



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:17 AM GMT

PDB ID : 2VAO  
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-  
ALCOHOL OXIDASE IN COMPLEX WITH ISOEUGENOL  
Authors : Mattevi, A.  
Deposited on : 1997-04-10  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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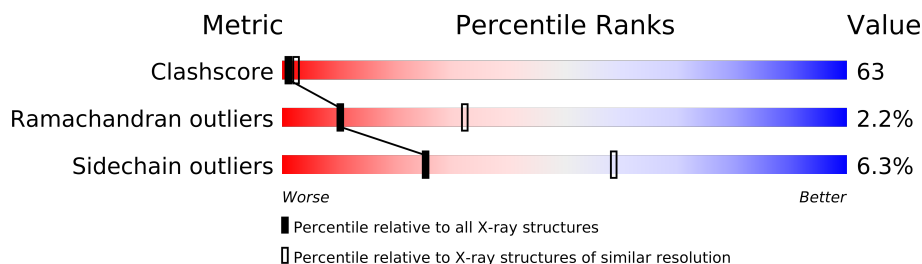
The following versions of software and data (see [references](#)) were used in the production of this report:

|                                |   |                          |
|--------------------------------|---|--------------------------|
| MolProbity                     | : | 4.02b-467                |
| Mogul                          | : | 1.15 2013                |
| Xtriage (Phenix)               | : | NOT EXECUTED             |
| EDS                            | : | NOT EXECUTED             |
| Percentile statistics          | : | 21963                    |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)      |
| Ideal geometry (DNA, RNA)      | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | stable22683              |

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 560    |                  |
| 1   | B     | 560    |                  |

## 2 Entry composition i

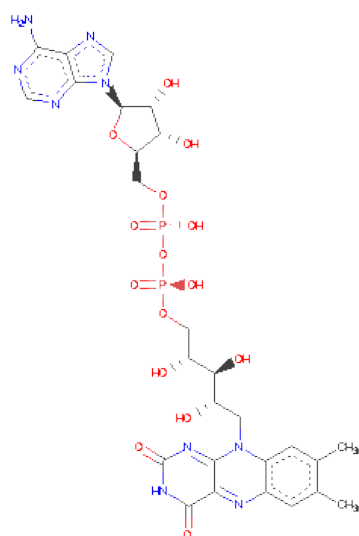
There are 4 unique types of molecules in this entry. The entry contains 8948 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

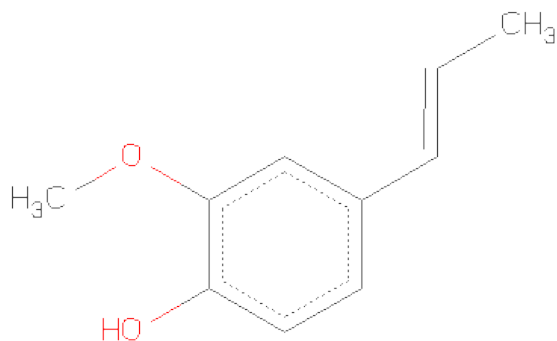
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 555      | Total | C    | N   | O   | S  | 51      | 0       | 0     |
|     |       |          | 4391  | 2817 | 751 | 799 | 24 |         |         |       |
| 1   | B     | 555      | Total | C    | N   | O   | S  | 51      | 0       | 0     |
|     |       |          | 4391  | 2817 | 751 | 799 | 24 |         |         |       |

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

- Molecule 3 is 2-METHOXY-4-VINYLPHENOL (three-letter code: EUG) (formula:  $C_{10}H_{12}O_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 9 | 2 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 9 | 2 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 4   | B     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |

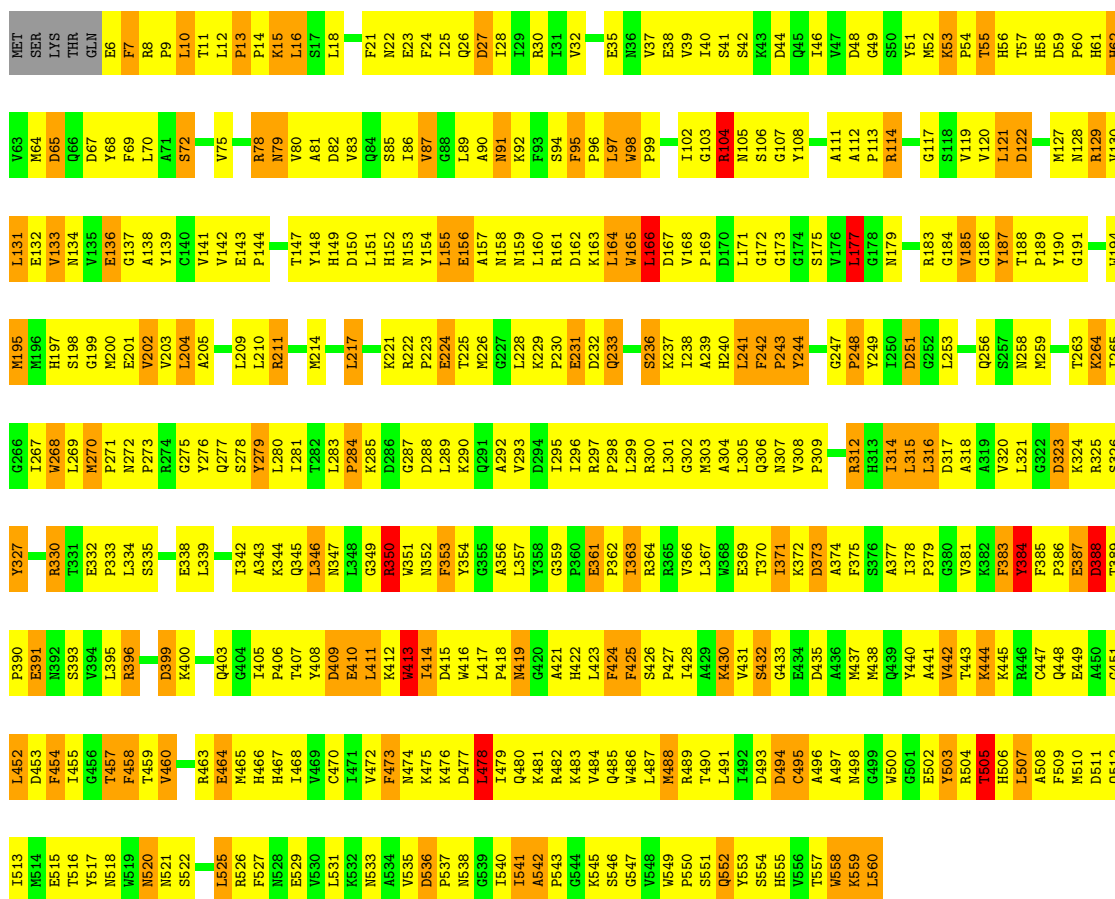
### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain A:



#### • Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:



|      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|
| E515 | F454 | S393 | R330 | W268 | H195 | V130 | V63  |
| T516 | I455 | V394 | T331 | L269 | H197 | L131 | M64  |
| N517 | G456 | L395 | E332 | M270 | S198 | E132 | D65  |
| N518 | T457 | R396 | P333 | P271 | G199 | V133 | Q66  |
| N519 | F458 |      | L334 | N272 | M200 | N134 | D67  |
| N520 | T459 | D399 | S335 | P273 | E201 | V135 | Y68  |
| N521 | V460 | K400 |      | R274 | V202 | E136 | F69  |
| S522 |      | T401 | E338 | Q275 | V203 | G137 | L70  |
|      |      | P402 | L339 | Y276 | L204 | A138 | A71  |
| L525 | R463 | Q403 |      | Q277 | A205 | Y139 | S72  |
| R526 | E464 | G404 | I342 | Z278 |      | C140 | A73  |
| R527 | M465 | I405 |      | Y279 | L209 | V141 | I74  |
| F528 | H466 | F406 | Q345 | L280 | L210 | V142 | W75  |
| H467 | T468 | T407 | L346 | I281 | R211 | E143 |      |
| I468 | V469 | Y408 | N347 | T282 |      | P144 |      |
| V469 | C470 | D409 | L348 | L283 | M214 |      |      |
| L531 | L471 | E410 | G349 | K284 |      | T147 | R78  |
| N533 | V472 | L411 | R350 | K285 | L217 | Y148 | V80  |
| A534 | F473 | K412 | V351 | D286 |      | H149 | A81  |
| V535 | M474 | R413 | R352 | G287 | K221 | D150 | D82  |
| D536 | K475 | I414 | F353 | D288 | R222 | H151 | Q84  |
| P537 | K476 | D415 | Y354 | L289 | P223 | H152 | S85  |
| N538 | D477 | W416 | G355 | K290 | E224 | N153 | I86  |
| G539 | L478 | L417 | A356 | Q291 | T225 | Y154 | V87  |
| I540 | I479 | P418 | L357 | A292 | M226 | L155 | G88  |
| I541 | Q480 | M419 | V358 | V293 | G227 | E156 | L89  |
| A542 | K481 | G420 | G359 | D294 | L228 | A157 | A90  |
|      | R482 | A421 | P360 | I295 | K229 | N158 | N91  |
| K545 | K483 | H422 | E361 | I296 | P230 | N159 | K92  |
| S546 | V484 | L423 | P362 | R297 | E231 | L160 | F93  |
| G547 | Q485 | F424 | I363 | P298 | D232 | R161 | S94  |
| V548 | W486 | F425 | R364 | L299 | Q233 | D162 | F95  |
| W549 | L487 | S426 | R365 | R300 |      | K163 | P96  |
| P550 | M488 | P427 | V366 | L301 | S236 | L164 | L97  |
| S551 | R489 | I428 | L367 | G302 | K237 | W165 | W98  |
| Q552 | T490 | A429 | K368 | M303 | I238 | L166 | P99  |
| Y553 | L491 | K430 | E369 | A304 | A239 |      |      |
| S554 | L492 | V431 | T370 | L305 | H240 | L171 | I102 |
| H555 | D493 | S432 | I371 | Q306 | L241 | G172 | G103 |
| V556 | D494 | G433 | K372 | N307 | F242 | G173 | R104 |
| T557 | C495 | E434 | D373 | V308 | P243 | G174 | N105 |
| W558 | A496 | D435 | A374 | P309 | Y244 | S175 | S106 |
| K559 | A497 | A436 | F375 |      |      | W176 | G107 |
| L560 | M498 | M437 | S376 | R312 | G247 | L177 | Y108 |
|      | G499 | M438 | A377 | H313 | P248 | G178 |      |
|      | W500 | Q439 | I378 | I314 | Y249 | N179 | A111 |
|      | G501 | Y440 | P379 | L315 | I250 |      | A112 |
| E502 | E502 | A441 | G380 | L316 | D251 |      | P113 |
| Y503 | R504 | V442 | V381 | D317 | G252 | R183 | R114 |
| R504 | T505 | T443 | K382 | A318 | L253 | G184 |      |
| T505 | H506 | K444 | F383 | A319 |      | V185 |      |
| L507 | L507 | K445 | Y384 | V320 | Q256 | G186 | G117 |
| A508 | F509 | R446 | F385 | L321 | S257 | Y187 | S118 |
| F509 | N510 | C447 | P386 | G322 | N258 | T188 | V119 |
| N510 | D511 | Q448 | E387 | D323 | M259 | P189 | V120 |
| D511 | Q512 | E449 | D388 | K324 |      | Y190 | L121 |
| Q512 | I513 | A450 | T389 | R325 | K264 | G191 | D122 |
| I513 | N514 | G451 | P390 | S326 | L265 |      |      |
|      |      | L452 | E391 | Y327 | G266 | W194 | M127 |
|      |      | D453 | N392 |      |      | M195 | N128 |
|      |      |      |      |      |      |      | R129 |

## 4 Data and refinement statistics

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

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | I 4   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 128.38Å 128.38Å 130.19Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 30.00 – 2.80                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 90.6 (30.00-2.80)                               | Depositor |
| $R_{merge}$  | (Not available)                                 | Depositor |
| $R_{sym}$  | 0.11  | Depositor |
| Refinement program                                       | TNT V. 5-E                                      | Depositor |
| R, $R_{free}$  | 0.214 , 0.290                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 8948  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 26.0  | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.81         | 3/4511 (0.1%) | 1.88        | 127/6131 (2.1%)  |
| 1   | B     | 0.81         | 2/4511 (0.0%) | 1.88        | 128/6131 (2.1%)  |
| All | All   | 0.81         | 5/9022 (0.1%) | 1.88        | 255/12262 (2.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 2                   | 0                   |
| 1   | B     | 2                   | 0                   |
| All | All   | 4                   | 0                   |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 268 | TRP  | CB-CG | -5.99 | 1.39        | 1.50     |
| 1   | B     | 156 | GLU  | CG-CD | 5.97  | 1.60        | 1.51     |
| 1   | B     | 268 | TRP  | CB-CG | -5.95 | 1.39        | 1.50     |
| 1   | A     | 156 | GLU  | CG-CD | 5.94  | 1.60        | 1.51     |
| 1   | A     | 244 | TYR  | CB-CG | -5.03 | 1.44        | 1.51     |

