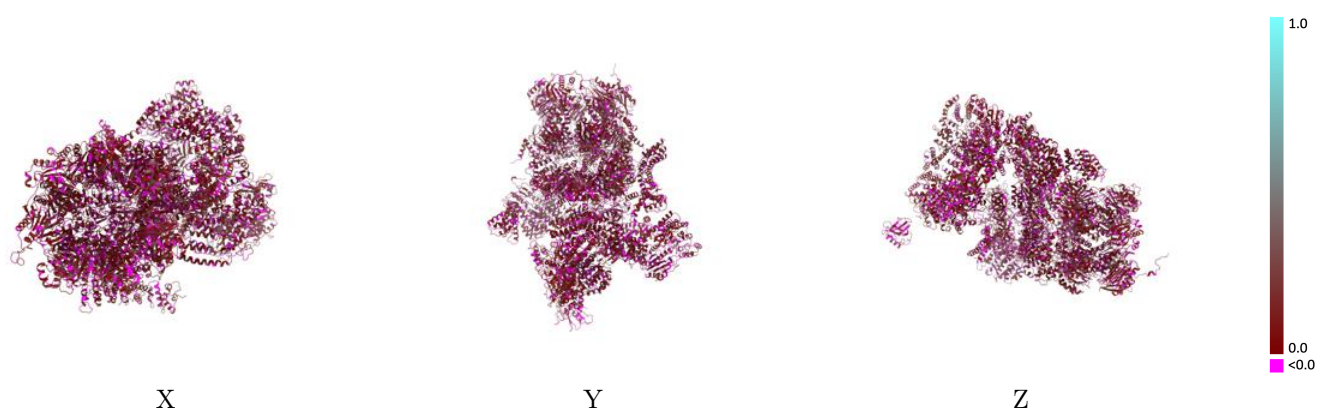
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2594 and PDB model 4CR2. Per-residue inclusion information can be found in section 3 on page 10.

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

This section was not generated.

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

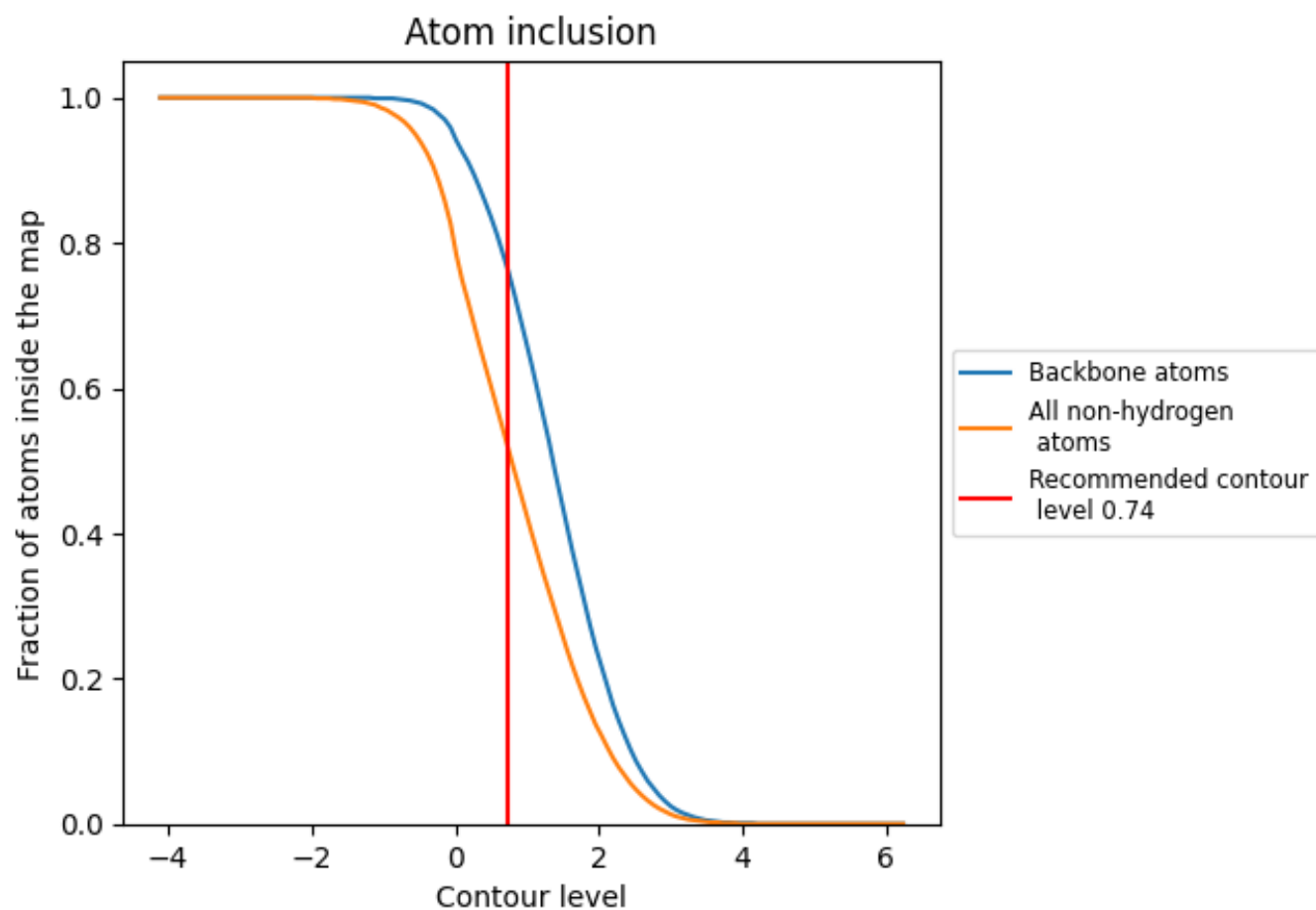


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 52% 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 (0.74) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.5170         | 0.1040  |
| 1     | 0.4940         | 0.0930  |
| 2     | 0.5130         | 0.1150  |
| 3     | 0.4720         | 0.1080  |
| 4     | 0.5410         | 0.1090  |
| 5     | 0.5530         | 0.1140  |
| 6     | 0.5220         | 0.1110  |
| 7     | 0.5160         | 0.1070  |
| A     | 0.4830         | 0.1150  |
| B     | 0.4500         | 0.1020  |
| C     | 0.4950         | 0.1170  |
| D     | 0.5000         | 0.1100  |
| E     | 0.4930         | 0.1110  |
| F     | 0.5150         | 0.1200  |
| G     | 0.4610         | 0.1070  |
| H     | 0.4420         | 0.0870  |
| I     | 0.4460         | 0.0970  |
| J     | 0.4920         | 0.1020  |
| K     | 0.4600         | 0.1050  |
| L     | 0.4870         | 0.1020  |
| M     | 0.4830         | 0.1080  |
| N     | 0.5620         | 0.1190  |
| O     | 0.5630         | 0.0940  |
| P     | 0.6250         | 0.1070  |
| Q     | 0.5850         | 0.1010  |
| R     | 0.5540         | 0.0930  |
| S     | 0.4810         | 0.0970  |
| T     | 0.6070         | 0.1120  |
| U     | 0.5490         | 0.1200  |
| V     | 0.5170         | 0.1040  |
| W     | 0.4580         | 0.0710  |
| X     | 0.4910         | 0.0420  |
| Y     | 0.5950         | 0.1020  |
| Z     | 0.5170         | 0.0930  |

