



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:41 AM UTC

PDB ID : 3DRS / pdb\_00003drs  
Title : HIV reverse transcriptase K103N mutant in complex with inhibitor R8D  
Authors : Yan, Y.; Prasad, S.  
Deposited on : 2008-07-11  
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

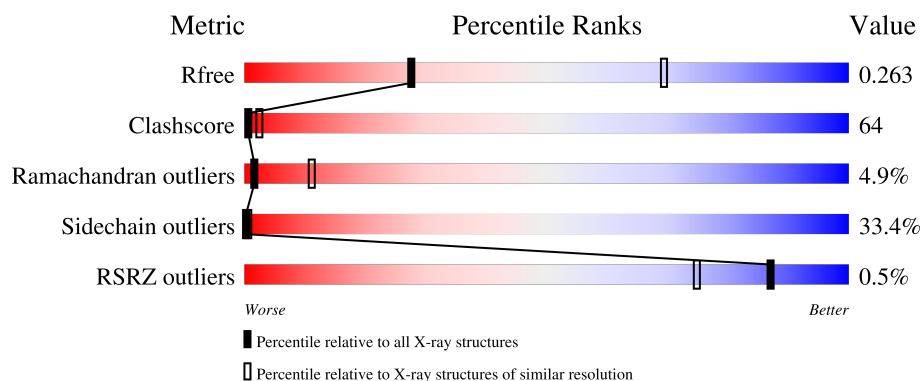
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2361 (3.20-3.12)                                      |
| Clashscore            | 190562                      | 2486 (3.20-3.12)                                      |
| Ramachandran outliers | 187476                      | 2405 (3.20-3.12)                                      |
| Sidechain outliers    | 187428                      | 2404 (3.20-3.12)                                      |
| RSRZ outliers         | 180081                      | 2361 (3.20-3.12)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                         |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------|
| 1   | A     | 563    | <br>20% 47% 26% . .  |
| 2   | B     | 443    | <br>22% 41% 25% . 9% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | R8D  | A     | 601 | -         | X        | X       | -                |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 549      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4475  | 2891 | 747 | 829 | 8 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | -2      | MET      | -      | expression tag      | UNP P04585 |
| A     | -1      | ASN      | -      | expression tag      | UNP P04585 |
| A     | 0       | SER      | -      | expression tag      | UNP P04585 |
| A     | 103     | ASN      | LYS    | engineered mutation | UNP P04585 |

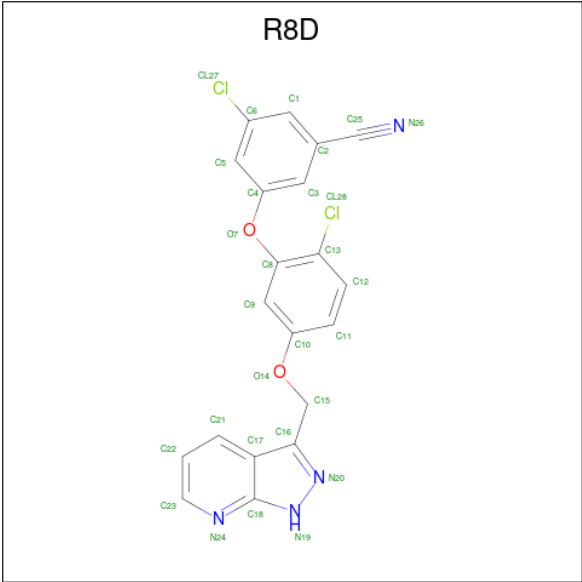
- Molecule 2 is a protein called p66 RT.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 405      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3351  | 2180 | 555 | 610 | 6 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | -2      | MET      | -      | expression tag      | UNP P04585 |
| B     | -1      | ASN      | -      | expression tag      | UNP P04585 |
| B     | 0       | SER      | -      | expression tag      | UNP P04585 |
| B     | 103     | ASN      | LYS    | engineered mutation | UNP P04585 |

- Molecule 3 is 3-chloro-5-[2-chloro-5-(1H-pyrazolo[3,4-b]pyridin-3-ylmethoxy)phenoxy]benzo nitrile (CCD ID: R8D) (formula: C<sub>20</sub>H<sub>12</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>2</sub>).