All (255) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | B     | 560 | LEU  | CB-CG-CD2 | -12.85 | 89.15       | 111.00   |
| 1   | A     | 560 | LEU  | CB-CG-CD2 | -12.83 | 89.19       | 111.00   |
| 1   | B     | 16  | LEU  | CA-CB-CG  | -11.58 | 88.66       | 115.30   |
| 1   | A     | 16  | LEU  | CA-CB-CG  | -11.56 | 88.70       | 115.30   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | B     | 495 | CYS  | CA-CB-SG  | -11.13 | 93.97       | 114.00   |
| 1   | A     | 495 | CYS  | CA-CB-SG  | -11.12 | 93.98       | 114.00   |
| 1   | A     | 177 | LEU  | CA-CB-CG  | 10.64  | 139.78      | 115.30   |
| 1   | B     | 177 | LEU  | CA-CB-CG  | 10.63  | 139.74      | 115.30   |
| 1   | B     | 505 | THR  | CB-CA-C   | -10.48 | 83.30       | 111.60   |
| 1   | A     | 505 | THR  | CB-CA-C   | -10.48 | 83.31       | 111.60   |
| 1   | A     | 411 | LEU  | CB-CA-C   | -10.15 | 90.91       | 110.20   |
| 1   | B     | 411 | LEU  | CB-CA-C   | -10.15 | 90.92       | 110.20   |
| 1   | A     | 122 | ASP  | CB-CG-OD1 | 10.10  | 127.39      | 118.30   |
| 1   | B     | 122 | ASP  | CB-CG-OD1 | 10.07  | 127.37      | 118.30   |
| 1   | A     | 366 | VAL  | CB-CA-C   | -9.83  | 92.73       | 111.40   |
| 1   | B     | 366 | VAL  | CB-CA-C   | -9.81  | 92.75       | 111.40   |
| 1   | B     | 452 | LEU  | CA-CB-CG  | -9.61  | 93.19       | 115.30   |
| 1   | A     | 452 | LEU  | CA-CB-CG  | -9.60  | 93.21       | 115.30   |
| 1   | A     | 202 | VAL  | CB-CA-C   | -8.86  | 94.56       | 111.40   |
| 1   | B     | 202 | VAL  | CB-CA-C   | -8.86  | 94.56       | 111.40   |
| 1   | A     | 316 | LEU  | CB-CG-CD2 | -8.80  | 96.04       | 111.00   |
| 1   | B     | 316 | LEU  | CB-CG-CD2 | -8.77  | 96.08       | 111.00   |
| 1   | B     | 460 | VAL  | CB-CA-C   | 8.74   | 128.02      | 111.40   |
| 1   | A     | 460 | VAL  | CB-CA-C   | 8.72   | 127.96      | 111.40   |
| 1   | B     | 97  | LEU  | CA-CB-CG  | -8.52  | 95.70       | 115.30   |
| 1   | A     | 97  | LEU  | CA-CB-CG  | -8.51  | 95.73       | 115.30   |
| 1   | A     | 129 | ARG  | N-CA-C    | 8.35   | 133.53      | 111.00   |
| 1   | B     | 129 | ARG  | N-CA-C    | 8.34   | 133.51      | 111.00   |
| 1   | B     | 518 | ASN  | N-CA-C    | 8.16   | 133.04      | 111.00   |
| 1   | A     | 518 | ASN  | N-CA-C    | 8.15   | 133.01      | 111.00   |
| 1   | B     | 457 | THR  | CB-CA-C   | -8.01  | 89.97       | 111.60   |
| 1   | A     | 457 | THR  | CB-CA-C   | -8.01  | 89.98       | 111.60   |
| 1   | B     | 242 | PHE  | C-N-CD    | -7.86  | 103.32      | 120.60   |
| 1   | A     | 242 | PHE  | C-N-CD    | -7.85  | 103.34      | 120.60   |
| 1   | B     | 142 | VAL  | CB-CA-C   | -7.56  | 97.03       | 111.40   |
| 1   | A     | 142 | VAL  | CB-CA-C   | -7.54  | 97.08       | 111.40   |
| 1   | B     | 244 | TYR  | CB-CA-C   | -7.51  | 95.38       | 110.40   |
| 1   | A     | 244 | TYR  | CB-CA-C   | -7.49  | 95.42       | 110.40   |
| 1   | B     | 473 | PHE  | N-CA-C    | -7.44  | 90.92       | 111.00   |
| 1   | A     | 473 | PHE  | N-CA-C    | -7.42  | 90.95       | 111.00   |
| 1   | B     | 558 | TRP  | N-CA-C    | 7.42   | 131.03      | 111.00   |
| 1   | A     | 558 | TRP  | N-CA-C    | 7.40   | 130.97      | 111.00   |
| 1   | A     | 162 | ASP  | CB-CA-C   | 7.38   | 125.17      | 110.40   |
| 1   | B     | 162 | ASP  | CB-CA-C   | 7.38   | 125.17      | 110.40   |
| 1   | A     | 195 | MET  | CA-CB-CG  | -7.37  | 100.78      | 113.30   |
| 1   | B     | 195 | MET  | CA-CB-CG  | -7.37  | 100.77      | 113.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 350 | ARG  | NE-CZ-NH2  | -7.31 | 116.65      | 120.30   |
| 1   | A     | 432 | SER  | N-CA-CB    | 7.30  | 121.45      | 110.50   |
| 1   | B     | 155 | LEU  | CA-CB-CG   | -7.29 | 98.52       | 115.30   |
| 1   | A     | 155 | LEU  | CA-CB-CG   | -7.29 | 98.54       | 115.30   |
| 1   | B     | 432 | SER  | N-CA-CB    | 7.29  | 121.43      | 110.50   |
| 1   | A     | 350 | ARG  | NE-CZ-NH2  | -7.27 | 116.66      | 120.30   |
| 1   | B     | 419 | ASN  | N-CA-C     | -7.15 | 91.70       | 111.00   |
| 1   | A     | 121 | LEU  | CA-CB-CG   | -7.15 | 98.86       | 115.30   |
| 1   | B     | 121 | LEU  | CA-CB-CG   | -7.15 | 98.86       | 115.30   |
| 1   | A     | 44  | ASP  | CB-CA-C    | 7.14  | 124.67      | 110.40   |
| 1   | A     | 327 | TYR  | CA-CB-CG   | 7.14  | 126.96      | 113.40   |
| 1   | B     | 72  | SER  | N-CA-C     | -7.14 | 91.73       | 111.00   |
| 1   | A     | 419 | ASN  | N-CA-C     | -7.13 | 91.74       | 111.00   |
| 1   | B     | 44  | ASP  | CB-CA-C    | 7.12  | 124.65      | 110.40   |
| 1   | A     | 511 | ASP  | CB-CG-OD1  | -7.12 | 111.89      | 118.30   |
| 1   | A     | 53  | LYS  | N-CA-CB    | 7.12  | 123.41      | 110.60   |
| 1   | A     | 72  | SER  | N-CA-C     | -7.12 | 91.79       | 111.00   |
| 1   | B     | 327 | TYR  | CA-CB-CG   | 7.11  | 126.91      | 113.40   |
| 1   | B     | 187 | TYR  | N-CA-C     | 7.09  | 130.16      | 111.00   |
| 1   | B     | 53  | LYS  | N-CA-CB    | 7.09  | 123.36      | 110.60   |
| 1   | A     | 187 | TYR  | N-CA-C     | 7.08  | 130.11      | 111.00   |
| 1   | B     | 430 | LYS  | CB-CA-C    | -7.05 | 96.29       | 110.40   |
| 1   | B     | 511 | ASP  | CB-CG-OD1  | -7.04 | 111.96      | 118.30   |
| 1   | A     | 430 | LYS  | CB-CA-C    | -7.03 | 96.33       | 110.40   |
| 1   | A     | 268 | TRP  | CB-CA-C    | -6.98 | 96.44       | 110.40   |
| 1   | B     | 268 | TRP  | CB-CA-C    | -6.97 | 96.45       | 110.40   |
| 1   | B     | 131 | LEU  | CA-CB-CG   | -6.97 | 99.27       | 115.30   |
| 1   | B     | 114 | ARG  | CB-CG-CD   | 6.96  | 129.68      | 111.60   |
| 1   | A     | 114 | ARG  | CB-CG-CD   | 6.95  | 129.68      | 111.60   |
| 1   | A     | 131 | LEU  | CA-CB-CG   | -6.95 | 99.32       | 115.30   |
| 1   | A     | 330 | ARG  | N-CA-CB    | -6.67 | 98.60       | 110.60   |
| 1   | B     | 330 | ARG  | N-CA-CB    | -6.65 | 98.62       | 110.60   |
| 1   | B     | 267 | ILE  | CB-CA-C    | -6.60 | 98.40       | 111.60   |
| 1   | B     | 306 | GLN  | N-CA-C     | 6.59  | 128.80      | 111.00   |
| 1   | A     | 267 | ILE  | CB-CA-C    | -6.59 | 98.42       | 111.60   |
| 1   | A     | 306 | GLN  | N-CA-C     | 6.59  | 128.79      | 111.00   |
| 1   | B     | 371 | ILE  | CG1-CB-CG2 | 6.57  | 125.85      | 111.40   |
| 1   | A     | 371 | ILE  | CG1-CB-CG2 | 6.57  | 125.84      | 111.40   |
| 1   | A     | 494 | ASP  | CB-CA-C    | -6.55 | 97.29       | 110.40   |
| 1   | B     | 363 | ILE  | CB-CA-C    | 6.54  | 124.69      | 111.60   |
| 1   | A     | 363 | ILE  | CB-CA-C    | 6.54  | 124.68      | 111.60   |
| 1   | B     | 478 | LEU  | CB-CA-C    | -6.54 | 97.77       | 110.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 494 | ASP  | CB-CA-C    | -6.53 | 97.33       | 110.40   |
| 1   | A     | 478 | LEU  | CB-CA-C    | -6.53 | 97.80       | 110.20   |
| 1   | B     | 130 | VAL  | N-CA-C     | -6.50 | 93.46       | 111.00   |
| 1   | A     | 130 | VAL  | N-CA-C     | -6.49 | 93.47       | 111.00   |
| 1   | B     | 241 | LEU  | CB-CA-C    | -6.48 | 97.89       | 110.20   |
| 1   | A     | 241 | LEU  | CB-CA-C    | -6.47 | 97.90       | 110.20   |
| 1   | A     | 414 | ILE  | CG1-CB-CG2 | 6.47  | 125.64      | 111.40   |
| 1   | B     | 414 | ILE  | CG1-CB-CG2 | 6.47  | 125.64      | 111.40   |
| 1   | A     | 62  | HIS  | N-CA-C     | 6.41  | 128.29      | 111.00   |
| 1   | B     | 62  | HIS  | N-CA-C     | 6.38  | 128.22      | 111.00   |
| 1   | B     | 87  | VAL  | CB-CA-C    | -6.35 | 99.34       | 111.40   |
| 1   | A     | 87  | VAL  | CB-CA-C    | -6.34 | 99.35       | 111.40   |
| 1   | A     | 164 | LEU  | N-CA-C     | 6.26  | 127.89      | 111.00   |
| 1   | A     | 476 | LYS  | CB-CA-C    | 6.26  | 122.91      | 110.40   |
| 1   | B     | 476 | LYS  | CB-CA-C    | 6.25  | 122.91      | 110.40   |
| 1   | B     | 164 | LEU  | N-CA-C     | 6.25  | 127.88      | 111.00   |
| 1   | A     | 384 | TYR  | CA-CB-CG   | 6.22  | 125.22      | 113.40   |
| 1   | A     | 410 | GLU  | N-CA-C     | 6.21  | 127.78      | 111.00   |
| 1   | B     | 384 | TYR  | CA-CB-CG   | 6.21  | 125.21      | 113.40   |
| 1   | B     | 410 | GLU  | N-CA-C     | 6.19  | 127.70      | 111.00   |
| 1   | A     | 396 | ARG  | CG-CD-NE   | -6.18 | 98.81       | 111.80   |
| 1   | B     | 396 | ARG  | CG-CD-NE   | -6.17 | 98.85       | 111.80   |
| 1   | A     | 185 | VAL  | CB-CA-C    | -6.16 | 99.70       | 111.40   |
| 1   | A     | 67  | ASP  | N-CA-CB    | -6.15 | 99.53       | 110.60   |
| 1   | B     | 67  | ASP  | N-CA-CB    | -6.15 | 99.53       | 110.60   |
| 1   | B     | 185 | VAL  | CB-CA-C    | -6.15 | 99.72       | 111.40   |
| 1   | A     | 304 | ALA  | N-CA-C     | -6.14 | 94.43       | 111.00   |
| 1   | B     | 304 | ALA  | N-CA-C     | -6.14 | 94.43       | 111.00   |
| 1   | A     | 541 | ILE  | CB-CA-C    | -6.11 | 99.37       | 111.60   |
| 1   | B     | 166 | LEU  | CB-CG-CD1  | 6.10  | 121.37      | 111.00   |
| 1   | B     | 541 | ILE  | CB-CA-C    | -6.09 | 99.42       | 111.60   |
| 1   | A     | 166 | LEU  | CB-CG-CD1  | 6.08  | 121.34      | 111.00   |
| 1   | A     | 155 | LEU  | CB-CA-C    | -6.06 | 98.68       | 110.20   |
| 1   | B     | 387 | GLU  | N-CA-CB    | -6.05 | 99.70       | 110.60   |
| 1   | A     | 452 | LEU  | N-CA-C     | 6.05  | 127.34      | 111.00   |
| 1   | B     | 155 | LEU  | CB-CA-C    | -6.05 | 98.70       | 110.20   |
| 1   | A     | 387 | GLU  | N-CA-CB    | -6.04 | 99.72       | 110.60   |
| 1   | B     | 452 | LEU  | N-CA-C     | 6.04  | 127.31      | 111.00   |
| 1   | B     | 425 | PHE  | CB-CA-C    | 6.04  | 122.48      | 110.40   |
| 1   | A     | 425 | PHE  | CB-CA-C    | 6.03  | 122.46      | 110.40   |
| 1   | B     | 231 | GLU  | CA-CB-CG   | -6.01 | 100.17      | 113.40   |
| 1   | A     | 231 | GLU  | CA-CB-CG   | -6.01 | 100.19      | 113.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 442 | VAL  | CB-CA-C   | -5.97 | 100.06      | 111.40   |
| 1   | B     | 312 | ARG  | CB-CG-CD  | -5.96 | 96.10       | 111.60   |
| 1   | A     | 312 | ARG  | CB-CG-CD  | -5.96 | 96.10       | 111.60   |
| 1   | A     | 442 | VAL  | CB-CA-C   | -5.96 | 100.08      | 111.40   |
| 1   | A     | 10  | LEU  | CB-CA-C   | -5.95 | 98.89       | 110.20   |
| 1   | B     | 10  | LEU  | CB-CA-C   | -5.95 | 98.90       | 110.20   |
| 1   | B     | 473 | PHE  | CA-C-N    | -5.88 | 104.26      | 117.20   |
| 1   | A     | 473 | PHE  | CA-C-N    | -5.88 | 104.27      | 117.20   |
| 1   | B     | 525 | LEU  | CA-CB-CG  | -5.87 | 101.79      | 115.30   |
| 1   | A     | 525 | LEU  | CA-CB-CG  | -5.86 | 101.83      | 115.30   |
| 1   | B     | 312 | ARG  | N-CA-C    | 5.85  | 126.80      | 111.00   |
| 1   | A     | 312 | ARG  | N-CA-C    | 5.85  | 126.78      | 111.00   |
| 1   | B     | 177 | LEU  | CB-CA-C   | 5.84  | 121.30      | 110.20   |
| 1   | B     | 204 | LEU  | CA-CB-CG  | -5.84 | 101.86      | 115.30   |
| 1   | A     | 177 | LEU  | CB-CA-C   | 5.83  | 121.28      | 110.20   |
| 1   | B     | 301 | LEU  | CB-CG-CD1 | 5.83  | 120.92      | 111.00   |
| 1   | A     | 204 | LEU  | CA-CB-CG  | -5.83 | 101.90      | 115.30   |
| 1   | A     | 301 | LEU  | CB-CG-CD1 | 5.83  | 120.90      | 111.00   |
| 1   | A     | 228 | LEU  | CB-CG-CD2 | -5.81 | 101.12      | 111.00   |
| 1   | A     | 458 | PHE  | CB-CA-C   | -5.80 | 98.79       | 110.40   |
| 1   | B     | 228 | LEU  | CB-CG-CD2 | -5.80 | 101.14      | 111.00   |
| 1   | B     | 413 | TRP  | CA-CB-CG  | 5.79  | 124.69      | 113.70   |
| 1   | B     | 458 | PHE  | CB-CA-C   | -5.78 | 98.84       | 110.40   |
| 1   | B     | 388 | ASP  | CB-CG-OD1 | -5.78 | 113.10      | 118.30   |
| 1   | A     | 413 | TRP  | CA-CB-CG  | 5.76  | 124.65      | 113.70   |
| 1   | A     | 444 | LYS  | N-CA-CB   | -5.76 | 100.23      | 110.60   |
| 1   | B     | 444 | LYS  | N-CA-CB   | -5.76 | 100.23      | 110.60   |
| 1   | A     | 388 | ASP  | CB-CG-OD1 | -5.75 | 113.12      | 118.30   |
| 1   | B     | 323 | ASP  | CB-CG-OD1 | -5.75 | 113.13      | 118.30   |
| 1   | A     | 323 | ASP  | CB-CG-OD1 | -5.72 | 113.15      | 118.30   |
| 1   | B     | 432 | SER  | N-CA-C    | -5.70 | 95.60       | 111.00   |
| 1   | A     | 432 | SER  | N-CA-C    | -5.69 | 95.63       | 111.00   |
| 1   | B     | 350 | ARG  | N-CA-C    | -5.67 | 95.68       | 111.00   |
| 1   | A     | 350 | ARG  | N-CA-C    | -5.67 | 95.69       | 111.00   |
| 1   | A     | 536 | ASP  | C-N-CD    | -5.67 | 108.12      | 120.60   |
| 1   | B     | 536 | ASP  | C-N-CD    | -5.66 | 108.15      | 120.60   |
| 1   | A     | 49  | GLY  | N-CA-C    | 5.65  | 127.23      | 113.10   |
| 1   | B     | 49  | GLY  | N-CA-C    | 5.64  | 127.21      | 113.10   |
| 1   | A     | 270 | MET  | CA-CB-CG  | -5.64 | 103.71      | 113.30   |
| 1   | B     | 384 | TYR  | CB-CA-C   | -5.64 | 99.12       | 110.40   |
| 1   | A     | 259 | MET  | CA-CB-CG  | -5.64 | 103.72      | 113.30   |
| 1   | A     | 384 | TYR  | CB-CA-C   | -5.64 | 99.13       | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 270 | MET  | CA-CB-CG  | -5.62 | 103.74      | 113.30   |
| 1   | B     | 259 | MET  | CA-CB-CG  | -5.62 | 103.75      | 113.30   |
| 1   | A     | 511 | ASP  | CB-CG-OD2 | 5.60  | 123.34      | 118.30   |
| 1   | B     | 211 | ARG  | NE-CZ-NH1 | -5.59 | 117.50      | 120.30   |
| 1   | A     | 211 | ARG  | NE-CZ-NH1 | -5.59 | 117.50      | 120.30   |
| 1   | B     | 315 | LEU  | CB-CG-CD2 | -5.59 | 101.50      | 111.00   |
| 1   | A     | 315 | LEU  | CB-CG-CD2 | -5.59 | 101.50      | 111.00   |
| 1   | A     | 383 | PHE  | N-CA-C    | 5.57  | 126.05      | 111.00   |
| 1   | B     | 217 | LEU  | N-CA-C    | -5.57 | 95.97       | 111.00   |
| 1   | B     | 383 | PHE  | N-CA-C    | 5.57  | 126.03      | 111.00   |
| 1   | A     | 217 | LEU  | N-CA-C    | -5.56 | 96.00       | 111.00   |
| 1   | A     | 129 | ARG  | CB-CA-C   | -5.55 | 99.30       | 110.40   |
| 1   | B     | 233 | GLN  | N-CA-CB   | -5.55 | 100.62      | 110.60   |
| 1   | A     | 233 | GLN  | N-CA-CB   | -5.54 | 100.62      | 110.60   |
| 1   | B     | 129 | ARG  | CB-CA-C   | -5.54 | 99.32       | 110.40   |
| 1   | A     | 98  | TRP  | CA-CB-CG  | -5.53 | 103.19      | 113.70   |
| 1   | A     | 165 | TRP  | N-CA-C    | 5.53  | 125.94      | 111.00   |
| 1   | B     | 98  | TRP  | CA-CB-CG  | -5.52 | 103.21      | 113.70   |
| 1   | B     | 165 | TRP  | N-CA-C    | 5.50  | 125.86      | 111.00   |
| 1   | B     | 384 | TYR  | N-CA-C    | 5.49  | 125.82      | 111.00   |
| 1   | A     | 384 | TYR  | N-CA-C    | 5.49  | 125.81      | 111.00   |
| 1   | B     | 511 | ASP  | CB-CG-OD2 | 5.48  | 123.23      | 118.30   |
| 1   | A     | 558 | TRP  | CA-CB-CG  | -5.46 | 103.33      | 113.70   |
| 1   | B     | 558 | TRP  | CA-CB-CG  | -5.45 | 103.34      | 113.70   |
| 1   | A     | 504 | ARG  | NE-CZ-NH2 | 5.44  | 123.02      | 120.30   |
| 1   | B     | 104 | ARG  | NE-CZ-NH1 | 5.44  | 123.02      | 120.30   |
| 1   | B     | 430 | LYS  | CB-CG-CD  | -5.43 | 97.48       | 111.60   |
| 1   | A     | 430 | LYS  | CB-CG-CD  | -5.42 | 97.50       | 111.60   |
| 1   | A     | 104 | ARG  | NE-CZ-NH1 | 5.42  | 123.01      | 120.30   |
| 1   | A     | 264 | LYS  | CB-CA-C   | -5.40 | 99.60       | 110.40   |
| 1   | B     | 264 | LYS  | CB-CA-C   | -5.38 | 99.63       | 110.40   |
| 1   | B     | 204 | LEU  | CB-CA-C   | -5.37 | 99.99       | 110.20   |
| 1   | A     | 204 | LEU  | CB-CA-C   | -5.37 | 100.00      | 110.20   |
| 1   | A     | 7   | PHE  | N-CA-C    | 5.35  | 125.44      | 111.00   |
| 1   | A     | 204 | LEU  | CB-CG-CD2 | -5.35 | 101.91      | 111.00   |
| 1   | A     | 236 | SER  | N-CA-CB   | -5.35 | 102.48      | 110.50   |
| 1   | B     | 7   | PHE  | N-CA-C    | 5.33  | 125.41      | 111.00   |
| 1   | B     | 204 | LEU  | CB-CG-CD2 | -5.33 | 101.94      | 111.00   |
| 1   | B     | 504 | ARG  | NE-CZ-NH2 | 5.33  | 122.97      | 120.30   |
| 1   | B     | 454 | PHE  | N-CA-C    | -5.32 | 96.63       | 111.00   |
| 1   | A     | 454 | PHE  | N-CA-C    | -5.31 | 96.67       | 111.00   |
| 1   | B     | 236 | SER  | N-CA-CB   | -5.31 | 102.54      | 110.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 452 | LEU  | CB-CA-C    | -5.29 | 100.14      | 110.20   |
| 1   | B     | 452 | LEU  | CB-CA-C    | -5.29 | 100.16      | 110.20   |
| 1   | A     | 507 | LEU  | CB-CA-C    | -5.26 | 100.21      | 110.20   |
| 1   | B     | 279 | TYR  | CB-CG-CD1  | -5.25 | 117.85      | 121.00   |
| 1   | B     | 507 | LEU  | CB-CA-C    | -5.23 | 100.27      | 110.20   |
| 1   | A     | 279 | TYR  | CB-CG-CD1  | -5.20 | 117.88      | 121.00   |
| 1   | B     | 560 | LEU  | CB-CG-CD1  | 5.19  | 119.83      | 111.00   |
| 1   | A     | 560 | LEU  | CB-CG-CD1  | 5.19  | 119.82      | 111.00   |
| 1   | B     | 346 | LEU  | N-CA-C     | 5.18  | 124.98      | 111.00   |
| 1   | B     | 11  | THR  | CB-CA-C    | -5.16 | 97.66       | 111.60   |
| 1   | A     | 346 | LEU  | N-CA-C     | 5.16  | 124.94      | 111.00   |
| 1   | A     | 11  | THR  | CB-CA-C    | -5.15 | 97.69       | 111.60   |
| 1   | B     | 13  | PRO  | N-CA-C     | -5.15 | 98.70       | 112.10   |
| 1   | A     | 55  | THR  | N-CA-CB    | 5.14  | 120.07      | 110.30   |
| 1   | A     | 211 | ARG  | NE-CZ-NH2  | 5.14  | 122.87      | 120.30   |
| 1   | A     | 13  | PRO  | N-CA-C     | -5.13 | 98.75       | 112.10   |
| 1   | B     | 399 | ASP  | CB-CG-OD2  | 5.13  | 122.92      | 118.30   |
| 1   | B     | 55  | THR  | N-CA-CB    | 5.12  | 120.03      | 110.30   |
| 1   | B     | 503 | TYR  | CB-CG-CD1  | 5.12  | 124.07      | 121.00   |
| 1   | B     | 211 | ARG  | NE-CZ-NH2  | 5.11  | 122.86      | 120.30   |
| 1   | B     | 133 | VAL  | N-CA-C     | -5.10 | 97.22       | 111.00   |
| 1   | A     | 121 | LEU  | CB-CG-CD1  | -5.10 | 102.34      | 111.00   |
| 1   | A     | 133 | VAL  | N-CA-C     | -5.10 | 97.24       | 111.00   |
| 1   | B     | 121 | LEU  | CB-CG-CD1  | -5.09 | 102.34      | 111.00   |
| 1   | A     | 353 | PHE  | N-CA-C     | 5.08  | 124.72      | 111.00   |
| 1   | B     | 353 | PHE  | N-CA-C     | 5.08  | 124.71      | 111.00   |
| 1   | A     | 399 | ASP  | CB-CG-OD2  | 5.07  | 122.86      | 118.30   |
| 1   | A     | 503 | TYR  | CB-CG-CD1  | 5.07  | 124.04      | 121.00   |
| 1   | B     | 424 | PHE  | CB-CA-C    | -5.06 | 100.28      | 110.40   |
| 1   | A     | 424 | PHE  | CB-CA-C    | -5.06 | 100.29      | 110.40   |
| 1   | A     | 156 | GLU  | OE1-CD-OE2 | -5.05 | 117.24      | 123.30   |
| 1   | A     | 453 | ASP  | CB-CG-OD1  | -5.04 | 113.76      | 118.30   |
| 1   | B     | 209 | LEU  | CB-CG-CD2  | -5.04 | 102.43      | 111.00   |
| 1   | B     | 15  | LYS  | N-CA-CB    | -5.04 | 101.53      | 110.60   |
| 1   | A     | 15  | LYS  | N-CA-CB    | -5.04 | 101.54      | 110.60   |
| 1   | A     | 209 | LEU  | CB-CG-CD2  | -5.03 | 102.45      | 111.00   |
| 1   | B     | 165 | TRP  | CA-C-N     | -5.02 | 106.15      | 117.20   |
| 1   | B     | 156 | GLU  | OE1-CD-OE2 | -5.02 | 117.28      | 123.30   |
| 1   | B     | 288 | ASP  | CB-CA-C    | 5.01  | 120.42      | 110.40   |
| 1   | B     | 401 | THR  | CB-CA-C    | 5.01  | 125.12      | 111.60   |
| 1   | A     | 165 | TRP  | CA-C-N     | -5.00 | 106.19      | 117.20   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 363 | ILE  | CA   |
| 1   | A     | 410 | GLU  | CA   |
| 1   | B     | 363 | ILE  | CA   |
| 1   | B     | 410 | GLU  | CA   |

There are no planarity outliers.

## 5.2 Close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4391  | 0        | 4330     | 550     | 0            |
| 1   | B     | 4391  | 0        | 4330     | 552     | 0            |
| 2   | A     | 53    | 0        | 31       | 17      | 0            |
| 2   | B     | 53    | 0        | 31       | 18      | 0            |
| 3   | A     | 11    | 0        | 7        | 4       | 0            |
| 3   | B     | 11    | 0        | 7        | 5       | 0            |
| 4   | A     | 14    | 0        | 0        | 2       | 0            |
| 4   | B     | 24    | 0        | 0        | 0       | 0            |
| All | All   | 8948  | 0        | 8736     | 1088    | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 63.

All (1088) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:422:HIS:NE2  | 2:B:600:FAD:HM81 | 1.45        | 1.12     |
| 1:A:422:HIS:NE2  | 2:A:600:FAD:HM82 | 1.42        | 1.10     |
| 2:B:600:FAD:H8A  | 2:B:600:FAD:H51A | 1.27        | 1.08     |
| 1:A:422:HIS:NE2  | 2:A:600:FAD:HM81 | 1.45        | 1.08     |
| 2:A:600:FAD:H8A  | 2:A:600:FAD:H51A | 1.27        | 1.08     |
| 1:B:422:HIS:NE2  | 2:B:600:FAD:HM82 | 1.42        | 1.08     |
| 1:B:550:PRO:HB2  | 1:B:552:GLN:HE21 | 1.18        | 1.08     |
| 1:A:253:LEU:HD21 | 1:B:253:LEU:HD21 | 1.31        | 1.07     |
| 1:B:177:LEU:HD22 | 1:B:265:ILE:HG22 | 1.35        | 1.07     |
| 1:A:177:LEU:HD22 | 1:A:265:ILE:HG22 | 1.35        | 1.05     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:550:PRO:HB2  | 1:A:552:GLN:HE21 | 1.18        | 1.05     |
| 1:B:361:GLU:N    | 1:B:364:ARG:HH21 | 1.57        | 1.02     |
| 1:A:422:HIS:CE1  | 2:A:600:FAD:HM81 | 1.95        | 1.01     |
| 1:A:361:GLU:N    | 1:A:364:ARG:HH21 | 1.57        | 1.01     |
| 1:B:422:HIS:CE1  | 2:B:600:FAD:HM81 | 1.95        | 1.00     |
| 1:A:422:HIS:CE1  | 2:A:600:FAD:C8M  | 2.46        | 0.99     |
| 1:B:422:HIS:CE1  | 2:B:600:FAD:C8M  | 2.46        | 0.98     |
| 1:A:133:VAL:HG21 | 1:A:154:TYR:CE1  | 2.00        | 0.97     |
| 1:B:133:VAL:HG21 | 1:B:154:TYR:CE1  | 2.00        | 0.97     |
| 1:A:422:HIS:CD2  | 2:A:600:FAD:HM82 | 2.02        | 0.94     |
| 1:B:422:HIS:CD2  | 2:B:600:FAD:HM82 | 2.02        | 0.93     |
| 1:B:78:ARG:HD3   | 1:B:82:ASP:OD2   | 1.69        | 0.93     |
| 1:B:40:ILE:HD11  | 1:B:57:THR:HG22  | 1.50        | 0.92     |
| 1:A:478:LEU:H    | 1:A:478:LEU:HD12 | 1.35        | 0.92     |
| 1:A:40:ILE:HD11  | 1:A:57:THR:HG22  | 1.50        | 0.91     |
| 1:A:78:ARG:HD3   | 1:A:82:ASP:OD2   | 1.69        | 0.91     |
| 1:B:419:ASN:O    | 1:B:474:ASN:HA   | 1.71        | 0.90     |
| 1:A:419:ASN:O    | 1:A:474:ASN:HA   | 1.71        | 0.90     |
| 1:B:478:LEU:HD12 | 1:B:478:LEU:H    | 1.35        | 0.90     |
| 1:B:56:HIS:HA    | 1:B:111:ALA:CB   | 2.03        | 0.89     |
| 1:A:91:ASN:ND2   | 1:A:538:ASN:HD22 | 1.71        | 0.88     |
| 1:B:205:ALA:HA   | 1:B:541:ILE:HD11 | 1.56        | 0.88     |
| 1:A:300:ARG:HH21 | 1:A:308:VAL:HA   | 1.37        | 0.88     |
| 1:A:205:ALA:HA   | 1:A:541:ILE:HD11 | 1.55        | 0.88     |
| 1:A:56:HIS:HA    | 1:A:111:ALA:CB   | 2.03        | 0.87     |
| 1:B:555:HIS:CG   | 1:B:559:LYS:HE3  | 2.09        | 0.87     |
| 1:B:91:ASN:ND2   | 1:B:538:ASN:HD22 | 1.71        | 0.87     |
| 1:A:443:THR:HA   | 1:A:491:LEU:HD21 | 1.57        | 0.86     |
| 1:A:555:HIS:CG   | 1:A:559:LYS:HE3  | 2.09        | 0.86     |
| 1:B:443:THR:HA   | 1:B:491:LEU:HD21 | 1.57        | 0.86     |
| 1:B:300:ARG:HH21 | 1:B:308:VAL:HA   | 1.37        | 0.86     |
| 1:A:457:THR:HG22 | 1:A:458:PHE:H    | 1.39        | 0.85     |
| 1:B:423:LEU:HD21 | 1:B:488:MET:HG3  | 1.57        | 0.85     |
| 1:B:457:THR:HG22 | 1:B:458:PHE:H    | 1.39        | 0.84     |
| 1:A:423:LEU:HD21 | 1:A:488:MET:HG3  | 1.57        | 0.84     |
| 2:A:600:FAD:H8A  | 2:A:600:FAD:C5B  | 2.08        | 0.84     |
| 1:A:431:VAL:HG22 | 1:A:465:MET:HG3  | 1.60        | 0.83     |
| 1:A:425:PHE:HB2  | 1:A:488:MET:CE   | 2.09        | 0.83     |
| 1:B:550:PRO:HB2  | 1:B:552:GLN:NE2  | 1.94        | 0.82     |
| 2:B:600:FAD:C5B  | 2:B:600:FAD:H8A  | 2.08        | 0.82     |
| 1:A:40:ILE:CD1   | 1:A:57:THR:HG22  | 2.10        | 0.82     |
| 1:B:550:PRO:CB   | 1:B:552:GLN:HE21 | 1.93        | 0.81     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:431:VAL:HG22 | 1:B:465:MET:HG3  | 1.60        | 0.81     |
| 1:A:247:GLY:O    | 1:B:183:ARG:NH2  | 2.12        | 0.81     |
| 1:B:425:PHE:HB2  | 1:B:488:MET:CE   | 2.09        | 0.81     |
| 1:A:459:THR:OG1  | 1:A:466:HIS:HB2  | 1.81        | 0.81     |
| 1:A:505:THR:HG22 | 1:A:506:HIS:H    | 1.45        | 0.81     |
| 1:A:156:GLU:HG3  | 1:A:161:ARG:CZ   | 2.10        | 0.80     |
| 1:A:550:PRO:CB   | 1:A:552:GLN:HE21 | 1.94        | 0.80     |
| 1:B:40:ILE:CD1   | 1:B:57:THR:HG22  | 2.10        | 0.80     |
| 1:B:505:THR:HG22 | 1:B:506:HIS:H    | 1.45        | 0.80     |
| 1:A:295:ILE:O    | 1:A:298:PRO:HD2  | 1.81        | 0.80     |
| 1:A:275:GLY:HA3  | 1:A:359:GLY:O    | 1.81        | 0.80     |
| 1:B:277:GLN:HB3  | 1:B:357:LEU:HD12 | 1.62        | 0.80     |
| 1:B:156:GLU:HG3  | 1:B:161:ARG:CZ   | 2.11        | 0.80     |
| 1:A:277:GLN:HB3  | 1:A:357:LEU:HD12 | 1.62        | 0.80     |
| 1:B:459:THR:OG1  | 1:B:466:HIS:HB2  | 1.81        | 0.80     |
| 1:B:295:ILE:O    | 1:B:298:PRO:HD2  | 1.81        | 0.80     |
| 2:A:600:FAD:C8A  | 2:A:600:FAD:H51A | 2.11        | 0.79     |
| 1:A:550:PRO:HB2  | 1:A:552:GLN:NE2  | 1.94        | 0.79     |
| 1:B:10:LEU:HD11  | 1:B:42:SER:HA    | 1.64        | 0.79     |
| 1:B:361:GLU:HG3  | 1:B:361:GLU:O    | 1.77        | 0.79     |
| 1:A:57:THR:O     | 1:A:70:LEU:HD12  | 1.83        | 0.79     |
| 1:A:378:ILE:O    | 1:A:381:VAL:HB   | 1.83        | 0.79     |
| 1:B:275:GLY:HA3  | 1:B:359:GLY:O    | 1.81        | 0.79     |
| 1:B:414:ILE:HD11 | 2:B:600:FAD:HM71 | 1.64        | 0.79     |
| 1:A:94:SER:HA    | 1:A:540:ILE:HD11 | 1.66        | 0.78     |
| 1:B:57:THR:O     | 1:B:70:LEU:HD12  | 1.83        | 0.78     |
| 1:B:378:ILE:O    | 1:B:381:VAL:HB   | 1.83        | 0.78     |
| 1:B:48:ASP:OD1   | 1:B:60:PRO:HA    | 1.84        | 0.78     |
| 1:A:377:ALA:O    | 1:A:379:PRO:HD3  | 1.84        | 0.78     |
| 1:A:414:ILE:HD11 | 2:A:600:FAD:HM71 | 1.64        | 0.78     |
| 1:A:132:GLU:HG2  | 1:A:133:VAL:N    | 1.99        | 0.78     |
| 1:A:10:LEU:HD11  | 1:A:42:SER:HA    | 1.64        | 0.77     |
| 1:A:479:ILE:O    | 1:A:483:LYS:HG3  | 1.84        | 0.77     |
| 1:B:377:ALA:O    | 1:B:379:PRO:HD3  | 1.84        | 0.77     |
| 1:A:85:SER:O     | 1:A:89:LEU:HD13  | 1.85        | 0.77     |
| 1:B:134:ASN:OD1  | 1:B:137:GLY:N    | 2.17        | 0.77     |
| 1:A:361:GLU:HG3  | 1:A:361:GLU:O    | 1.77        | 0.77     |
| 1:B:132:GLU:HG2  | 1:B:133:VAL:N    | 1.99        | 0.77     |
| 1:A:32:VAL:HA    | 1:A:78:ARG:HD2   | 1.67        | 0.77     |
| 1:B:56:HIS:HA    | 1:B:111:ALA:HB1  | 1.67        | 0.77     |
| 1:B:479:ILE:O    | 1:B:483:LYS:HG3  | 1.84        | 0.77     |
| 1:A:507:LEU:HD23 | 1:A:510:MET:HE3  | 1.67        | 0.77     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:85:SER:O     | 1:B:89:LEU:HD13  | 1.85        | 0.77     |
| 2:B:600:FAD:C8A  | 2:B:600:FAD:H51A | 2.11        | 0.76     |
| 1:A:357:LEU:HB3  | 1:A:364:ARG:HG2  | 1.66        | 0.76     |
| 1:A:48:ASP:OD1   | 1:A:60:PRO:HA    | 1.84        | 0.76     |
| 1:A:102:ILE:HG12 | 1:A:175:SER:HB2  | 1.68        | 0.76     |
| 1:B:357:LEU:HB3  | 1:B:364:ARG:HG2  | 1.66        | 0.76     |
| 1:B:94:SER:HA    | 1:B:540:ILE:HD11 | 1.66        | 0.76     |
| 1:A:425:PHE:HB2  | 1:A:488:MET:HE1  | 1.66        | 0.76     |
| 1:A:56:HIS:HA    | 1:A:111:ALA:HB1  | 1.66        | 0.76     |
| 1:B:507:LEU:HD23 | 1:B:510:MET:HE3  | 1.68        | 0.75     |
| 1:A:134:ASN:OD1  | 1:A:137:GLY:N    | 2.17        | 0.75     |
| 1:B:32:VAL:HA    | 1:B:78:ARG:HD2   | 1.67        | 0.75     |
| 1:A:443:THR:HA   | 1:A:491:LEU:CD2  | 2.17        | 0.75     |
| 1:A:183:ARG:NH2  | 1:B:247:GLY:O    | 2.20        | 0.75     |
| 1:B:443:THR:HA   | 1:B:491:LEU:CD2  | 2.17        | 0.75     |
| 1:A:423:LEU:HD21 | 1:A:488:MET:CG   | 2.16        | 0.74     |
| 1:A:248:PRO:HD3  | 1:B:256:GLN:O    | 1.87        | 0.74     |
| 1:A:244:TYR:OH   | 1:B:195:MET:HG3  | 1.86        | 0.74     |
| 1:B:423:LEU:HD21 | 1:B:488:MET:CG   | 2.16        | 0.74     |
| 2:B:600:FAD:N5   | 3:B:601:EUG:H7   | 2.02        | 0.74     |
| 1:B:527:PHE:CE2  | 1:B:531:LEU:HD11 | 2.23        | 0.74     |
| 1:A:79:ASN:HD21  | 1:A:81:ALA:HB3   | 1.52        | 0.74     |
| 1:B:79:ASN:HD21  | 1:B:81:ALA:HB3   | 1.52        | 0.74     |
| 1:A:527:PHE:CE2  | 1:A:531:LEU:HD11 | 2.23        | 0.74     |
| 2:A:600:FAD:N5   | 3:A:601:EUG:H7   | 2.02        | 0.74     |
| 1:B:385:PHE:HB3  | 1:B:386:PRO:HD2  | 1.70        | 0.74     |
| 1:A:284:PRO:HD2  | 1:A:288:ASP:OD2  | 1.87        | 0.73     |
| 1:B:361:GLU:N    | 1:B:364:ARG:NH2  | 2.36        | 0.73     |
| 1:B:507:LEU:HA   | 1:B:510:MET:CE   | 2.18        | 0.73     |
| 1:B:284:PRO:HD2  | 1:B:288:ASP:OD2  | 1.87        | 0.73     |
| 1:B:419:ASN:H    | 1:B:474:ASN:ND2  | 1.86        | 0.73     |
| 1:A:244:TYR:CD2  | 1:B:183:ARG:HD2  | 2.23        | 0.73     |
| 1:B:102:ILE:HG12 | 1:B:175:SER:HB2  | 1.68        | 0.73     |
| 1:A:339:LEU:HD12 | 1:A:350:ARG:CZ   | 2.19        | 0.73     |
| 1:A:205:ALA:CA   | 1:A:541:ILE:HD11 | 2.19        | 0.73     |
| 1:A:507:LEU:HA   | 1:A:510:MET:CE   | 2.18        | 0.73     |
| 1:A:487:LEU:HD11 | 1:A:491:LEU:HD11 | 1.70        | 0.73     |
| 1:B:102:ILE:CG1  | 1:B:175:SER:HB2  | 2.19        | 0.73     |
| 1:A:419:ASN:H    | 1:A:474:ASN:ND2  | 1.86        | 0.72     |
| 1:A:102:ILE:CG1  | 1:A:175:SER:HB2  | 2.19        | 0.72     |
| 1:B:52:MET:O     | 1:B:53:LYS:HG3   | 1.90        | 0.72     |
| 1:A:187:TYR:O    | 1:A:307:ASN:HB2  | 1.89        | 0.72     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:187:TYR:O    | 1:B:307:ASN:HB2  | 1.89        | 0.72     |
| 1:B:96:PRO:O     | 1:B:97:LEU:HD23  | 1.89        | 0.72     |
| 1:A:487:LEU:HG   | 1:A:491:LEU:HD12 | 1.72        | 0.72     |
| 1:B:425:PHE:CZ   | 1:B:427:PRO:HG3  | 2.25        | 0.72     |
| 1:A:418:PRO:HD2  | 1:A:474:ASN:HD22 | 1.53        | 0.72     |
| 1:B:312:ARG:HH22 | 1:B:410:GLU:CD   | 1.93        | 0.72     |
| 1:B:418:PRO:HD2  | 1:B:474:ASN:HD22 | 1.53        | 0.72     |
| 1:B:487:LEU:HD11 | 1:B:491:LEU:HD11 | 1.71        | 0.72     |
| 1:B:223:PRO:HG2  | 1:B:224:GLU:OE2  | 1.89        | 0.72     |
| 1:A:425:PHE:CZ   | 1:A:427:PRO:HG3  | 2.25        | 0.72     |
| 1:B:339:LEU:HD12 | 1:B:350:ARG:CZ   | 2.19        | 0.72     |
| 1:A:223:PRO:HG2  | 1:A:224:GLU:OE2  | 1.89        | 0.71     |
| 1:B:205:ALA:CA   | 1:B:541:ILE:HD11 | 2.19        | 0.71     |
| 1:A:550:PRO:HG2  | 1:A:553:TYR:CD1  | 2.26        | 0.71     |
| 1:B:13:PRO:HG2   | 1:B:16:LEU:HB2   | 1.72        | 0.71     |
| 1:A:183:ARG:HD2  | 1:B:244:TYR:CD2  | 2.26        | 0.71     |
| 2:B:600:FAD:C5X  | 3:B:601:EUG:H7   | 2.21        | 0.71     |
| 1:B:217:LEU:O    | 1:B:236:SER:HB2  | 1.91        | 0.71     |
| 1:A:52:MET:O     | 1:A:53:LYS:HG3   | 1.90        | 0.71     |
| 1:B:18:LEU:HD12  | 1:B:21:PHE:HB3   | 1.73        | 0.71     |
| 1:A:96:PRO:O     | 1:A:97:LEU:HD23  | 1.89        | 0.71     |
| 1:B:309:PRO:HG2  | 1:B:460:VAL:HB   | 1.73        | 0.71     |
| 1:A:385:PHE:HB3  | 1:A:386:PRO:HD2  | 1.70        | 0.71     |
| 1:A:299:LEU:HB2  | 1:A:305:LEU:HD12 | 1.72        | 0.71     |
| 1:A:238:ILE:HG21 | 1:B:428:ILE:HG21 | 1.72        | 0.71     |
| 1:A:217:LEU:O    | 1:A:236:SER:HB2  | 1.91        | 0.71     |
| 2:A:600:FAD:C5X  | 3:A:601:EUG:H7   | 2.21        | 0.71     |
| 1:B:61:HIS:ND1   | 1:B:422:HIS:ND1  | 2.39        | 0.71     |
| 1:B:55:THR:HG21  | 1:B:58:HIS:CE1   | 2.26        | 0.71     |
| 1:A:21:PHE:O     | 1:A:25:ILE:HG22  | 1.91        | 0.70     |
| 1:A:309:PRO:HG2  | 1:A:460:VAL:HB   | 1.73        | 0.70     |
| 1:B:487:LEU:HG   | 1:B:491:LEU:HD12 | 1.72        | 0.70     |
| 1:B:200:MET:HE1  | 1:B:251:ASP:HB3  | 1.73        | 0.70     |
| 1:B:21:PHE:O     | 1:B:25:ILE:HG22  | 1.91        | 0.70     |
| 1:B:391:GLU:HA   | 1:B:396:ARG:HD2  | 1.73        | 0.70     |
| 1:B:550:PRO:HG2  | 1:B:553:TYR:CD1  | 2.26        | 0.70     |
| 1:B:292:ALA:O    | 1:B:296:ILE:HG13 | 1.91        | 0.70     |
| 1:A:312:ARG:HH22 | 1:A:410:GLU:CD   | 1.93        | 0.70     |
| 1:B:299:LEU:HB2  | 1:B:305:LEU:HD12 | 1.72        | 0.70     |
| 1:B:507:LEU:HA   | 1:B:510:MET:HE3  | 1.73        | 0.70     |
| 1:A:391:GLU:HA   | 1:A:396:ARG:HD2  | 1.73        | 0.70     |
| 1:A:61:HIS:ND1   | 1:A:422:HIS:ND1  | 2.39        | 0.69     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:422:HIS:CE1  | 2:B:600:FAD:HM82 | 2.21        | 0.69     |
| 1:A:361:GLU:N    | 1:A:364:ARG:NH2  | 2.35        | 0.69     |
| 1:A:292:ALA:O    | 1:A:296:ILE:HG13 | 1.91        | 0.69     |
| 1:A:13:PRO:HG2   | 1:A:16:LEU:HB2   | 1.72        | 0.69     |
| 1:A:419:ASN:N    | 1:A:474:ASN:ND2  | 2.40        | 0.69     |
| 1:A:59:ASP:N     | 1:A:112:ALA:HB2  | 2.07        | 0.69     |
| 1:B:59:ASP:N     | 1:B:112:ALA:HB2  | 2.07        | 0.69     |
| 1:A:55:THR:HG21  | 1:A:58:HIS:CE1   | 2.26        | 0.69     |
| 1:B:214:MET:HB2  | 1:B:239:ALA:HA   | 1.74        | 0.69     |
| 1:A:164:LEU:HD23 | 1:A:271:PRO:HA   | 1.74        | 0.69     |
| 1:B:426:SER:N    | 1:B:427:PRO:HD3  | 2.08        | 0.69     |
| 1:B:464:GLU:HG2  | 1:B:465:MET:N    | 2.08        | 0.69     |
| 1:A:18:LEU:HD12  | 1:A:21:PHE:HB3   | 1.73        | 0.69     |
| 1:B:419:ASN:N    | 1:B:474:ASN:ND2  | 2.40        | 0.68     |
| 1:A:195:MET:HG3  | 1:B:244:TYR:OH   | 1.93        | 0.68     |
| 1:A:297:ARG:HB3  | 1:A:298:PRO:HD3  | 1.75        | 0.68     |
| 1:A:222:ARG:HB2  | 1:A:223:PRO:HD2  | 1.74        | 0.68     |
| 1:B:494:ASP:O    | 1:B:498:ASN:ND2  | 2.26        | 0.68     |
| 1:A:61:HIS:CE1   | 1:A:422:HIS:HD1  | 2.11        | 0.68     |
| 1:B:61:HIS:CE1   | 1:B:422:HIS:HD1  | 2.11        | 0.68     |
| 1:B:502:GLU:N    | 1:B:502:GLU:OE1  | 2.26        | 0.68     |
| 1:A:464:GLU:HG2  | 1:A:465:MET:N    | 2.08        | 0.68     |
| 1:B:48:ASP:OD1   | 1:B:58:HIS:NE2   | 2.24        | 0.68     |
| 1:A:200:MET:HE1  | 1:A:251:ASP:HB3  | 1.74        | 0.68     |
| 1:B:316:LEU:O    | 1:B:320:VAL:HG23 | 1.94        | 0.68     |
| 1:B:297:ARG:HB3  | 1:B:298:PRO:HD3  | 1.75        | 0.68     |
| 1:B:222:ARG:HB2  | 1:B:223:PRO:HD2  | 1.74        | 0.68     |
| 1:A:427:PRO:HD2  | 1:A:467:HIS:O    | 1.93        | 0.68     |
| 1:B:427:PRO:HD2  | 1:B:467:HIS:O    | 1.93        | 0.68     |
| 1:B:164:LEU:HD23 | 1:B:271:PRO:HA   | 1.74        | 0.68     |
| 1:A:214:MET:HB2  | 1:A:239:ALA:HA   | 1.74        | 0.68     |
| 1:A:316:LEU:O    | 1:A:320:VAL:HG23 | 1.94        | 0.68     |
| 1:A:494:ASP:O    | 1:A:498:ASN:ND2  | 2.26        | 0.68     |
| 1:A:502:GLU:N    | 1:A:502:GLU:OE1  | 2.26        | 0.68     |
| 1:A:324:LYS:HA   | 1:A:416:TRP:CH2  | 2.29        | 0.68     |
| 1:B:112:ALA:O    | 1:B:507:LEU:HD11 | 1.94        | 0.67     |
| 1:A:506:HIS:CE1  | 1:A:508:ALA:H    | 2.13        | 0.67     |
| 1:A:147:THR:O    | 1:A:150:ASP:HB2  | 1.95        | 0.67     |
| 1:A:426:SER:N    | 1:A:427:PRO:HD3  | 2.08        | 0.67     |