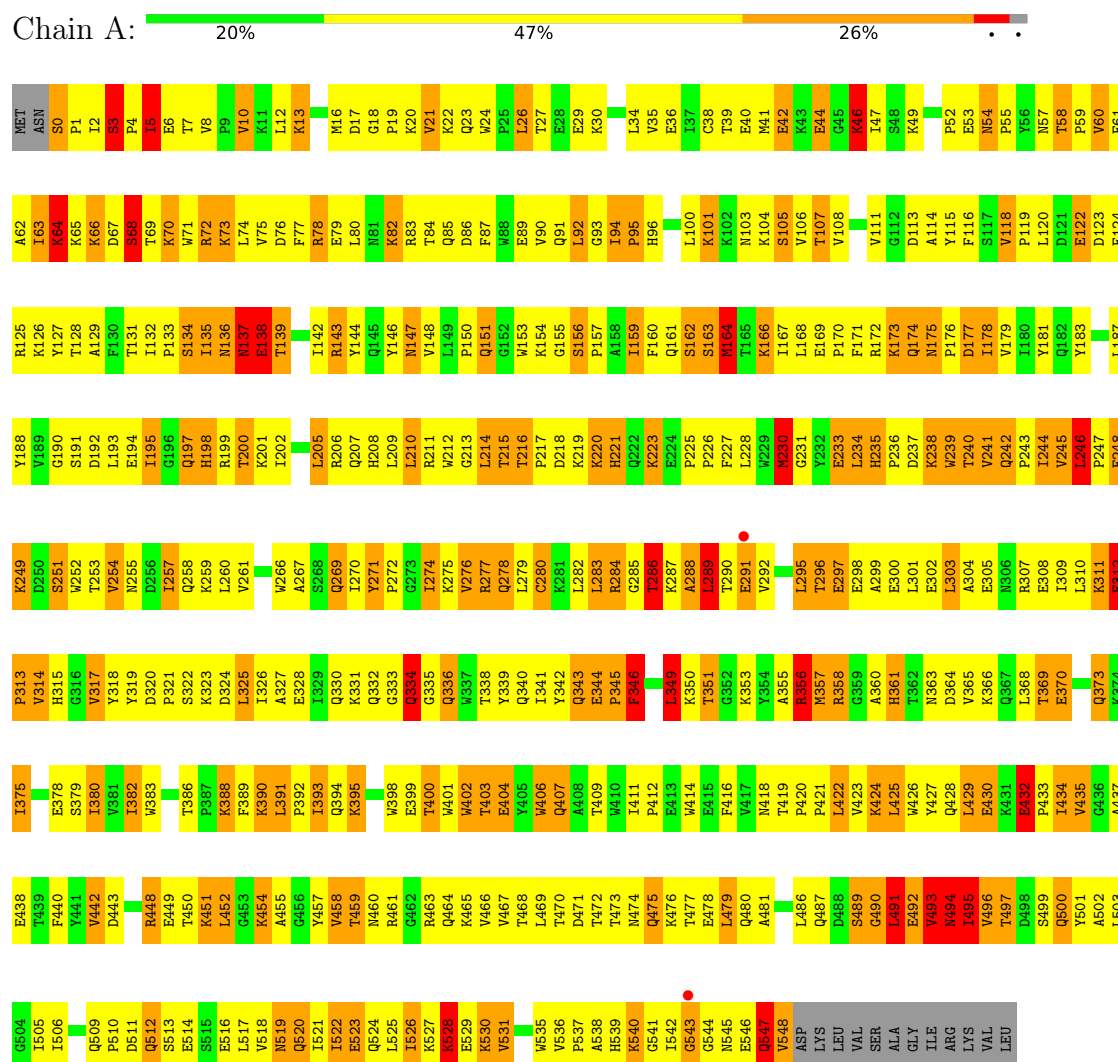


| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
|     |       |          | Total | C  | Cl | N | O |         |         |
| 3   | A     | 1        | 28    | 20 | 2  | 4 | 2 | 0       | 0       |