| 1:A:200:MET:CE   | 1:A:251:ASP:HB3  | 2.25        | 0.67     |
| 1:B:324:LYS:HA   | 1:B:416:TRP:CH2  | 2.29        | 0.67     |
| 1:B:147:THR:O    | 1:B:150:ASP:HB2  | 1.95        | 0.67     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:425:PHE:HB2  | 1:B:488:MET:HE1  | 1.75        | 0.67     |
| 1:A:112:ALA:O    | 1:A:507:LEU:HD11 | 1.94        | 0.67     |
| 1:A:507:LEU:HA   | 1:A:510:MET:HE3  | 1.74        | 0.67     |
| 1:B:9:PRO:HG3    | 1:B:21:PHE:CZ    | 2.30        | 0.67     |
| 1:B:425:PHE:HB2  | 1:B:488:MET:HE3  | 1.77        | 0.67     |
| 1:B:152:HIS:CE1  | 1:B:161:ARG:HH21 | 2.13        | 0.66     |
| 1:A:522:SER:O    | 1:A:526:ARG:HG2  | 1.95        | 0.66     |
| 1:B:205:ALA:HB2  | 1:B:541:ILE:HD12 | 1.77        | 0.66     |
| 1:A:238:ILE:HG21 | 1:B:428:ILE:CG2  | 2.25        | 0.66     |
| 1:B:506:HIS:CE1  | 1:B:508:ALA:H    | 2.12        | 0.66     |
| 1:B:295:ILE:HD12 | 1:B:378:ILE:HD11 | 1.77        | 0.66     |
| 1:B:486:TRP:O    | 1:B:490:THR:OG1  | 2.14        | 0.66     |
| 1:B:522:SER:O    | 1:B:526:ARG:HG2  | 1.95        | 0.66     |
| 1:A:9:PRO:HG3    | 1:A:21:PHE:CZ    | 2.30        | 0.66     |
| 1:A:95:PHE:HD1   | 1:A:96:PRO:CD    | 2.09        | 0.66     |
| 1:A:457:THR:CG2  | 1:A:458:PHE:H    | 2.01        | 0.66     |
| 1:B:351:TRP:O    | 1:B:352:ASN:ND2  | 2.29        | 0.66     |
| 1:A:422:HIS:CE1  | 2:A:600:FAD:HM82 | 2.21        | 0.66     |
| 1:B:200:MET:CE   | 1:B:251:ASP:HB3  | 2.25        | 0.66     |
| 1:B:95:PHE:O     | 1:B:540:ILE:HD12 | 1.96        | 0.66     |
| 1:B:95:PHE:HD1   | 1:B:96:PRO:CD    | 2.09        | 0.66     |
| 1:B:283:LEU:HB2  | 1:B:351:TRP:HB2  | 1.78        | 0.66     |
| 1:B:270:MET:CG   | 1:B:271:PRO:HD2  | 2.26        | 0.66     |
| 1:A:205:ALA:HB2  | 1:A:541:ILE:HD12 | 1.77        | 0.65     |
| 1:A:486:TRP:O    | 1:A:490:THR:OG1  | 2.14        | 0.65     |
| 1:A:479:ILE:HG22 | 1:A:483:LYS:CE   | 2.27        | 0.65     |
| 1:B:289:LEU:HD23 | 1:B:437:MET:SD   | 2.37        | 0.65     |
| 1:A:95:PHE:O     | 1:A:540:ILE:HD12 | 1.96        | 0.65     |
| 1:A:270:MET:CG   | 1:A:271:PRO:HD2  | 2.26        | 0.65     |
| 1:A:152:HIS:CE1  | 1:A:161:ARG:HH21 | 2.13        | 0.65     |
| 1:A:289:LEU:HD23 | 1:A:437:MET:SD   | 2.37        | 0.65     |
| 1:A:479:ILE:HG22 | 1:A:483:LYS:HE3  | 1.77        | 0.65     |
| 1:B:149:HIS:O    | 1:B:153:ASN:ND2  | 2.29        | 0.65     |
| 1:A:351:TRP:O    | 1:A:352:ASN:ND2  | 2.29        | 0.65     |
| 1:A:295:ILE:HD12 | 1:A:378:ILE:HD11 | 1.77        | 0.65     |
| 1:B:425:PHE:C    | 1:B:427:PRO:HD3  | 2.17        | 0.65     |
| 1:A:224:GLU:H    | 1:A:224:GLU:CD   | 2.01        | 0.65     |
| 1:B:224:GLU:CD   | 1:B:224:GLU:H    | 2.01        | 0.64     |
| 1:B:479:ILE:HG22 | 1:B:483:LYS:CE   | 2.27        | 0.64     |
| 1:A:555:HIS:CB   | 1:A:559:LYS:HE3  | 2.27        | 0.64     |
| 1:A:312:ARG:NH2  | 1:A:410:GLU:OE2  | 2.30        | 0.64     |
| 1:B:312:ARG:NH2  | 1:B:410:GLU:OE2  | 2.30        | 0.64     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:91:ASN:HD22  | 1:B:538:ASN:HD22 | 1.45        | 0.64     |
| 1:A:425:PHE:CD1  | 1:A:488:MET:HE1  | 2.33        | 0.64     |
| 1:A:95:PHE:HD1   | 1:A:96:PRO:N     | 1.96        | 0.64     |
| 1:B:550:PRO:HG2  | 1:B:553:TYR:HD1  | 1.62        | 0.64     |
| 1:A:108:TYR:O    | 1:A:506:HIS:HA   | 1.98        | 0.64     |
| 1:B:506:HIS:ND1  | 1:B:508:ALA:N    | 2.39        | 0.64     |
| 1:A:283:LEU:HB2  | 1:A:351:TRP:HB2  | 1.78        | 0.64     |
| 1:B:151:LEU:O    | 1:B:151:LEU:HD12 | 1.98        | 0.64     |
| 1:B:95:PHE:HD1   | 1:B:96:PRO:N     | 1.96        | 0.64     |
| 1:B:555:HIS:CB   | 1:B:559:LYS:HE3  | 2.27        | 0.64     |
| 1:A:91:ASN:HD22  | 1:A:538:ASN:HD22 | 1.45        | 0.64     |
| 1:A:149:HIS:O    | 1:A:153:ASN:ND2  | 2.30        | 0.63     |
| 1:A:269:LEU:O    | 1:B:463:ARG:NH2  | 2.31        | 0.63     |
| 1:B:479:ILE:HG22 | 1:B:483:LYS:HE3  | 1.77        | 0.63     |
| 1:A:425:PHE:C    | 1:A:427:PRO:HD3  | 2.17        | 0.63     |
| 1:A:555:HIS:HB3  | 1:A:559:LYS:HE3  | 1.80        | 0.63     |
| 1:B:309:PRO:HB2  | 1:B:353:PHE:CE1  | 2.33        | 0.63     |
| 1:A:309:PRO:HB2  | 1:A:353:PHE:CE1  | 2.33        | 0.63     |
| 1:B:425:PHE:CD1  | 1:B:488:MET:HE1  | 2.32        | 0.63     |
| 1:B:349:GLY:H    | 1:B:352:ASN:HD21 | 1.47        | 0.63     |
| 1:B:411:LEU:O    | 1:B:414:ILE:HB   | 1.99        | 0.63     |
| 1:A:151:LEU:HD12 | 1:A:151:LEU:O    | 1.98        | 0.63     |
| 1:A:559:LYS:O    | 1:A:560:LEU:HG   | 1.99        | 0.63     |
| 1:A:48:ASP:OD1   | 1:A:58:HIS:NE2   | 2.24        | 0.63     |
| 1:B:393:SER:OG   | 1:B:396:ARG:HG3  | 1.99        | 0.63     |
| 1:A:197:HIS:HB2  | 1:A:265:ILE:HD11 | 1.81        | 0.63     |
| 1:A:349:GLY:H    | 1:A:352:ASN:HD21 | 1.47        | 0.63     |
| 1:B:79:ASN:HD22  | 1:B:81:ALA:H     | 1.46        | 0.62     |
| 1:A:185:VAL:HG12 | 1:A:186:GLY:N    | 2.15        | 0.62     |
| 1:A:79:ASN:HD22  | 1:A:81:ALA:H     | 1.46        | 0.62     |
| 1:A:256:GLN:O    | 1:B:248:PRO:HD3  | 1.98        | 0.62     |
| 1:B:555:HIS:HB3  | 1:B:559:LYS:HE3  | 1.80        | 0.62     |
| 1:A:393:SER:OG   | 1:A:396:ARG:HG3  | 1.99        | 0.62     |
| 1:B:108:TYR:O    | 1:B:506:HIS:HA   | 1.98        | 0.62     |
| 1:A:411:LEU:O    | 1:A:414:ILE:HB   | 1.99        | 0.62     |
| 1:B:559:LYS:O    | 1:B:560:LEU:HG   | 1.99        | 0.62     |
| 1:B:324:LYS:HA   | 1:B:416:TRP:CZ3  | 2.34        | 0.62     |
| 1:B:24:PHE:CE1   | 1:B:28:ILE:HD12  | 2.34        | 0.62     |
| 1:B:10:LEU:HD11  | 1:B:42:SER:CA    | 2.30        | 0.62     |
| 1:B:280:LEU:HB2  | 1:B:395:LEU:HD13 | 1.81        | 0.62     |
| 1:A:148:TYR:HB2  | 1:A:172:GLY:O    | 2.00        | 0.62     |
| 1:A:24:PHE:CE1   | 1:A:28:ILE:HD12  | 2.34        | 0.62     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:167:ASP:OD1  | 1:B:186:GLY:HA3  | 2.00        | 0.62     |
| 1:B:197:HIS:HB2  | 1:B:265:ILE:HD11 | 1.81        | 0.62     |
| 1:A:550:PRO:HG2  | 1:A:553:TYR:HD1  | 1.62        | 0.62     |
| 1:B:148:TYR:HB2  | 1:B:172:GLY:O    | 2.00        | 0.62     |
| 1:B:13:PRO:HG3   | 1:B:95:PHE:CE1   | 2.35        | 0.62     |
| 1:A:315:LEU:HA   | 1:A:318:ALA:HB3  | 1.82        | 0.62     |
| 1:B:6:GLU:N      | 1:B:39:VAL:HG21  | 2.15        | 0.61     |
| 1:A:506:HIS:ND1  | 1:A:508:ALA:N    | 2.39        | 0.61     |
| 1:B:189:PRO:HA   | 1:B:307:ASN:HA   | 1.82        | 0.61     |
| 1:A:280:LEU:HB2  | 1:A:395:LEU:HD13 | 1.81        | 0.61     |
| 1:A:13:PRO:HG3   | 1:A:95:PHE:CE1   | 2.35        | 0.61     |
| 1:B:285:LYS:O    | 1:B:288:ASP:HB2  | 2.00        | 0.61     |
| 1:A:485:GLN:O    | 1:A:489:ARG:HG3  | 2.00        | 0.61     |
| 1:A:6:GLU:N      | 1:A:39:VAL:HG21  | 2.15        | 0.61     |
| 1:B:485:GLN:O    | 1:B:489:ARG:HG3  | 2.00        | 0.61     |
| 1:A:167:ASP:OD1  | 1:A:186:GLY:HA3  | 2.00        | 0.61     |
| 1:A:189:PRO:HA   | 1:A:307:ASN:HA   | 1.82        | 0.61     |
| 1:A:505:THR:HG22 | 1:A:506:HIS:N    | 2.15        | 0.61     |
| 1:B:61:HIS:CE1   | 1:B:422:HIS:ND1  | 2.69        | 0.61     |
| 1:B:149:HIS:O    | 1:B:152:HIS:HB3  | 2.01        | 0.61     |
| 1:B:505:THR:HG22 | 1:B:506:HIS:N    | 2.15        | 0.61     |
| 1:A:316:LEU:HD11 | 1:A:413:TRP:NE1  | 2.16        | 0.61     |
| 1:A:61:HIS:CE1   | 1:A:422:HIS:ND1  | 2.69        | 0.61     |
| 1:A:10:LEU:HD11  | 1:A:42:SER:CA    | 2.30        | 0.61     |
| 1:A:285:LYS:O    | 1:A:288:ASP:HB2  | 2.00        | 0.61     |
| 1:B:416:TRP:CE3  | 1:B:416:TRP:HA   | 2.36        | 0.61     |
| 1:B:185:VAL:HG12 | 1:B:186:GLY:N    | 2.15        | 0.61     |
| 1:A:39:VAL:HG12  | 1:A:40:ILE:H     | 1.66        | 0.61     |
| 1:A:324:LYS:HA   | 1:A:416:TRP:CZ3  | 2.34        | 0.61     |
| 1:A:230:PRO:HA   | 1:A:233:GLN:CD   | 2.21        | 0.61     |
| 1:A:426:SER:O    | 1:A:502:GLU:HA   | 2.01        | 0.61     |
| 1:B:315:LEU:HA   | 1:B:318:ALA:HB3  | 1.82        | 0.60     |
| 1:B:230:PRO:HA   | 1:B:233:GLN:CD   | 2.21        | 0.60     |
| 1:B:316:LEU:HD11 | 1:B:413:TRP:NE1  | 2.16        | 0.60     |
| 1:B:39:VAL:HG12  | 1:B:40:ILE:H     | 1.66        | 0.60     |
| 1:B:82:ASP:O     | 1:B:86:ILE:HG13  | 2.01        | 0.60     |
| 1:A:24:PHE:CD2   | 1:A:95:PHE:HD2   | 2.20        | 0.60     |
| 1:B:129:ARG:HB2  | 1:B:131:LEU:HD21 | 1.83        | 0.60     |
| 1:A:136:GLU:H    | 1:A:136:GLU:CD   | 2.05        | 0.60     |
| 1:A:149:HIS:O    | 1:A:152:HIS:HB3  | 2.01        | 0.60     |
| 1:A:549:TRP:CZ2  | 1:A:558:TRP:HB3  | 2.37        | 0.60     |
| 1:B:24:PHE:CD2   | 1:B:95:PHE:HD2   | 2.20        | 0.60     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:37:VAL:HG12  | 1:B:38:GLU:N     | 2.17        | 0.60     |
| 1:B:549:TRP:CZ2  | 1:B:558:TRP:HB3  | 2.37        | 0.60     |
| 1:A:445:LYS:O    | 1:A:449:GLU:HG3  | 2.02        | 0.60     |
| 1:B:426:SER:O    | 1:B:502:GLU:HA   | 2.01        | 0.60     |
| 1:A:37:VAL:HG12  | 1:A:38:GLU:N     | 2.17        | 0.59     |
| 1:B:96:PRO:C     | 1:B:97:LEU:HD23  | 2.22        | 0.59     |
| 1:A:478:LEU:H    | 1:A:478:LEU:CD1  | 2.12        | 0.59     |
| 1:B:445:LYS:O    | 1:B:449:GLU:HG3  | 2.02        | 0.59     |
| 1:A:96:PRO:C     | 1:A:97:LEU:HD23  | 2.22        | 0.59     |
| 1:A:129:ARG:HB2  | 1:A:131:LEU:HD21 | 1.83        | 0.59     |
| 1:A:425:PHE:CB   | 1:A:488:MET:HE1  | 2.32        | 0.59     |
| 1:A:554:SER:HB3  | 1:A:557:THR:HB   | 1.84        | 0.59     |
| 1:A:82:ASP:O     | 1:A:86:ILE:HG13  | 2.01        | 0.59     |
| 1:A:242:PHE:CD1  | 1:A:243:PRO:HD2  | 2.37        | 0.59     |
| 1:A:416:TRP:CE3  | 1:A:416:TRP:HA   | 2.36        | 0.59     |
| 1:A:39:VAL:HG12  | 1:A:40:ILE:N     | 2.17        | 0.59     |
| 1:A:430:LYS:O    | 1:A:465:MET:HE2  | 2.03        | 0.59     |
| 1:B:136:GLU:H    | 1:B:136:GLU:CD   | 2.05        | 0.59     |
| 1:B:430:LYS:O    | 1:B:465:MET:HE2  | 2.02        | 0.59     |
| 1:A:299:LEU:HB2  | 1:A:305:LEU:CD1  | 2.33        | 0.59     |
| 1:A:243:PRO:HD2  | 1:A:244:TYR:H    | 1.68        | 0.59     |
| 1:B:242:PHE:CD1  | 1:B:243:PRO:HD2  | 2.37        | 0.59     |
| 1:B:283:LEU:HD12 | 1:B:351:TRP:HB3  | 1.85        | 0.58     |
| 1:A:332:GLU:CB   | 1:A:333:PRO:HD2  | 2.33        | 0.58     |
| 1:B:243:PRO:HD2  | 1:B:244:TYR:H    | 1.68        | 0.58     |
| 1:B:554:SER:HB3  | 1:B:557:THR:HB   | 1.84        | 0.58     |
| 1:A:411:LEU:HA   | 1:A:414:ILE:HD12 | 1.86        | 0.58     |
| 1:B:154:TYR:HD1  | 1:B:155:LEU:HD23 | 1.68        | 0.58     |
| 1:B:222:ARG:CB   | 1:B:223:PRO:HD2  | 2.30        | 0.58     |
| 1:A:230:PRO:HD2  | 1:A:231:GLU:H    | 1.68        | 0.58     |
| 1:B:299:LEU:HB2  | 1:B:305:LEU:CD1  | 2.33        | 0.58     |
| 1:B:230:PRO:HD2  | 1:B:231:GLU:H    | 1.68        | 0.58     |
| 1:A:525:LEU:O    | 1:A:525:LEU:HD12 | 2.04        | 0.58     |
| 1:B:475:LYS:O    | 1:B:481:LYS:HD2  | 2.04        | 0.58     |
| 1:B:272:ASN:OD1  | 1:B:273:PRO:HD2  | 2.04        | 0.58     |
| 1:B:51:TYR:CZ    | 1:B:104:ARG:HD3  | 2.39        | 0.58     |
| 1:A:154:TYR:HD1  | 1:A:155:LEU:HD23 | 1.68        | 0.58     |
| 1:B:35:GLU:HA    | 1:B:35:GLU:OE1   | 2.04        | 0.58     |
| 1:B:332:GLU:CB   | 1:B:333:PRO:HD2  | 2.33        | 0.58     |
| 1:A:475:LYS:O    | 1:A:481:LYS:HD2  | 2.04        | 0.57     |
| 1:A:272:ASN:OD1  | 1:A:273:PRO:HD2  | 2.04        | 0.57     |
| 1:A:61:HIS:CE1   | 1:A:422:HIS:CE1  | 2.93        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:51:TYR:CZ    | 1:A:104:ARG:HD3  | 2.39        | 0.57     |
| 1:B:13:PRO:HD3   | 1:B:117:GLY:O    | 2.04        | 0.57     |
| 1:A:24:PHE:CE1   | 1:A:28:ILE:CD1   | 2.87        | 0.57     |
| 1:B:39:VAL:HG12  | 1:B:40:ILE:N     | 2.17        | 0.57     |
| 1:A:65:ASP:N     | 1:A:65:ASP:OD1   | 2.37        | 0.57     |
| 1:B:83:VAL:O     | 1:B:87:VAL:HG23  | 2.04        | 0.57     |
| 1:A:283:LEU:HD12 | 1:A:351:TRP:HB3  | 1.85        | 0.57     |
| 1:A:13:PRO:HD3   | 1:A:117:GLY:O    | 2.04        | 0.57     |
| 1:B:411:LEU:HA   | 1:B:414:ILE:HD12 | 1.86        | 0.57     |
| 1:B:24:PHE:CE1   | 1:B:28:ILE:CD1   | 2.88        | 0.57     |
| 1:B:393:SER:O    | 1:B:396:ARG:HB2  | 2.05        | 0.57     |
| 1:B:421:ALA:O    | 1:B:472:VAL:HA   | 2.05        | 0.57     |
| 1:A:83:VAL:O     | 1:A:87:VAL:HG23  | 2.04        | 0.57     |
| 1:A:425:PHE:HB2  | 1:A:488:MET:HE3  | 1.86        | 0.57     |
| 1:A:332:GLU:CG   | 1:A:333:PRO:HD2  | 2.35        | 0.57     |
| 1:A:222:ARG:CB   | 1:A:223:PRO:HD2  | 2.30        | 0.56     |
| 1:A:280:LEU:O    | 1:A:280:LEU:HG   | 2.05        | 0.56     |
| 1:B:165:TRP:HB2  | 1:B:270:MET:O    | 2.05        | 0.56     |
| 1:B:525:LEU:O    | 1:B:525:LEU:HD12 | 2.04        | 0.56     |
| 1:A:48:ASP:HA    | 1:A:58:HIS:CE1   | 2.40        | 0.56     |
| 1:A:393:SER:O    | 1:A:396:ARG:HB2  | 2.05        | 0.56     |
| 1:A:165:TRP:HB2  | 1:A:270:MET:O    | 2.05        | 0.56     |
| 1:B:444:LYS:O    | 1:B:447:CYS:N    | 2.39        | 0.56     |
| 1:A:448:GLN:O    | 1:A:451:GLY:N    | 2.33        | 0.56     |
| 1:A:421:ALA:O    | 1:A:472:VAL:HA   | 2.05        | 0.56     |
| 1:B:61:HIS:CE1   | 1:B:422:HIS:CE1  | 2.93        | 0.56     |
| 1:B:418:PRO:HB2  | 1:B:474:ASN:ND2  | 2.21        | 0.56     |
| 1:B:478:LEU:CD1  | 1:B:478:LEU:H    | 2.12        | 0.56     |
| 1:B:48:ASP:HA    | 1:B:58:HIS:CE1   | 2.40        | 0.56     |
| 1:B:389:THR:HB   | 1:B:390:PRO:HD2  | 1.86        | 0.56     |
| 1:B:332:GLU:CG   | 1:B:333:PRO:HD2  | 2.35        | 0.56     |
| 1:A:35:GLU:OE1   | 1:A:35:GLU:HA    | 2.04        | 0.56     |
| 1:A:223:PRO:O    | 1:A:226:MET:HG2  | 2.06        | 0.56     |
| 1:A:389:THR:HB   | 1:A:390:PRO:CD   | 2.36        | 0.56     |
| 1:A:156:GLU:C    | 1:A:158:ASN:H    | 2.09        | 0.56     |
| 1:B:389:THR:HB   | 1:B:390:PRO:CD   | 2.36        | 0.56     |
| 1:B:223:PRO:O    | 1:B:226:MET:HG2  | 2.06        | 0.56     |
| 1:A:389:THR:HB   | 1:A:390:PRO:HD2  | 1.86        | 0.56     |
| 1:A:400:LYS:HB3  | 1:A:405:ILE:HB   | 1.87        | 0.56     |
| 1:A:237:LYS:NZ   | 1:B:500:TRP:CZ2  | 2.73        | 0.56     |
| 1:A:10:LEU:HD13  | 1:A:40:ILE:O     | 2.06        | 0.56     |
| 1:A:545:LYS:HG3  | 1:A:546:SER:N    | 2.20        | 0.56     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:B:156:GLU:C   | 1:B:158:ASN:H    | 2.09        | 0.56     |
| 1:B:229:LYS:HB3 | 1:B:230:PRO:CD   | 2.36        | 0.56     |
| 1:B:201:GLU:HG2 | 1:B:202:VAL:N    | 2.19        | 0.56     |
| 1:A:27:ASP:OD1  | 1:A:27:ASP:N     | 2.39        | 0.56     |
| 1:B:10:LEU:HD13 | 1:B:40:ILE:O     | 2.06        | 0.56     |
| 1:B:280:LEU:HG  | 1:B:280:LEU:O    | 2.05        | 0.56     |
| 1:A:494:ASP:O   | 1:A:497:ALA:HB3  | 2.06        | 0.56     |
| 1:A:444:LYS:O   | 1:A:447:CYS:N    | 2.39        | 0.56     |
| 1:B:59:ASP:O    | 1:B:62:HIS:HB3   | 2.07        | 0.55     |
| 1:A:270:MET:HG3 | 1:A:271:PRO:HD2  | 1.87        | 0.55     |
| 1:B:555:HIS:HB3 | 1:B:559:LYS:CE   | 2.37        | 0.55     |
| 1:B:494:ASP:O   | 1:B:497:ALA:HB3  | 2.06        | 0.55     |
| 1:B:65:ASP:OD1  | 1:B:65:ASP:N     | 2.37        | 0.55     |
| 1:B:425:PHE:CE2 | 1:B:427:PRO:HG3  | 2.41        | 0.55     |
| 1:B:270:MET:HG3 | 1:B:271:PRO:HD2  | 1.87        | 0.55     |
| 1:A:201:GLU:HG2 | 1:A:202:VAL:N    | 2.20        | 0.55     |
| 1:A:425:PHE:CE2 | 1:A:427:PRO:HG3  | 2.41        | 0.55     |
| 1:A:59:ASP:O    | 1:A:62:HIS:HB3   | 2.07        | 0.55     |
| 1:B:143:GLU:HB3 | 1:B:144:PRO:HD2  | 1.89        | 0.55     |
| 1:B:545:LYS:HG3 | 1:B:546:SER:N    | 2.20        | 0.55     |
| 1:B:164:LEU:C   | 1:B:165:TRP:HD1  | 2.10        | 0.55     |
| 1:A:549:TRP:CH2 | 1:A:558:TRP:HB3  | 2.42        | 0.55     |
| 1:B:403:GLN:HG3 | 1:B:405:ILE:HG13 | 1.89        | 0.55     |
| 1:A:418:PRO:HB2 | 1:A:474:ASN:ND2  | 2.21        | 0.55     |
| 1:B:276:TYR:OH  | 1:B:399:ASP:O    | 2.19        | 0.55     |
| 1:A:229:LYS:HB3 | 1:A:230:PRO:CD   | 2.36        | 0.55     |
| 1:B:549:TRP:CH2 | 1:B:558:TRP:HB3  | 2.42        | 0.55     |
| 1:A:361:GLU:N   | 1:A:362:PRO:HD2  | 2.22        | 0.55     |
| 1:A:75:VAL:O    | 1:A:122:ASP:N    | 2.37        | 0.55     |
| 1:A:18:LEU:HD12 | 1:A:18:LEU:O     | 2.07        | 0.55     |
| 1:A:317:ASP:O   | 1:A:321:LEU:HG   | 2.08        | 0.54     |
| 1:A:463:ARG:NH2 | 1:B:269:LEU:O    | 2.40        | 0.54     |
| 1:A:270:MET:HG2 | 1:A:271:PRO:HD2  | 1.88        | 0.54     |
| 1:B:270:MET:HG2 | 1:B:271:PRO:HD2  | 1.88        | 0.54     |
| 1:A:422:HIS:CD2 | 1:A:424:PHE:CZ   | 2.95        | 0.54     |
| 1:B:97:LEU:CD2  | 1:B:119:VAL:HB   | 2.37        | 0.54     |
| 1:B:505:THR:CG2 | 1:B:506:HIS:N    | 2.71        | 0.54     |
| 1:A:554:SER:HB3 | 1:A:557:THR:CB   | 2.37        | 0.54     |
| 1:B:422:HIS:CD2 | 1:B:424:PHE:CZ   | 2.95        | 0.54     |
| 1:A:555:HIS:HB3 | 1:A:559:LYS:CE   | 2.37        | 0.54     |
| 1:B:312:ARG:NH1 | 1:B:317:ASP:OD1  | 2.40        | 0.54     |
| 1:B:361:GLU:N   | 1:B:362:PRO:HD2  | 2.22        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:9:PRO:HG3    | 1:A:21:PHE:CE2   | 2.42        | 0.54     |
| 1:B:478:LEU:O    | 1:B:482:ARG:HG3  | 2.08        | 0.54     |
| 1:B:89:LEU:CD1   | 1:B:89:LEU:N     | 2.71        | 0.54     |
| 1:B:400:LYS:HB3  | 1:B:405:ILE:HB   | 1.87        | 0.54     |
| 1:B:7:PHE:HB3    | 1:B:8:ARG:HG3    | 1.89        | 0.54     |
| 1:B:9:PRO:HG3    | 1:B:21:PHE:CE2   | 2.42        | 0.54     |
| 1:A:7:PHE:HB3    | 1:A:8:ARG:HG3    | 1.89        | 0.54     |
| 1:B:506:HIS:ND1  | 1:B:507:LEU:N    | 2.56        | 0.54     |
| 1:B:312:ARG:HD2  | 1:B:354:TYR:CE1  | 2.43        | 0.54     |
| 1:A:164:LEU:C    | 1:A:165:TRP:HD1  | 2.10        | 0.54     |
| 1:A:229:LYS:O    | 1:A:233:GLN:HG3  | 2.08        | 0.54     |
| 1:B:503:TYR:OH   | 3:B:601:EUG:O4   | 2.15        | 0.54     |
| 1:A:143:GLU:HB3  | 1:A:144:PRO:HD2  | 1.89        | 0.54     |
| 1:B:533:ASN:OD1  | 1:B:552:GLN:NE2  | 2.41        | 0.54     |
| 1:A:506:HIS:ND1  | 1:A:507:LEU:N    | 2.56        | 0.54     |
| 1:A:312:ARG:HD2  | 1:A:354:TYR:CE1  | 2.43        | 0.54     |
| 1:B:317:ASP:O    | 1:B:321:LEU:HG   | 2.08        | 0.54     |
| 1:B:217:LEU:HD13 | 1:B:217:LEU:C    | 2.28        | 0.54     |
| 1:B:229:LYS:O    | 1:B:233:GLN:HG3  | 2.08        | 0.54     |
| 1:A:97:LEU:CD2   | 1:A:119:VAL:HB   | 2.37        | 0.54     |
| 1:B:221:LYS:O    | 1:B:222:ARG:HB3  | 2.08        | 0.54     |
| 1:A:505:THR:CG2  | 1:A:506:HIS:N    | 2.71        | 0.54     |
| 1:B:18:LEU:HD12  | 1:B:18:LEU:O     | 2.07        | 0.54     |
| 1:A:388:ASP:OD1  | 1:A:388:ASP:N    | 2.41        | 0.54     |
| 1:A:296:ILE:HG21 | 1:A:460:VAL:HG11 | 1.90        | 0.53     |
| 1:B:388:ASP:N    | 1:B:388:ASP:OD1  | 2.41        | 0.53     |
| 1:A:221:LYS:O    | 1:A:222:ARG:HB3  | 2.08        | 0.53     |
| 1:B:554:SER:HB3  | 1:B:557:THR:CB   | 2.37        | 0.53     |
| 1:A:403:GLN:HG3  | 1:A:405:ILE:HG13 | 1.89        | 0.53     |
| 1:A:464:GLU:OE2  | 1:A:466:HIS:ND1  | 2.41        | 0.53     |
| 1:A:79:ASN:ND2   | 1:A:81:ALA:H     | 2.06        | 0.53     |
| 1:A:533:ASN:OD1  | 1:A:552:GLN:NE2  | 2.41        | 0.53     |
| 1:B:194:TRP:O    | 1:B:197:HIS:CD2  | 2.62        | 0.53     |
| 1:A:478:LEU:O    | 1:A:482:ARG:HG3  | 2.08        | 0.53     |
| 1:A:205:ALA:CB   | 1:A:536:ASP:HB2  | 2.39        | 0.53     |
| 1:A:217:LEU:HD13 | 1:A:217:LEU:C    | 2.28        | 0.53     |
| 1:B:27:ASP:OD1   | 1:B:27:ASP:N     | 2.39        | 0.53     |
| 1:B:422:HIS:HD2  | 1:B:424:PHE:CZ   | 2.27        | 0.53     |
| 1:B:422:HIS:NE2  | 2:B:600:FAD:C8   | 2.64        | 0.53     |
| 1:A:89:LEU:N     | 1:A:89:LEU:CD1   | 2.71        | 0.53     |
| 1:A:136:GLU:OE1  | 1:A:136:GLU:N    | 2.34        | 0.53     |
| 1:B:23:GLU:O     | 1:B:27:ASP:OD1   | 2.27        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:205:ALA:CB   | 1:B:536:ASP:HB2  | 2.39        | 0.53     |
| 1:A:7:PHE:HA     | 1:A:22:ASN:OD1   | 2.09        | 0.53     |
| 1:A:509:PHE:O    | 1:A:513:ILE:HG13 | 2.09        | 0.53     |
| 1:A:23:GLU:O     | 1:A:27:ASP:OD1   | 2.27        | 0.53     |
| 1:A:495:CYS:HB2  | 4:A:605:HOH:O    | 2.07        | 0.53     |
| 1:A:422:HIS:HD2  | 1:A:424:PHE:CZ   | 2.27        | 0.53     |
| 1:A:194:TRP:O    | 1:A:197:HIS:CD2  | 2.62        | 0.53     |
| 1:B:509:PHE:O    | 1:B:513:ILE:HG13 | 2.09        | 0.53     |
| 1:B:390:PRO:O    | 1:B:393:SER:HB3  | 2.09        | 0.53     |
| 1:B:79:ASN:ND2   | 1:B:81:ALA:H     | 2.06        | 0.53     |
| 1:A:390:PRO:O    | 1:A:393:SER:HB3  | 2.09        | 0.53     |
| 1:B:194:TRP:O    | 1:B:197:HIS:HD2  | 1.91        | 0.53     |
| 1:A:160:LEU:O    | 1:A:163:LYS:N    | 2.37        | 0.53     |
| 1:A:419:ASN:O    | 1:A:475:LYS:N    | 2.38        | 0.53     |
| 1:B:62:HIS:O     | 1:B:62:HIS:ND1   | 2.39        | 0.53     |
| 1:A:472:VAL:HG12 | 1:A:473:PHE:N    | 2.24        | 0.53     |
| 1:B:7:PHE:HA     | 1:B:22:ASN:OD1   | 2.09        | 0.52     |
| 1:B:419:ASN:O    | 1:B:475:LYS:N    | 2.38        | 0.52     |
| 1:A:247:GLY:HA2  | 1:B:546:SER:OG   | 2.09        | 0.52     |
| 1:B:349:GLY:N    | 1:B:352:ASN:HD21 | 2.07        | 0.52     |
| 1:A:165:TRP:N    | 1:A:270:MET:O    | 2.39        | 0.52     |
| 1:A:194:TRP:O    | 1:A:197:HIS:HD2  | 1.91        | 0.52     |
| 1:A:55:THR:HG21  | 1:A:58:HIS:ND1   | 2.25        | 0.52     |
| 1:A:62:HIS:O     | 1:A:62:HIS:ND1   | 2.39        | 0.52     |
| 1:A:349:GLY:N    | 1:A:352:ASN:HD21 | 2.07        | 0.52     |
| 1:B:457:THR:CG2  | 1:B:458:PHE:H    | 2.01        | 0.52     |
| 1:B:464:GLU:OE2  | 1:B:466:HIS:ND1  | 2.41        | 0.52     |
| 1:B:383:PHE:C    | 1:B:384:TYR:CD1  | 2.82        | 0.52     |
| 1:B:296:ILE:HG21 | 1:B:460:VAL:HG11 | 1.90        | 0.52     |
| 1:B:165:TRP:N    | 1:B:270:MET:O    | 2.39        | 0.52     |
| 1:A:369:GLU:O    | 1:A:373:ASP:HB3  | 2.10        | 0.52     |
| 1:B:369:GLU:O    | 1:B:373:ASP:HB3  | 2.10        | 0.52     |
| 1:A:507:LEU:HA   | 1:A:510:MET:HE2  | 1.92        | 0.52     |
| 1:A:383:PHE:C    | 1:A:384:TYR:CD1  | 2.82        | 0.52     |
| 1:B:371:ILE:O    | 1:B:374:ALA:HB3  | 2.10        | 0.52     |
| 1:B:243:PRO:CD   | 1:B:244:TYR:H    | 2.23        | 0.52     |
| 1:B:156:GLU:O    | 1:B:158:ASN:N    | 2.43        | 0.52     |
| 1:A:243:PRO:CD   | 1:A:244:TYR:H    | 2.23        | 0.52     |
| 1:A:312:ARG:NH1  | 1:A:317:ASP:OD1  | 2.40        | 0.52     |
| 1:A:371:ILE:O    | 1:A:374:ALA:HB3  | 2.10        | 0.52     |
| 1:B:55:THR:HG21  | 1:B:58:HIS:ND1   | 2.25        | 0.52     |
| 1:A:132:GLU:HG2  | 1:A:133:VAL:H    | 1.75        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:515:GLU:HA   | 1:B:515:GLU:OE1  | 2.11        | 0.51     |
| 1:A:323:ASP:OD1  | 1:A:326:SER:HB3  | 2.10        | 0.51     |
| 1:B:323:ASP:OD1  | 1:B:326:SER:HB3  | 2.10        | 0.51     |
| 1:A:505:THR:HG21 | 1:A:509:PHE:HB2  | 1.91        | 0.51     |
| 1:A:409:ASP:HA   | 1:A:412:LYS:HE3  | 1.92        | 0.51     |
| 1:B:472:VAL:HG12 | 1:B:473:PHE:N    | 2.24        | 0.51     |
| 1:B:442:VAL:O    | 1:B:445:LYS:HB3  | 2.11        | 0.51     |
| 1:B:433:GLY:O    | 1:B:437:MET:HB2  | 2.11        | 0.51     |
| 1:B:200:MET:O    | 1:B:211:ARG:HA   | 2.11        | 0.51     |
| 1:B:409:ASP:OD1  | 1:B:409:ASP:N    | 2.44        | 0.51     |
| 1:A:411:LEU:HA   | 1:A:414:ILE:CD1  | 2.41        | 0.51     |
| 1:A:533:ASN:HD21 | 1:A:551:SER:H    | 1.59        | 0.51     |
| 1:B:95:PHE:CD1   | 1:B:96:PRO:CD    | 2.94        | 0.51     |
| 1:B:418:PRO:CD   | 1:B:474:ASN:HD22 | 2.22        | 0.51     |
| 1:B:300:ARG:NH2  | 1:B:308:VAL:HA   | 2.18        | 0.51     |
| 1:B:505:THR:HG21 | 1:B:509:PHE:HB2  | 1.91        | 0.51     |
| 1:B:107:GLY:HA2  | 1:B:422:HIS:O    | 2.11        | 0.51     |
| 1:A:484:VAL:O    | 1:A:487:LEU:HB3  | 2.11        | 0.51     |
| 1:A:425:PHE:CE1  | 1:A:502:GLU:CG   | 2.94        | 0.51     |
| 1:B:425:PHE:CE1  | 1:B:502:GLU:CG   | 2.94        | 0.51     |
| 1:B:507:LEU:HA   | 1:B:510:MET:HE2  | 1.93        | 0.51     |
| 1:A:433:GLY:O    | 1:A:437:MET:HB2  | 2.11        | 0.51     |
| 1:B:289:LEU:HB2  | 1:B:351:TRP:NE1  | 2.26        | 0.51     |
| 1:B:136:GLU:N    | 1:B:136:GLU:OE1  | 2.34        | 0.51     |
| 1:B:409:ASP:HA   | 1:B:412:LYS:HE3  | 1.92        | 0.51     |
| 1:A:277:GLN:O    | 1:A:357:LEU:N    | 2.29        | 0.50     |
| 1:A:156:GLU:O    | 1:A:158:ASN:N    | 2.43        | 0.50     |
| 1:A:133:VAL:HG21 | 1:A:154:TYR:CZ   | 2.44        | 0.50     |
| 1:A:351:TRP:CE3  | 1:A:351:TRP:HA   | 2.47        | 0.50     |
| 1:A:289:LEU:HB2  | 1:A:351:TRP:NE1  | 2.26        | 0.50     |
| 1:A:409:ASP:OD1  | 1:A:409:ASP:N    | 2.44        | 0.50     |
| 1:B:533:ASN:HD21 | 1:B:551:SER:H    | 1.59        | 0.50     |
| 1:A:300:ARG:HE   | 1:A:309:PRO:HD2  | 1.76        | 0.50     |
| 1:A:442:VAL:O    | 1:A:445:LYS:HB3  | 2.11        | 0.50     |
| 1:A:223:PRO:HG2  | 1:A:224:GLU:CD   | 2.32        | 0.50     |
| 1:A:371:ILE:O    | 1:A:374:ALA:N    | 2.44        | 0.50     |
| 1:B:179:ASN:OD1  | 1:B:184:GLY:HA3  | 2.11        | 0.50     |
| 1:B:411:LEU:HA   | 1:B:414:ILE:CD1  | 2.41        | 0.50     |
| 1:A:144:PRO:HA   | 1:A:177:LEU:HG   | 1.93        | 0.50     |
| 1:B:28:ILE:O     | 1:B:32:VAL:HG22  | 2.12        | 0.50     |
| 1:A:22:ASN:HA    | 1:A:25:ILE:HG22  | 1.94        | 0.50     |
| 1:B:448:GLN:O    | 1:B:451:GLY:N    | 2.33        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:277:GLN:O    | 1:B:357:LEU:N    | 2.29        | 0.50     |
| 1:B:24:PHE:CE2   | 1:B:95:PHE:CD2   | 3.00        | 0.50     |
| 1:A:24:PHE:CE2   | 1:A:95:PHE:CD2   | 3.00        | 0.50     |
| 1:A:349:GLY:CA   | 1:A:352:ASN:HD21 | 2.25        | 0.50     |
| 1:A:385:PHE:HB2  | 1:A:387:GLU:OE1  | 2.11        | 0.50     |
| 1:B:425:PHE:CB   | 1:B:488:MET:HE1  | 2.40        | 0.50     |
| 1:B:351:TRP:HA   | 1:B:351:TRP:CE3  | 2.47        | 0.50     |
| 1:A:200:MET:O    | 1:A:211:ARG:HA   | 2.11        | 0.50     |
| 1:B:324:LYS:HE2  | 1:B:334:LEU:HD21 | 1.94        | 0.50     |
| 1:B:371:ILE:O    | 1:B:374:ALA:N    | 2.44        | 0.50     |
| 1:B:75:VAL:O     | 1:B:122:ASP:N    | 2.37        | 0.50     |
| 1:B:51:TYR:CE1   | 1:B:171:LEU:HD13 | 2.47        | 0.50     |
| 1:B:144:PRO:HA   | 1:B:177:LEU:HG   | 1.93        | 0.50     |
| 1:A:425:PHE:HE1  | 1:A:502:GLU:CG   | 2.25        | 0.50     |
| 1:B:484:VAL:O    | 1:B:487:LEU:HB3  | 2.11        | 0.50     |
| 1:B:385:PHE:HB2  | 1:B:387:GLU:OE1  | 2.11        | 0.50     |
| 1:A:107:GLY:HA2  | 1:A:422:HIS:O    | 2.11        | 0.49     |
| 1:B:205:ALA:HB2  | 1:B:541:ILE:CD1  | 2.42        | 0.49     |
| 1:B:223:PRO:HG2  | 1:B:224:GLU:CD   | 2.32        | 0.49     |
| 1:A:179:ASN:OD1  | 1:A:184:GLY:HA3  | 2.11        | 0.49     |
| 1:B:132:GLU:HG2  | 1:B:133:VAL:H    | 1.75        | 0.49     |
| 1:B:155:LEU:O    | 1:B:160:LEU:N    | 2.40        | 0.49     |
| 1:A:205:ALA:HB2  | 1:A:541:ILE:CD1  | 2.42        | 0.49     |
| 1:B:279:TYR:HB3  | 1:B:385:PHE:CE1  | 2.47        | 0.49     |
| 1:A:152:HIS:CE1  | 1:A:161:ARG:NH2  | 2.79        | 0.49     |
| 1:B:58:HIS:C     | 1:B:112:ALA:HB2  | 2.32        | 0.49     |
| 1:A:279:TYR:HB3  | 1:A:385:PHE:CE1  | 2.47        | 0.49     |
| 1:A:515:GLU:HA   | 1:A:515:GLU:OE1  | 2.11        | 0.49     |
| 1:A:51:TYR:CE1   | 1:A:171:LEU:HD13 | 2.47        | 0.49     |
| 1:B:133:VAL:HG21 | 1:B:154:TYR:CZ   | 2.44        | 0.49     |
| 1:B:297:ARG:HB3  | 1:B:298:PRO:CD   | 2.42        | 0.49     |
| 1:B:349:GLY:CA   | 1:B:352:ASN:HD21 | 2.25        | 0.49     |
| 1:B:22:ASN:HA    | 1:B:25:ILE:HG22  | 1.94        | 0.49     |
| 1:A:28:ILE:O     | 1:A:32:VAL:HG22  | 2.12        | 0.49     |
| 1:B:217:LEU:HD22 | 1:B:217:LEU:HA   | 1.41        | 0.49     |
| 1:B:454:PHE:CD1  | 1:B:455:ILE:N    | 2.81        | 0.49     |
| 1:A:428:ILE:HG21 | 1:B:238:ILE:HG21 | 1.93        | 0.49     |
| 1:B:309:PRO:HB2  | 1:B:353:PHE:HE1  | 1.78        | 0.49     |
| 1:B:103:GLY:C    | 1:B:105:ASN:H    | 2.16        | 0.49     |
| 1:B:300:ARG:HE   | 1:B:309:PRO:HD2  | 1.76        | 0.49     |
| 1:A:244:TYR:CD1  | 1:A:244:TYR:N    | 2.77        | 0.49     |
| 1:A:58:HIS:C     | 1:A:112:ALA:HB2  | 2.32        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:526:ARG:NH1  | 1:A:529:GLU:OE1  | 2.46        | 0.49     |
| 1:B:526:ARG:NH1  | 1:B:529:GLU:OE1  | 2.46        | 0.49     |
| 1:B:186:GLY:O    | 1:B:191:GLY:HA3  | 2.13        | 0.49     |
| 1:A:324:LYS:HE2  | 1:A:334:LEU:HD21 | 1.94        | 0.49     |
| 1:A:361:GLU:CA   | 1:A:364:ARG:NH2  | 2.76        | 0.48     |
| 1:A:478:LEU:HB2  | 1:A:479:ILE:HD12 | 1.95        | 0.48     |
| 1:B:425:PHE:HE1  | 1:B:502:GLU:CG   | 2.25        | 0.48     |
| 1:A:243:PRO:CD   | 1:A:244:TYR:N    | 2.76        | 0.48     |
| 1:B:147:THR:HG23 | 1:B:150:ASP:OD2  | 2.13        | 0.48     |
| 1:A:454:PHE:CD1  | 1:A:455:ILE:N    | 2.81        | 0.48     |
| 1:A:186:GLY:O    | 1:A:191:GLY:HA3  | 2.13        | 0.48     |
| 1:A:103:GLY:C    | 1:A:105:ASN:H    | 2.16        | 0.48     |
| 1:A:422:HIS:NE2  | 2:A:600:FAD:C8   | 2.64        | 0.48     |