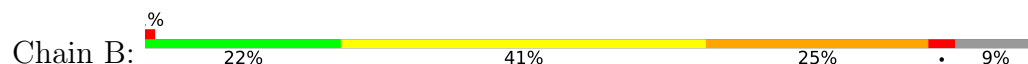
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

#### • Molecule 1: Reverse transcriptase/ribonuclease H



#### • Molecule 2: p66 RT



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| T386 | P387 | K388 | F389 | K390 | L391 | P392 | I393 | Q394 | K395 | E396 | T397 | K398 | E399 | T400 | W401 | W402 | T403 | W404 | E405 | W406 | A407 | A408 | T409 | W410 | I411 | P412 | E413 | W414 | E415 | F416 | W417 | W418 | T419 | P420 | P421 | L422 | W423 | K424 | L425 | W426 | Y427 | Q428 | LEU  | GLU  | LYS  | GLU  | PRO  | ILE  | VAL  | GLY  | ALA  | THR  | PHE  |      |      |      |      |      |      |
| Y319 | D320 | P321 | S322 | K323 | E328 | I329 | Q330 | K331 | Q332 | E396 | Q333 | Q334 | G335 | Q336 | W337 | T338 | Y339 | Q340 | T341 | Y342 | Q343 | E344 | P345 | F346 | K347 | N348 | L349 | G352 | K353 | Y354 | A355 | R356 | MET  | ARG  | GLY  | ALA  | H361 | T362 | K366 | Q367 | L368 | T369 | E370 | Q373 | K374 | T375 | T376 | T377 | E378 | S379 | I380 | P381 | I382 | W383 | G384 | K385 |      |      |      |
| Q288 | K289 | L260 | V261 | G262 | K263 | L264 | N265 | W266 | A267 | S268 | Q269 | I270 | Y271 | P272 | G273 | I274 | Y275 | W276 | R277 | Q278 | L279 | C280 | K281 | L282 | L283 | R284 | G285 | T286 | K287 | A288 | L289 | T290 | E291 | V292 | L293 | P294 | L295 | T296 | E297 | E298 | A299 | E300 | L301 | E302 | L303 | A304 | E305 | N306 | R307 | E308 | I309 | L310 | K311 | S251 | E312 | P313 | V314 | V317 | Y318 |
| G196 | Q197 | H198 | R199 | T200 | K201 | I202 | E203 | E204 | L205 | R206 | Q207 | W208 | L209 | L210 | R211 | L214 | T215 | THR  | PRO  | ASP  | LYS  | LYS  | HIS  | GLN  | LYS  | GLU  | PRO  | PHE  | LEU  | TRP  | MET  | G231 | V232 | E233 | L234 | H235 | P236 | D237 | T240 | V241 | Q242 | P243 | I244 | V245 | L246 | P247 | E248 | K249 | D250 | S251 | W252 | T253 | V254 | N255 | D256 | I257 |      |      |      |
| P133 | S134 | I135 | N136 | E137 | E138 | T139 | T142 | K143 | Y144 | Q145 | Y146 | N147 | V148 | L149 | P150 | Q151 | G152 | W153 | K154 | G155 | A158 | I159 | F160 | Q161 | S162 | I163 | M164 | T165 | K166 | I167 | L168 | E169 | P170 | F171 | R172 | K173 | Q174 | N175 | P176 | D177 | I178 | Y179 | I180 | Y181 | Q182 | Y183 | M184 | L187 | Y188 | V189 | R125 | G190 | S191 | D192 | L193 | E194 | I195 |      |      |
| 163  | K64  | K65  | R66  | D67  | S68  | T69  | R72  | K73  | L74  | E79  | L80  | N81  | K82  | R83  | T84  | O85  | D86  | F87  | W88  | E89  | V90  | Q91  | L92  | G93  | I94  | P95  | H96  | P97  | A98  | G99  | L100 | K101 | K102 | N103 | K104 | S105 | V111 | A114 | Y115 | F116 | S117 | V118 | P119 | L120 | D121 | E122 | D123 | K125 | K126 | Y127 | T128 | T131 | I132 |      |      |      |      |      |      |
| MET  | ASN  | SER  | PRO  | ILE  | SER  | PRO  | I5   | E6   | T7   | V8   | P9   | V10  | K11  | L12  | K13  | P14  | G15  | M16  | D17  | G18  | P19  | K20  | V21  | W24  | P25  | L26  | T27  | E28  | E29  | K30  | I31  | K32  | A33  | L34  | V35  | E36  | I37  | E40  | E44  | G45  | K46  | L47  | S48  | K49  | I50  | G51  | P52  | E53  | N54  | P55  | Y56  | W57  | T58  | P59  | V60  |      |      |      |      |