| 1:B:149:HIS:C    | 1:B:153:ASN:HD22 | 2.17        | 0.48     |
| 1:A:321:LEU:HD12 | 1:A:346:LEU:CD2  | 2.43        | 0.48     |
| 1:A:190:TYR:CE1  | 1:A:270:MET:HG3  | 2.48        | 0.48     |
| 1:B:323:ASP:N    | 1:B:323:ASP:OD1  | 2.46        | 0.48     |
| 1:A:6:GLU:N      | 1:A:39:VAL:CG2   | 2.76        | 0.48     |
| 1:A:147:THR:HG23 | 1:A:150:ASP:OD2  | 2.13        | 0.48     |
| 1:A:229:LYS:O    | 1:A:232:ASP:N    | 2.43        | 0.48     |
| 1:B:361:GLU:CA   | 1:B:364:ARG:NH2  | 2.76        | 0.48     |
| 1:B:321:LEU:HD12 | 1:B:346:LEU:CD2  | 2.43        | 0.48     |
| 1:A:270:MET:HA   | 1:A:271:PRO:HD3  | 1.72        | 0.48     |
| 1:B:167:ASP:OD2  | 1:B:191:GLY:N    | 2.47        | 0.48     |
| 1:B:158:ASN:O    | 1:B:160:LEU:HG   | 2.13        | 0.48     |
| 1:B:160:LEU:O    | 1:B:163:LYS:N    | 2.37        | 0.48     |
| 1:A:87:VAL:O     | 1:A:91:ASN:N     | 2.44        | 0.48     |
| 1:A:238:ILE:N    | 1:A:238:ILE:HD13 | 2.28        | 0.48     |
| 1:B:422:HIS:CD2  | 2:B:600:FAD:C8M  | 2.73        | 0.48     |
| 1:B:148:TYR:O    | 1:B:152:HIS:N    | 2.45        | 0.48     |
| 1:B:6:GLU:N      | 1:B:39:VAL:CG2   | 2.76        | 0.48     |
| 1:A:69:PHE:HB3   | 1:A:113:PRO:O    | 2.14        | 0.48     |
| 1:A:463:ARG:HH21 | 1:B:138:ALA:CB   | 2.27        | 0.48     |
| 1:B:244:TYR:N    | 1:B:244:TYR:CD1  | 2.77        | 0.48     |
| 1:A:324:LYS:CE   | 1:A:334:LEU:HD21 | 2.44        | 0.48     |
| 1:A:158:ASN:O    | 1:A:160:LEU:HG   | 2.13        | 0.48     |
| 1:B:190:TYR:CE1  | 1:B:270:MET:HG3  | 2.48        | 0.48     |
| 1:A:149:HIS:C    | 1:A:153:ASN:HD22 | 2.17        | 0.48     |
| 1:A:472:VAL:HG12 | 1:A:473:PHE:H    | 1.79        | 0.48     |
| 1:B:478:LEU:HB2  | 1:B:479:ILE:HD12 | 1.95        | 0.48     |
| 1:B:87:VAL:O     | 1:B:91:ASN:N     | 2.44        | 0.48     |
| 1:B:108:TYR:HD1  | 1:B:505:THR:C    | 2.17        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:279:TYR:CD2  | 1:B:280:LEU:N    | 2.82        | 0.48     |
| 1:A:53:LYS:HA    | 1:A:54:PRO:HD3   | 1.70        | 0.48     |
| 1:A:496:ALA:N    | 4:A:605:HOH:O    | 2.46        | 0.48     |
| 1:A:148:TYR:O    | 1:A:152:HIS:N    | 2.44        | 0.47     |
| 1:B:24:PHE:CD2   | 1:B:95:PHE:CD2   | 3.01        | 0.47     |
| 1:B:484:VAL:O    | 1:B:488:MET:N    | 2.31        | 0.47     |
| 1:A:268:TRP:O    | 1:A:269:LEU:HD23 | 2.13        | 0.47     |
| 1:A:217:LEU:HB2  | 1:B:517:TYR:CE1  | 2.50        | 0.47     |
| 1:A:167:ASP:OD2  | 1:A:191:GLY:N    | 2.47        | 0.47     |
| 1:B:201:GLU:HA   | 1:B:210:LEU:O    | 2.14        | 0.47     |
| 1:A:201:GLU:HA   | 1:A:210:LEU:O    | 2.14        | 0.47     |
| 1:B:383:PHE:CD1  | 1:B:383:PHE:N    | 2.82        | 0.47     |
| 1:B:99:PRO:HA    | 1:B:121:LEU:HB3  | 1.97        | 0.47     |
| 1:B:268:TRP:O    | 1:B:269:LEU:HD23 | 2.14        | 0.47     |
| 1:B:243:PRO:CD   | 1:B:244:TYR:N    | 2.76        | 0.47     |
| 1:B:468:ILE:HG22 | 1:B:470:CYS:SG   | 2.54        | 0.47     |
| 1:A:9:PRO:HA     | 1:A:40:ILE:O     | 2.15        | 0.47     |
| 1:B:59:ASP:HA    | 1:B:60:PRO:HD2   | 1.67        | 0.47     |
| 1:B:324:LYS:CE   | 1:B:334:LEU:HD21 | 2.43        | 0.47     |
| 1:A:99:PRO:HA    | 1:A:121:LEU:HB3  | 1.96        | 0.47     |
| 1:A:95:PHE:CD1   | 1:A:96:PRO:CD    | 2.94        | 0.47     |
| 1:A:108:TYR:HD1  | 1:A:505:THR:C    | 2.17        | 0.47     |
| 1:A:61:HIS:N     | 1:A:61:HIS:CD2   | 2.82        | 0.47     |
| 1:A:160:LEU:HA   | 1:A:160:LEU:HD23 | 1.72        | 0.47     |
| 1:A:300:ARG:NH2  | 1:A:308:VAL:HA   | 2.18        | 0.47     |
| 1:A:283:LEU:HA   | 1:A:284:PRO:HD3  | 1.65        | 0.47     |
| 1:A:383:PHE:N    | 1:A:383:PHE:CD1  | 2.82        | 0.47     |
| 1:B:148:TYR:O    | 1:B:151:LEU:N    | 2.48        | 0.47     |
| 1:A:8:ARG:O      | 1:A:41:SER:HA    | 2.15        | 0.47     |
| 1:A:244:TYR:HH   | 1:B:195:MET:HG3  | 1.79        | 0.47     |
| 1:A:494:ASP:O    | 1:A:497:ALA:N    | 2.48        | 0.47     |
| 1:B:8:ARG:O      | 1:B:41:SER:HA    | 2.15        | 0.47     |
| 1:B:69:PHE:HB3   | 1:B:113:PRO:O    | 2.14        | 0.47     |
| 1:A:290:LYS:HG3  | 1:A:433:GLY:HA3  | 1.97        | 0.47     |
| 1:A:279:TYR:CD2  | 1:A:280:LEU:N    | 2.82        | 0.47     |
| 1:A:489:ARG:NE   | 1:A:512:GLN:OE1  | 2.46        | 0.47     |
| 1:B:229:LYS:O    | 1:B:232:ASP:N    | 2.43        | 0.47     |
| 1:B:37:VAL:CG1   | 1:B:38:GLU:N     | 2.78        | 0.47     |
| 1:B:238:ILE:HD13 | 1:B:238:ILE:N    | 2.28        | 0.47     |
| 1:A:204:LEU:HD23 | 1:A:204:LEU:HA   | 1.65        | 0.47     |
| 1:A:468:ILE:HG22 | 1:A:470:CYS:SG   | 2.54        | 0.47     |
| 1:B:152:HIS:CE1  | 1:B:161:ARG:NH2  | 2.80        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:24:PHE:CD2   | 1:A:95:PHE:CD2   | 3.01        | 0.47     |
| 1:A:418:PRO:CD   | 1:A:474:ASN:HD22 | 2.22        | 0.47     |
| 1:A:327:TYR:HB3  | 1:A:342:ILE:HD11 | 1.97        | 0.47     |
| 1:A:323:ASP:OD1  | 1:A:323:ASP:N    | 2.46        | 0.47     |
| 1:A:520:ASN:O    | 1:A:521:ASN:HB2  | 2.15        | 0.47     |
| 1:A:342:ILE:HA   | 1:A:345:GLN:HG3  | 1.97        | 0.47     |
| 1:A:14:PRO:C     | 1:A:16:LEU:N     | 2.69        | 0.47     |
| 1:B:290:LYS:HG3  | 1:B:433:GLY:HA3  | 1.97        | 0.47     |
| 1:A:79:ASN:ND2   | 1:A:81:ALA:N     | 2.63        | 0.47     |
| 1:B:494:ASP:C    | 1:B:498:ASN:HD22 | 2.18        | 0.47     |
| 1:B:472:VAL:HG12 | 1:B:473:PHE:H    | 1.79        | 0.47     |
| 1:B:99:PRO:HD3   | 1:B:542:ALA:HB2  | 1.97        | 0.46     |
| 1:A:242:PHE:HA   | 1:A:243:PRO:HD3  | 1.49        | 0.46     |
| 1:B:314:ILE:HB   | 1:B:350:ARG:O    | 2.15        | 0.46     |
| 1:B:441:ALA:O    | 1:B:444:LYS:HB3  | 2.15        | 0.46     |
| 1:A:143:GLU:HB3  | 1:A:144:PRO:CD   | 2.45        | 0.46     |
| 1:A:173:GLY:N    | 1:A:408:TYR:HE1  | 2.13        | 0.46     |
| 1:B:79:ASN:HD22  | 1:B:81:ALA:N     | 2.14        | 0.46     |
| 1:A:222:ARG:HG2  | 1:A:225:THR:OG1  | 2.16        | 0.46     |
| 1:B:361:GLU:N    | 1:B:362:PRO:CD   | 2.78        | 0.46     |
| 1:A:148:TYR:O    | 1:A:151:LEU:N    | 2.48        | 0.46     |
| 1:B:189:PRO:CA   | 1:B:307:ASN:HA   | 2.45        | 0.46     |
| 1:B:494:ASP:O    | 1:B:497:ALA:N    | 2.48        | 0.46     |
| 1:B:278:SER:HA   | 1:B:356:ALA:HA   | 1.97        | 0.46     |
| 1:B:541:ILE:O    | 1:B:541:ILE:HG22 | 2.16        | 0.46     |
| 1:A:155:LEU:O    | 1:A:160:LEU:N    | 2.40        | 0.46     |
| 1:B:8:ARG:HA     | 1:B:9:PRO:HD3    | 1.78        | 0.46     |
| 1:A:416:TRP:HE3  | 1:A:416:TRP:HA   | 1.79        | 0.46     |
| 1:A:276:TYR:OH   | 1:A:399:ASP:O    | 2.19        | 0.46     |
| 1:A:367:LEU:O    | 1:A:370:THR:HB   | 2.15        | 0.46     |
| 1:B:21:PHE:CE2   | 1:B:25:ILE:HG21  | 2.50        | 0.46     |
| 1:A:21:PHE:CE2   | 1:A:25:ILE:HG21  | 2.50        | 0.46     |
| 1:A:425:PHE:CG   | 1:A:488:MET:HE1  | 2.50        | 0.46     |
| 1:A:297:ARG:HB3  | 1:A:298:PRO:CD   | 2.43        | 0.46     |
| 1:A:321:LEU:HD12 | 1:A:346:LEU:HD23 | 1.97        | 0.46     |
| 1:B:399:ASP:O    | 1:B:403:GLN:HG2  | 2.15        | 0.46     |
| 1:A:413:TRP:CZ2  | 2:A:600:FAD:HM72 | 2.51        | 0.46     |
| 1:B:61:HIS:CD2   | 1:B:61:HIS:N     | 2.82        | 0.46     |
| 1:A:505:THR:OG1  | 1:A:513:ILE:HD12 | 2.16        | 0.46     |
| 1:B:321:LEU:HD12 | 1:B:346:LEU:HD23 | 1.96        | 0.46     |
| 1:B:137:GLY:O    | 1:B:138:ALA:HB3  | 2.16        | 0.46     |
| 1:B:428:ILE:HD13 | 1:B:428:ILE:HA   | 1.62        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:399:ASP:O    | 1:A:403:GLN:HG2  | 2.15        | 0.46     |
| 1:B:79:ASN:ND2   | 1:B:81:ALA:N     | 2.63        | 0.46     |
| 1:B:533:ASN:HD21 | 1:B:551:SER:N    | 2.14        | 0.46     |
| 1:A:99:PRO:HD3   | 1:A:542:ALA:HB2  | 1.97        | 0.46     |
| 1:A:309:PRO:HB2  | 1:A:353:PHE:HE1  | 1.78        | 0.46     |
| 1:A:484:VAL:O    | 1:A:488:MET:N    | 2.31        | 0.46     |
| 1:B:222:ARG:HG2  | 1:B:225:THR:OG1  | 2.16        | 0.46     |
| 1:A:217:LEU:HD22 | 1:A:217:LEU:HA   | 1.41        | 0.46     |
| 1:A:139:TYR:CD1  | 1:A:139:TYR:C    | 2.90        | 0.46     |
| 1:B:327:TYR:HB3  | 1:B:342:ILE:HD11 | 1.97        | 0.46     |
| 1:A:332:GLU:CB   | 1:A:333:PRO:CD   | 2.94        | 0.46     |
| 1:B:173:GLY:N    | 1:B:408:TYR:HE1  | 2.13        | 0.46     |
| 1:B:560:LEU:HD23 | 1:B:560:LEU:HA   | 1.50        | 0.46     |
| 1:B:280:LEU:HD12 | 1:B:281:ILE:N    | 2.31        | 0.46     |
| 1:A:164:LEU:C    | 1:A:165:TRP:CD1  | 2.89        | 0.46     |
| 1:A:441:ALA:O    | 1:A:444:LYS:HB3  | 2.15        | 0.46     |
| 1:B:367:LEU:O    | 1:B:370:THR:HB   | 2.15        | 0.46     |
| 1:A:533:ASN:HD21 | 1:A:551:SER:N    | 2.14        | 0.45     |
| 1:A:425:PHE:CE1  | 1:A:502:GLU:HG3  | 2.52        | 0.45     |
| 1:A:137:GLY:O    | 1:A:138:ALA:HB3  | 2.16        | 0.45     |
| 1:B:489:ARG:NE   | 1:B:512:GLN:OE1  | 2.46        | 0.45     |
| 1:A:230:PRO:HD2  | 1:A:231:GLU:HG2  | 1.99        | 0.45     |
| 1:A:37:VAL:CG1   | 1:A:38:GLU:N     | 2.78        | 0.45     |
| 1:A:428:ILE:CG2  | 1:B:238:ILE:HG21 | 2.46        | 0.45     |
| 1:B:143:GLU:HB3  | 1:B:144:PRO:CD   | 2.45        | 0.45     |
| 1:B:9:PRO:HA     | 1:B:40:ILE:O     | 2.15        | 0.45     |
| 1:A:189:PRO:CA   | 1:A:307:ASN:HA   | 2.45        | 0.45     |
| 1:B:342:ILE:HA   | 1:B:345:GLN:HG3  | 1.97        | 0.45     |
| 1:B:424:PHE:HD2  | 1:B:468:ILE:HG23 | 1.82        | 0.45     |
| 1:A:361:GLU:N    | 1:A:362:PRO:CD   | 2.78        | 0.45     |
| 1:B:425:PHE:CE1  | 1:B:502:GLU:HG3  | 2.52        | 0.45     |
| 1:A:141:VAL:HG21 | 1:A:240:HIS:CE1  | 2.52        | 0.45     |
| 1:B:141:VAL:HG21 | 1:B:240:HIS:CE1  | 2.52        | 0.45     |
| 1:A:14:PRO:HB2   | 1:A:15:LYS:HE3   | 1.99        | 0.45     |
| 1:A:16:LEU:HA    | 1:A:16:LEU:HD12  | 1.51        | 0.45     |
| 1:B:243:PRO:CG   | 1:B:244:TYR:N    | 2.79        | 0.45     |
| 1:A:314:ILE:HB   | 1:A:350:ARG:O    | 2.15        | 0.45     |
| 1:A:280:LEU:HD12 | 1:A:281:ILE:N    | 2.31        | 0.45     |
| 1:B:416:TRP:HE3  | 1:B:416:TRP:HA   | 1.79        | 0.45     |
| 1:A:278:SER:HA   | 1:A:356:ALA:HA   | 1.97        | 0.45     |
| 1:B:164:LEU:C    | 1:B:165:TRP:CD1  | 2.89        | 0.45     |
| 1:B:424:PHE:CE2  | 3:B:601:EUG:H6   | 2.51        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:413:TRP:CZ2  | 2:B:600:FAD:HM72 | 2.51        | 0.45     |
| 1:A:487:LEU:HD11 | 1:A:491:LEU:CD1  | 2.44        | 0.45     |
| 1:A:243:PRO:CG   | 1:A:244:TYR:N    | 2.79        | 0.45     |
| 1:B:139:TYR:CD1  | 1:B:139:TYR:C    | 2.90        | 0.45     |
| 1:B:25:ILE:HD12  | 1:B:25:ILE:HA    | 1.78        | 0.45     |
| 1:A:56:HIS:O     | 1:A:111:ALA:HB1  | 2.17        | 0.45     |
| 1:B:269:LEU:HD23 | 1:B:269:LEU:HA   | 1.81        | 0.45     |
| 1:B:267:ILE:HG22 | 1:B:267:ILE:O    | 2.10        | 0.45     |
| 1:A:424:PHE:CE2  | 3:A:601:EUG:H6   | 2.51        | 0.45     |
| 1:A:149:HIS:HB2  | 1:A:408:TYR:OH   | 2.17        | 0.45     |
| 1:B:56:HIS:O     | 1:B:111:ALA:HB1  | 2.17        | 0.45     |
| 1:A:487:LEU:CD1  | 1:A:491:LEU:CD1  | 2.95        | 0.45     |
| 1:B:487:LEU:CD1  | 1:B:491:LEU:CD1  | 2.95        | 0.45     |
| 1:A:112:ALA:HA   | 1:A:113:PRO:HD3  | 1.69        | 0.45     |
| 1:A:513:ILE:HA   | 1:A:516:THR:HG23 | 1.98        | 0.45     |
| 1:A:284:PRO:HG2  | 1:A:379:PRO:O    | 2.17        | 0.45     |
| 1:A:287:GLY:HA2  | 1:A:437:MET:CE   | 2.47        | 0.45     |
| 1:A:171:LEU:HD21 | 2:A:600:FAD:HM73 | 1.99        | 0.45     |
| 1:B:550:PRO:HB2  | 1:B:552:GLN:HG2  | 1.99        | 0.45     |
| 1:B:149:HIS:HB2  | 1:B:408:TYR:OH   | 2.17        | 0.45     |
| 1:A:10:LEU:HD11  | 1:A:41:SER:C     | 2.37        | 0.45     |
| 1:B:505:THR:OG1  | 1:B:513:ILE:HD12 | 2.16        | 0.45     |
| 1:B:513:ILE:HA   | 1:B:516:THR:HG23 | 1.98        | 0.45     |
| 1:B:287:GLY:HA2  | 1:B:437:MET:CE   | 2.47        | 0.45     |
| 1:B:293:VAL:C    | 1:B:295:ILE:N    | 2.68        | 0.45     |
| 1:A:79:ASN:HD22  | 1:A:81:ALA:N     | 2.14        | 0.45     |
| 1:B:438:MET:O    | 1:B:442:VAL:HG23 | 2.17        | 0.45     |
| 1:A:405:ILE:HA   | 1:A:406:PRO:HD2  | 1.79        | 0.45     |
| 1:B:204:LEU:HD23 | 1:B:204:LEU:HA   | 1.65        | 0.45     |
| 1:A:263:THR:HG1  | 1:A:263:THR:H    | 1.46        | 0.45     |
| 1:B:348:LEU:HD23 | 1:B:348:LEU:HA   | 1.69        | 0.45     |
| 1:B:520:ASN:O    | 1:B:521:ASN:HB2  | 2.15        | 0.45     |
| 1:B:171:LEU:HD21 | 2:B:600:FAD:HM73 | 1.99        | 0.44     |
| 1:B:10:LEU:HD11  | 1:B:41:SER:C     | 2.37        | 0.44     |
| 1:A:185:VAL:CG1  | 1:A:186:GLY:N    | 2.80        | 0.44     |
| 1:B:40:ILE:O     | 1:B:40:ILE:HG22  | 2.18        | 0.44     |
| 1:B:287:GLY:HA2  | 1:B:437:MET:HE2  | 1.99        | 0.44     |
| 1:A:89:LEU:N     | 1:A:89:LEU:HD12  | 2.33        | 0.44     |
| 1:B:385:PHE:HA   | 1:B:386:PRO:HD3  | 1.68        | 0.44     |
| 1:B:279:TYR:O    | 1:B:395:LEU:HD11 | 2.17        | 0.44     |
| 1:A:339:LEU:O    | 1:A:342:ILE:N    | 2.51        | 0.44     |
| 1:B:230:PRO:HD2  | 1:B:231:GLU:OE2  | 2.18        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:267:ILE:HA   | 1:B:267:ILE:HD13 | 1.57        | 0.44     |
| 1:A:151:LEU:HD12 | 1:A:151:LEU:C    | 2.37        | 0.44     |
| 1:A:155:LEU:HD23 | 1:A:155:LEU:HA   | 1.63        | 0.44     |
| 1:B:14:PRO:C     | 1:B:16:LEU:N     | 2.68        | 0.44     |
| 1:B:72:SER:HB3   | 1:B:117:GLY:O    | 2.17        | 0.44     |
| 1:A:283:LEU:HD12 | 1:A:351:TRP:CB   | 2.47        | 0.44     |
| 1:B:283:LEU:HA   | 1:B:284:PRO:HD3  | 1.65        | 0.44     |
| 1:B:89:LEU:O     | 1:B:92:LYS:N     | 2.51        | 0.44     |
| 1:B:53:LYS:HA    | 1:B:54:PRO:HD3   | 1.70        | 0.44     |
| 1:A:279:TYR:O    | 1:A:395:LEU:HD11 | 2.17        | 0.44     |
| 1:B:230:PRO:HD2  | 1:B:231:GLU:HG2  | 1.98        | 0.44     |
| 1:B:372:LYS:HA   | 1:B:383:PHE:CE2  | 2.52        | 0.44     |
| 1:A:372:LYS:HA   | 1:A:383:PHE:CE2  | 2.52        | 0.44     |
| 1:B:97:LEU:O     | 1:B:542:ALA:HA   | 2.17        | 0.44     |
| 1:B:487:LEU:CD1  | 1:B:491:LEU:HD11 | 2.44        | 0.44     |
| 1:B:284:PRO:HG2  | 1:B:379:PRO:O    | 2.17        | 0.44     |
| 1:A:214:MET:CB   | 1:A:239:ALA:HA   | 2.46        | 0.44     |
| 1:A:541:ILE:O    | 1:A:541:ILE:HG22 | 2.16        | 0.44     |
| 1:B:387:GLU:HG3  | 1:B:387:GLU:H    | 1.22        | 0.44     |
| 1:B:188:THR:HB   | 1:B:189:PRO:HD2  | 1.99        | 0.44     |
| 1:A:424:PHE:HD2  | 1:A:468:ILE:HG23 | 1.82        | 0.44     |
| 1:B:72:SER:HB3   | 1:B:117:GLY:HA2  | 1.99        | 0.44     |
| 1:A:97:LEU:HD23  | 1:A:97:LEU:HA    | 1.48        | 0.44     |
| 1:A:438:MET:O    | 1:A:442:VAL:HG23 | 2.17        | 0.44     |
| 1:A:72:SER:HB3   | 1:A:117:GLY:HA2  | 1.99        | 0.44     |
| 1:A:90:ALA:HB2   | 1:A:97:LEU:HD11  | 2.00        | 0.44     |
| 1:B:487:LEU:HD11 | 1:B:491:LEU:CD1  | 2.44        | 0.44     |
| 1:B:283:LEU:HD12 | 1:B:351:TRP:CB   | 2.48        | 0.44     |
| 1:B:89:LEU:HD12  | 1:B:89:LEU:N     | 2.33        | 0.44     |
| 1:B:270:MET:HA   | 1:B:271:PRO:HD3  | 1.72        | 0.44     |
| 1:A:332:GLU:HB3  | 1:A:333:PRO:HD2  | 1.98        | 0.44     |
| 1:B:535:VAL:C    | 1:B:537:PRO:HD3  | 2.38        | 0.44     |
| 1:A:535:VAL:C    | 1:A:537:PRO:HD3  | 2.38        | 0.44     |
| 1:A:550:PRO:HB2  | 1:A:552:GLN:HG2  | 1.99        | 0.44     |
| 1:A:545:LYS:C    | 1:A:547:GLY:N    | 2.71        | 0.44     |
| 1:B:332:GLU:HB3  | 1:B:333:PRO:HD2  | 1.98        | 0.44     |
| 1:A:97:LEU:O     | 1:A:542:ALA:HA   | 2.17        | 0.44     |
| 1:A:80:VAL:O     | 1:A:83:VAL:HB    | 2.17        | 0.44     |
| 1:A:378:ILE:HA   | 1:A:379:PRO:HD2  | 1.83        | 0.44     |
| 1:B:102:ILE:HG13 | 1:B:175:SER:HB2  | 1.99        | 0.44     |
| 1:A:389:THR:CB   | 1:A:390:PRO:CD   | 2.95        | 0.44     |
| 1:A:330:ARG:HH22 | 1:A:335:SER:HB3  | 1.83        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:177:LEU:HD22 | 1:A:265:ILE:CG2  | 2.26        | 0.43     |
| 1:B:16:LEU:HD12  | 1:B:16:LEU:HA    | 1.51        | 0.43     |
| 1:B:90:ALA:HB2   | 1:B:97:LEU:HD11  | 2.00        | 0.43     |
| 1:A:72:SER:HB3   | 1:A:117:GLY:C    | 2.39        | 0.43     |
| 1:A:546:SER:OG   | 1:B:247:GLY:HA2  | 2.17        | 0.43     |
| 1:A:552:GLN:CD   | 1:A:552:GLN:H    | 2.22        | 0.43     |
| 1:B:80:VAL:O     | 1:B:83:VAL:HB    | 2.17        | 0.43     |
| 1:B:339:LEU:O    | 1:B:342:ILE:N    | 2.51        | 0.43     |
| 1:A:494:ASP:C    | 1:A:498:ASN:HD22 | 2.18        | 0.43     |
| 1:B:23:GLU:O     | 1:B:26:GLN:N     | 2.51        | 0.43     |
| 1:B:330:ARG:HH22 | 1:B:335:SER:HB3  | 1.83        | 0.43     |
| 1:B:72:SER:HB3   | 1:B:117:GLY:C    | 2.39        | 0.43     |
| 1:A:72:SER:HB3   | 1:A:117:GLY:O    | 2.17        | 0.43     |
| 1:A:487:LEU:CD1  | 1:A:491:LEU:HD11 | 2.44        | 0.43     |
| 1:A:346:LEU:O    | 1:A:347:ASN:HB2  | 2.19        | 0.43     |
| 1:B:272:ASN:HA   | 1:B:273:PRO:HD3  | 1.64        | 0.43     |
| 1:A:27:ASP:O     | 1:A:30:ARG:HB3   | 2.18        | 0.43     |
| 1:B:27:ASP:O     | 1:B:30:ARG:HB3   | 2.18        | 0.43     |
| 1:B:432:SER:OG   | 1:B:435:ASP:HB2  | 2.19        | 0.43     |
| 1:A:537:PRO:O    | 1:A:552:GLN:NE2  | 2.51        | 0.43     |
| 1:A:560:LEU:HA   | 1:A:560:LEU:HD23 | 1.50        | 0.43     |
| 1:B:440:TYR:O    | 1:B:444:LYS:HB2  | 2.19        | 0.43     |
| 1:A:417:LEU:HD22 | 1:A:473:PHE:HA   | 2.00        | 0.43     |
| 1:B:14:PRO:HB2   | 1:B:15:LYS:HE3   | 1.99        | 0.43     |
| 1:B:545:LYS:C    | 1:B:547:GLY:N    | 2.71        | 0.43     |
| 1:A:58:HIS:HA    | 1:A:112:ALA:HB2  | 2.01        | 0.43     |
| 1:A:188:THR:HB   | 1:A:189:PRO:CD   | 2.49        | 0.43     |
| 1:A:323:ASP:OD2  | 1:A:325:ARG:HB3  | 2.18        | 0.43     |
| 1:B:537:PRO:O    | 1:B:552:GLN:NE2  | 2.52        | 0.43     |
| 1:A:10:LEU:HD12  | 1:A:10:LEU:N     | 2.34        | 0.43     |
| 1:A:134:ASN:HB3  | 1:A:139:TYR:CZ   | 2.54        | 0.43     |
| 1:A:230:PRO:HD2  | 1:A:231:GLU:OE2  | 2.18        | 0.43     |
| 1:B:417:LEU:HD22 | 1:B:473:PHE:HA   | 2.00        | 0.43     |
| 1:A:428:ILE:HA   | 1:A:428:ILE:HD13 | 1.62        | 0.43     |
| 1:B:536:ASP:HA   | 1:B:537:PRO:HD3  | 1.34        | 0.43     |
| 1:B:56:HIS:HA    | 1:B:111:ALA:HB2  | 1.97        | 0.43     |
| 1:B:464:GLU:CG   | 1:B:465:MET:N    | 2.80        | 0.43     |
| 1:A:89:LEU:O     | 1:A:92:LYS:N     | 2.51        | 0.43     |
| 1:A:241:LEU:HB3  | 1:B:463:ARG:O    | 2.19        | 0.43     |
| 1:A:188:THR:HB   | 1:A:189:PRO:HD2  | 1.99        | 0.43     |
| 1:A:418:PRO:HB2  | 1:A:474:ASN:HD21 | 1.84        | 0.43     |
| 1:A:452:LEU:HA   | 1:A:452:LEU:HD23 | 1.18        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:40:ILE:HG22  | 1:A:40:ILE:O     | 2.17        | 0.43     |
| 2:B:600:FAD:N1   | 2:B:600:FAD:O3'  | 2.28        | 0.43     |
| 1:A:98:TRP:CD2   | 1:A:113:PRO:HA   | 2.54        | 0.43     |
| 1:B:395:LEU:HD12 | 1:B:395:LEU:HA   | 1.93        | 0.43     |
| 1:B:188:THR:HB   | 1:B:189:PRO:CD   | 2.49        | 0.43     |
| 1:A:51:TYR:CE1   | 1:A:104:ARG:HD3  | 2.54        | 0.42     |
| 1:B:413:TRP:HE3  | 1:B:413:TRP:C    | 2.22        | 0.42     |
| 1:B:14:PRO:CB    | 1:B:15:LYS:HE3   | 2.49        | 0.42     |
| 1:B:425:PHE:CG   | 1:B:488:MET:HE1  | 2.54        | 0.42     |
| 1:A:233:GLN:HG3  | 1:A:233:GLN:H    | 1.32        | 0.42     |
| 1:B:323:ASP:OD2  | 1:B:325:ARG:HB3  | 2.18        | 0.42     |
| 1:B:413:TRP:C    | 1:B:415:ASP:N    | 2.72        | 0.42     |
| 1:A:177:LEU:CD2  | 1:A:265:ILE:HG22 | 2.26        | 0.42     |
| 1:B:346:LEU:O    | 1:B:347:ASN:HB2  | 2.19        | 0.42     |
| 1:B:134:ASN:HB3  | 1:B:139:TYR:CZ   | 2.54        | 0.42     |
| 1:B:386:PRO:N    | 1:B:395:LEU:HD23 | 2.34        | 0.42     |
| 1:B:332:GLU:HB3  | 1:B:333:PRO:CD   | 2.50        | 0.42     |
| 1:B:335:SER:OG   | 1:B:338:GLU:N    | 2.42        | 0.42     |
| 1:B:552:GLN:H    | 1:B:552:GLN:CD   | 2.22        | 0.42     |
| 1:A:14:PRO:CB    | 1:A:15:LYS:HE3   | 2.49        | 0.42     |
| 1:A:312:ARG:O    | 1:A:352:ASN:N    | 2.53        | 0.42     |
| 1:A:249:TYR:CE1  | 1:A:251:ASP:CG   | 2.93        | 0.42     |
| 1:A:104:ARG:C    | 1:A:106:SER:H    | 2.23        | 0.42     |
| 1:A:413:TRP:C    | 1:A:415:ASP:N    | 2.72        | 0.42     |
| 1:B:505:THR:CG2  | 1:B:513:ILE:HD12 | 2.50        | 0.42     |
| 1:A:386:PRO:N    | 1:A:395:LEU:HD23 | 2.34        | 0.42     |
| 1:B:104:ARG:C    | 1:B:106:SER:H    | 2.23        | 0.42     |
| 1:B:177:LEU:HD22 | 1:B:265:ILE:CG2  | 2.26        | 0.42     |
| 1:B:152:HIS:CE1  | 1:B:156:GLU:OE1  | 2.73        | 0.42     |
| 1:A:463:ARG:NH2  | 1:B:138:ALA:HB3  | 2.34        | 0.42     |
| 1:A:440:TYR:O    | 1:A:444:LYS:HB2  | 2.19        | 0.42     |
| 1:B:330:ARG:CZ   | 1:B:338:GLU:OE1  | 2.68        | 0.42     |
| 1:A:413:TRP:C    | 1:A:413:TRP:HE3  | 2.22        | 0.42     |
| 1:B:102:ILE:HD13 | 1:B:102:ILE:HA   | 1.87        | 0.42     |
| 1:A:200:MET:CE   | 1:A:251:ASP:CB   | 2.97        | 0.42     |
| 1:B:324:LYS:N    | 1:B:416:TRP:CE3  | 2.88        | 0.42     |
| 1:B:454:PHE:C    | 1:B:454:PHE:CD1  | 2.93        | 0.42     |
| 1:A:156:GLU:O    | 1:A:159:ASN:N    | 2.43        | 0.42     |
| 1:B:10:LEU:N     | 1:B:10:LEU:HD12  | 2.33        | 0.42     |
| 1:B:108:TYR:CD1  | 1:B:505:THR:C    | 2.93        | 0.42     |
| 1:B:58:HIS:HA    | 1:B:112:ALA:HB2  | 2.01        | 0.42     |
| 1:B:98:TRP:CD2   | 1:B:113:PRO:HA   | 2.54        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:293:VAL:C    | 1:A:295:ILE:N    | 2.68        | 0.42     |
| 1:A:295:ILE:HD12 | 1:A:378:ILE:CD1  | 2.48        | 0.42     |
| 2:A:600:FAD:C4   | 3:A:601:EUG:C2   | 2.97        | 0.42     |
| 1:A:296:ILE:H    | 1:A:296:ILE:HG13 | 1.57        | 0.42     |
| 1:B:332:GLU:CB   | 1:B:333:PRO:CD   | 2.94        | 0.42     |
| 1:A:23:GLU:O     | 1:A:26:GLN:N     | 2.51        | 0.42     |
| 1:A:432:SER:OG   | 1:A:435:ASP:HB2  | 2.19        | 0.42     |
| 2:B:600:FAD:C4   | 3:B:601:EUG:C2   | 2.97        | 0.42     |
| 1:A:58:HIS:CA    | 1:A:112:ALA:HB2  | 2.50        | 0.42     |
| 1:B:249:TYR:CE1  | 1:B:251:ASP:CG   | 2.93        | 0.42     |
| 1:B:299:LEU:HB3  | 1:B:305:LEU:HG   | 2.02        | 0.42     |
| 1:B:202:VAL:HG12 | 1:B:203:VAL:N    | 2.34        | 0.42     |
| 1:B:418:PRO:HB2  | 1:B:474:ASN:HD21 | 1.84        | 0.42     |
| 1:A:324:LYS:N    | 1:A:416:TRP:CE3  | 2.88        | 0.42     |
| 1:B:493:ASP:O    | 1:B:496:ALA:HB3  | 2.20        | 0.42     |
| 1:A:12:LEU:HD13  | 1:A:16:LEU:O     | 2.20        | 0.41     |
| 1:B:479:ILE:C    | 1:B:483:LYS:HE3  | 2.40        | 0.41     |
| 1:A:505:THR:CG2  | 1:A:513:ILE:HD12 | 2.50        | 0.41     |
| 1:B:242:PHE:HA   | 1:B:243:PRO:HD3  | 1.49        | 0.41     |
| 1:B:229:LYS:CB   | 1:B:230:PRO:CD   | 2.98        | 0.41     |
| 1:A:332:GLU:HB3  | 1:A:333:PRO:CD   | 2.50        | 0.41     |
| 1:A:201:GLU:HB3  | 1:A:264:LYS:HB2  | 2.02        | 0.41     |
| 1:A:422:HIS:HD1  | 1:A:422:HIS:H    | 1.68        | 0.41     |
| 1:B:411:LEU:O    | 1:B:414:ILE:N    | 2.46        | 0.41     |
| 1:B:422:HIS:H    | 1:B:422:HIS:HD1  | 1.68        | 0.41     |
| 1:B:536:ASP:N    | 1:B:537:PRO:HD3  | 2.26        | 0.41     |
| 1:A:479:ILE:C    | 1:A:483:LYS:HE3  | 2.40        | 0.41     |
| 1:A:463:ARG:HH21 | 1:B:138:ALA:HB3  | 1.85        | 0.41     |
| 1:B:367:LEU:O    | 1:B:370:THR:N    | 2.53        | 0.41     |
| 1:B:378:ILE:HA   | 1:B:379:PRO:HD2  | 1.83        | 0.41     |
| 1:B:185:VAL:CG1  | 1:B:186:GLY:N    | 2.80        | 0.41     |
| 1:B:10:LEU:HD11  | 1:B:42:SER:N     | 2.35        | 0.41     |
| 1:B:278:SER:OG   | 1:B:399:ASP:OD2  | 2.30        | 0.41     |
| 1:A:493:ASP:O    | 1:A:496:ALA:HB3  | 2.20        | 0.41     |
| 1:A:454:PHE:CD1  | 1:A:454:PHE:C    | 2.93        | 0.41     |
| 1:B:68:TYR:CD1   | 1:B:68:TYR:C     | 2.94        | 0.41     |
| 1:A:168:VAL:HA   | 1:A:169:PRO:HD3  | 1.75        | 0.41     |
| 1:A:411:LEU:O    | 1:A:414:ILE:N    | 2.46        | 0.41     |
| 1:A:535:VAL:CG1  | 1:B:531:LEU:HD21 | 2.50        | 0.41     |
| 1:A:152:HIS:CE1  | 1:A:156:GLU:OE1  | 2.73        | 0.41     |
| 1:B:151:LEU:HA   | 1:B:151:LEU:HD12 | 1.75        | 0.41     |
| 1:B:160:LEU:HA   | 1:B:160:LEU:HD23 | 1.72        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:12:LEU:HD13  | 1:B:16:LEU:O     | 2.20        | 0.41     |
| 1:A:10:LEU:HD11  | 1:A:42:SER:N     | 2.35        | 0.41     |
| 1:A:108:TYR:CD1  | 1:A:505:THR:C    | 2.93        | 0.41     |
| 1:B:60:PRO:C     | 1:B:62:HIS:H     | 2.24        | 0.41     |
| 1:A:330:ARG:CZ   | 1:A:338:GLU:OE1  | 2.68        | 0.41     |
| 1:A:363:ILE:HG12 | 1:B:363:ILE:HG12 | 2.02        | 0.41     |
| 1:A:139:TYR:HA   | 1:A:269:LEU:H    | 1.86        | 0.41     |
| 1:B:281:ILE:HG21 | 1:B:375:PHE:CD2  | 2.56        | 0.41     |
| 1:B:385:PHE:O    | 1:B:388:ASP:N    | 2.54        | 0.41     |
| 1:A:202:VAL:HG12 | 1:A:203:VAL:N    | 2.34        | 0.41     |
| 1:A:367:LEU:O    | 1:A:370:THR:N    | 2.53        | 0.41     |
| 1:B:316:LEU:HD11 | 1:B:413:TRP:CE2  | 2.55        | 0.41     |
| 1:B:58:HIS:CA    | 1:B:112:ALA:HB2  | 2.50        | 0.41     |
| 1:B:112:ALA:HA   | 1:B:113:PRO:HD3  | 1.69        | 0.41     |
| 1:A:385:PHE:HA   | 1:A:386:PRO:HD3  | 1.68        | 0.41     |
| 1:B:164:LEU:O    | 1:B:165:TRP:HD1  | 2.04        | 0.41     |
| 1:B:201:GLU:HB3  | 1:B:264:LYS:HB2  | 2.02        | 0.41     |
| 1:B:452:LEU:HD23 | 1:B:452:LEU:HA   | 1.18        | 0.41     |
| 1:A:316:LEU:HD11 | 1:A:413:TRP:CE2  | 2.55        | 0.41     |
| 1:B:51:TYR:CE1   | 1:B:104:ARG:HD3  | 2.54        | 0.41     |
| 1:B:39:VAL:CG1   | 1:B:40:ILE:N     | 2.84        | 0.41     |
| 1:A:387:GLU:HG3  | 1:A:387:GLU:H    | 1.22        | 0.41     |
| 1:B:156:GLU:C    | 1:B:158:ASN:N    | 2.74        | 0.41     |
| 1:B:258:ASN:HB3  | 1:B:542:ALA:O    | 2.21        | 0.41     |
| 1:A:540:ILE:HA   | 1:A:540:ILE:HD13 | 1.71        | 0.41     |
| 1:A:542:ALA:HA   | 1:A:543:PRO:HD2  | 1.78        | 0.41     |
| 1:A:505:THR:CG2  | 1:A:513:ILE:CD1  | 2.99        | 0.41     |
| 1:A:59:ASP:HA    | 1:A:60:PRO:HD2   | 1.67        | 0.41     |
| 1:A:60:PRO:C     | 1:A:62:HIS:H     | 2.24        | 0.41     |
| 1:B:283:LEU:O    | 1:B:349:GLY:CA   | 2.69        | 0.41     |
| 1:A:281:ILE:HG21 | 1:A:375:PHE:CD2  | 2.56        | 0.41     |
| 1:A:230:PRO:O    | 1:B:519:TRP:HZ2  | 2.02        | 0.41     |
| 1:B:444:LYS:HB3  | 1:B:445:LYS:H    | 1.66        | 0.41     |
| 1:A:409:ASP:O    | 1:A:412:LYS:HG3  | 2.21        | 0.41     |
| 1:B:74:ILE:HG22  | 1:B:75:VAL:N     | 2.35        | 0.41     |
| 1:A:419:ASN:C    | 1:A:474:ASN:HA   | 2.39        | 0.41     |
| 1:A:283:LEU:O    | 1:A:349:GLY:CA   | 2.69        | 0.41     |
| 1:B:312:ARG:O    | 1:B:352:ASN:N    | 2.53        | 0.41     |
| 1:B:139:TYR:HA   | 1:B:269:LEU:H    | 1.86        | 0.41     |
| 1:B:200:MET:CE   | 1:B:251:ASP:CB   | 2.97        | 0.41     |
| 1:A:164:LEU:O    | 1:A:165:TRP:HD1  | 2.04        | 0.41     |
| 1:A:495:CYS:HA   | 1:A:500:TRP:HE3  | 1.86        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:330:ARG:NH1  | 1:B:338:GLU:OE1  | 2.54        | 0.41     |
| 1:B:214:MET:CB   | 1:B:239:ALA:HA   | 2.46        | 0.40     |
| 1:A:166:LEU:HA   | 1:A:166:LEU:HD23 | 1.82        | 0.40     |
| 1:A:104:ARG:N    | 2:A:600:FAD:O2P  | 2.55        | 0.40     |
| 1:A:339:LEU:O    | 1:A:343:ALA:N    | 2.49        | 0.40     |
| 1:A:68:TYR:CD1   | 1:A:68:TYR:C     | 2.94        | 0.40     |
| 1:A:279:TYR:HB2  | 1:A:280:LEU:H    | 1.60        | 0.40     |
| 1:B:129:ARG:HB2  | 1:B:131:LEU:CD2  | 2.51        | 0.40     |
| 1:B:198:SER:O    | 1:B:240:HIS:HD2  | 2.04        | 0.40     |
| 1:A:330:ARG:NH1  | 1:A:338:GLU:OE1  | 2.54        | 0.40     |
| 1:A:302:GLY:O    | 1:A:303:MET:HB2  | 2.21        | 0.40     |
| 1:A:258:ASN:HB3  | 1:A:542:ALA:O    | 2.21        | 0.40     |
| 1:B:419:ASN:C    | 1:B:474:ASN:HA   | 2.39        | 0.40     |
| 1:A:385:PHE:O    | 1:A:388:ASP:N    | 2.54        | 0.40     |
| 1:B:400:LYS:O    | 1:B:403:GLN:HG2  | 2.21        | 0.40     |
| 1:A:198:SER:O    | 1:A:240:HIS:HD2  | 2.04        | 0.40     |
| 1:B:477:ASP:OD2  | 1:B:480:GLN:HB2  | 2.21        | 0.40     |
| 1:B:302:GLY:O    | 1:B:303:MET:HB2  | 2.21        | 0.40     |
| 1:A:154:TYR:CD1  | 1:A:154:TYR:C    | 2.95        | 0.40     |
| 1:B:119:VAL:HG12 | 1:B:120:VAL:N    | 2.37        | 0.40     |
| 1:A:10:LEU:CD1   | 1:A:41:SER:C     | 2.90        | 0.40     |
| 1:A:119:VAL:HG12 | 1:A:120:VAL:N    | 2.37        | 0.40     |
| 1:A:24:PHE:CE1   | 1:A:28:ILE:HD11  | 2.56        | 0.40     |
| 1:B:502:GLU:N    | 1:B:502:GLU:CD   | 2.75        | 0.40     |
| 1:A:344:LYS:C    | 1:A:346:LEU:N    | 2.75        | 0.40     |
| 1:B:314:ILE:HG23 | 1:B:315:LEU:N    | 2.36        | 0.40     |
| 1:A:385:PHE:CB   | 1:A:386:PRO:CD   | 2.97        | 0.40     |
| 1:A:477:ASP:OD2  | 1:A:480:GLN:HB2  | 2.21        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 1   | A     | 553/560 (99%) | 472 (85%) | 69 (12%) | 12 (2%)  | 10 32       |

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| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 1   | B     | 553/560 (99%)   | 472 (85%) | 69 (12%)  | 12 (2%)  | 10          | 32 |
| All | All   | 1106/1120 (99%) | 944 (85%) | 138 (12%) | 24 (2%)  | 10          | 32 |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | ILE  |
| 1   | A     | 559 | LYS  |
| 1   | B     | 46  | ILE  |
| 1   | B     | 559 | LYS  |
| 1   | A     | 157 | ALA  |
| 1   | B     | 157 | ALA  |
| 1   | A     | 391 | GLU  |
| 1   | A     | 517 | TYR  |
| 1   | B     | 391 | GLU  |
| 1   | B     | 517 | TYR  |
| 1   | A     | 127 | MET  |
| 1   | A     | 166 | LEU  |
| 1   | B     | 127 | MET  |
| 1   | B     | 166 | LEU  |
| 1   | A     | 104 | ARG  |
| 1   | A     | 388 | ASP  |
| 1   | B     | 104 | ARG  |
| 1   | B     | 388 | ASP  |
| 1   | A     | 199 | GLY  |
| 1   | A     | 284 | PRO  |
| 1   | B     | 199 | GLY  |
| 1   | B     | 284 | PRO  |
| 1   | A     | 542 | ALA  |
| 1   | B     | 542 | ALA  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 475/482 (98%) | 445 (94%) | 30 (6%)  | 25          | 59 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | B     | 475/482 (98%) | 445 (94%) | 30 (6%)  | 25          | 59 |
| All | All   | 950/964 (98%) | 890 (94%) | 60 (6%)  | 25          | 59 |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 27  | ASP  |
| 1   | A     | 64  | MET  |
| 1   | A     | 65  | ASP  |
| 1   | A     | 78  | ARG  |
| 1   | A     | 79  | ASN  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 95  | PHE  |
| 1   | A     | 114 | ARG  |
| 1   | A     | 128 | ASN  |
| 1   | A     | 136 | GLU  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 224 | GLU  |
| 1   | A     | 243 | PRO  |
| 1   | A     | 248 | PRO  |
| 1   | A     | 251 | ASP  |
| 1   | A     | 314 | ILE  |
| 1   | A     | 350 | ARG  |
| 1   | A     | 361 | GLU  |
| 1   | A     | 373 | ASP  |
| 1   | A     | 384 | TYR  |
| 1   | A     | 407 | THR  |
| 1   | A     | 409 | ASP  |
| 1   | A     | 413 | TRP  |
| 1   | A     | 464 | GLU  |
| 1   | A     | 478 | LEU  |
| 1   | A     | 488 | MET  |
| 1   | A     | 503 | TYR  |
| 1   | A     | 505 | THR  |
| 1   | A     | 520 | ASN  |
| 1   | A     | 552 | GLN  |
| 1   | B     | 27  | ASP  |
| 1   | B     | 64  | MET  |
| 1   | B     | 65  | ASP  |
| 1   | B     | 78  | ARG  |
| 1   | B     | 79  | ASN  |
| 1   | B     | 91  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 95  | PHE  |
| 1   | B     | 114 | ARG  |
| 1   | B     | 128 | ASN  |
| 1   | B     | 136 | GLU  |
| 1   | B     | 177 | LEU  |
| 1   | B     | 224 | GLU  |
| 1   | B     | 243 | PRO  |
| 1   | B     | 248 | PRO  |
| 1   | B     | 251 | ASP  |
| 1   | B     | 314 | ILE  |
| 1   | B     | 350 | ARG  |
| 1   | B     | 361 | GLU  |
| 1   | B     | 373 | ASP  |
| 1   | B     | 384 | TYR  |
| 1   | B     | 407 | THR  |
| 1   | B     | 409 | ASP  |
| 1   | B     | 413 | TRP  |
| 1   | B     | 464 | GLU  |
| 1   | B     | 478 | LEU  |
| 1   | B     | 488 | MET  |
| 1   | B     | 503 | TYR  |
| 1   | B     | 505 | THR  |
| 1   | B     | 520 | ASN  |
| 1   | B     | 552 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 79  | ASN  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 152 | HIS  |
| 1   | A     | 153 | ASN  |
| 1   | A     | 197 | HIS  |
| 1   | A     | 240 | HIS  |
| 1   | A     | 352 | ASN  |
| 1   | A     | 403 | GLN  |
| 1   | A     | 467 | HIS  |
| 1   | A     | 474 | ASN  |
| 1   | A     | 485 | GLN  |
| 1   | A     | 520 | ASN  |
| 1   | A     | 528 | ASN  |
| 1   | A     | 533 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 552 | GLN  |
| 1   | B     | 79  | ASN  |
| 1   | B     | 91  | ASN  |
| 1   | B     | 152 | HIS  |
| 1   | B     | 153 | ASN  |
| 1   | B     | 197 | HIS  |
| 1   | B     | 240 | HIS  |
| 1   | B     | 352 | ASN  |
| 1   | B     | 403 | GLN  |
| 1   | B     | 474 | ASN  |
| 1   | B     | 485 | GLN  |
| 1   | B     | 520 | ASN  |
| 1   | B     | 528 | ASN  |
| 1   | B     | 533 | ASN  |
| 1   | B     | 552 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | FAD  | A     | 600 | 1    | 58,58,58     | 0.90 | 2 (3%)   | 85,89,89    | 1.21 | 6 (7%)   |
| 3   | EUG  | A     | 601 | -    | 10,11,12     | 0.41 | 0        | 13,14,15    | 1.63 | 2 (15%)  |
| 2   | FAD  | B     | 600 | 1    | 58,58,58     | 0.89 | 2 (3%)   | 85,89,89    | 1.22 | 5 (5%)   |
| 3   | EUG  | B     | 601 | -    | 10,11,12     | 0.42 | 0        | 13,14,15    | 1.64 | 2 (15%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | FAD  | A     | 600 | 1    | -       | 0/34/50/50 | 0/1/6/6 |
| 3   | EUG  | A     | 601 | -    | -       | 0/4/4/5    | 0/1/1/1 |
| 2   | FAD  | B     | 600 | 1    | -       | 0/34/50/50 | 0/1/6/6 |
| 3   | EUG  | B     | 601 | -    | -       | 0/4/4/5    | 0/1/1/1 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 600 | FAD  | C1'-C2' | 2.42  | 1.53        | 1.51     |
| 2   | B     | 600 | FAD  | C1'-C2' | 2.37  | 1.53        | 1.51     |
| 2   | B     | 600 | FAD  | O5B-C5B | -2.25 | 1.35        | 1.44     |
| 2   | A     | 600 | FAD  | O5B-C5B | -2.23 | 1.35        | 1.44     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 600 | FAD  | C2-N1-C10   | 5.47  | 120.49      | 114.98   |
| 2   | A     | 600 | FAD  | C2-N1-C10   | 5.44  | 120.46      | 114.98   |
| 3   | B     | 601 | EUG  | O3-C3-C4    | 4.40  | 120.38      | 114.57   |
| 3   | A     | 601 | EUG  | O3-C3-C4    | 4.36  | 120.33      | 114.57   |
| 2   | B     | 600 | FAD  | O4B-C1B-N9A | 3.93  | 112.10      | 108.44   |
| 2   | A     | 600 | FAD  | O4B-C1B-N9A | 3.89  | 112.06      | 108.44   |
| 2   | B     | 600 | FAD  | C1'-N10-C9A | 2.84  | 121.63      | 118.87   |
| 2   | A     | 600 | FAD  | C1'-N10-C9A | 2.83  | 121.62      | 118.87   |
| 2   | B     | 600 | FAD  | C6-C5X-N5   | -2.51 | 116.05      | 118.97   |
| 2   | A     | 600 | FAD  | C6-C5X-N5   | -2.49 | 116.07      | 118.97   |
| 3   | B     | 601 | EUG  | C9-O3-C3    | 2.38  | 121.11      | 117.59   |
| 3   | A     | 601 | EUG  | C9-O3-C3    | 2.37  | 121.10      | 117.59   |
| 2   | B     | 600 | FAD  | C9A-N10-C10 | -2.35 | 119.46      | 121.77   |
| 2   | A     | 600 | FAD  | C9A-N10-C10 | -2.28 | 119.53      | 121.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 600 | FAD  | C4X-C10-N10 | -2.06 | 119.48      | 120.51   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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