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 118.55Å 154.63Å 154.12Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 37.50 – 3.15<br>37.50 – 3.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.4 (37.50-3.15)<br>99.4 (37.50-3.15)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.98 (at 3.18Å)                                             | Xtriage          |
| Refinement program                                                      | BUSTER-TNT 2.1.1                                            | Depositor        |
| R, $R_{free}$                                                           | 0.184 , 0.250<br>0.192 , 0.263                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1255 reflections (5.08%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 68.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.051                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 80.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 7854                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R8D

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         | 0/4592      | 1.43        | 71/6242 (1.1%)   |
| 2   | B     | 0.81         | 0/3445      | 1.52        | 65/4682 (1.4%)   |
| All | All   | 0.81         | 0/8037      | 1.47        | 136/10924 (1.2%) |

There are no bond length outliers.

All (136) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 312 | GLU  | CA-C-N | -16.74 | 98.91       | 119.84   |
| 1   | A     | 312 | GLU  | C-N-CA | -16.74 | 98.91       | 119.84   |
| 2   | B     | 18  | GLY  | CA-C-N | 15.17  | 135.83      | 119.90   |
| 2   | B     | 18  | GLY  | C-N-CA | 15.17  | 135.83      | 119.90   |
| 2   | B     | 271 | TYR  | CA-C-N | 12.30  | 132.82      | 119.90   |
| 2   | B     | 271 | TYR  | C-N-CA | 12.30  | 132.82      | 119.90   |
| 1   | A     | 242 | GLN  | CA-C-N | 11.96  | 134.79      | 119.84   |
| 1   | A     | 242 | GLN  | C-N-CA | 11.96  | 134.79      | 119.84   |
| 2   | B     | 312 | GLU  | CA-C-N | 11.74  | 134.51      | 119.84   |
| 2   | B     | 312 | GLU  | C-N-CA | 11.74  | 134.51      | 119.84   |
| 1   | A     | 118 | VAL  | CA-C-N | 11.57  | 134.31      | 119.84   |
| 1   | A     | 118 | VAL  | C-N-CA | 11.57  | 134.31      | 119.84   |
| 2   | B     | 8   | VAL  | CA-C-N | 11.45  | 131.92      | 119.90   |
| 2   | B     | 8   | VAL  | C-N-CA | 11.45  | 131.92      | 119.90   |
| 2   | B     | 344 | GLU  | C-N-CD | -11.35 | 78.46       | 125.00   |
| 2   | B     | 58  | THR  | CA-C-N | -10.86 | 109.66      | 120.31   |
| 2   | B     | 58  | THR  | C-N-CA | -10.86 | 109.66      | 120.31   |
| 1   | A     | 419 | THR  | CA-C-N | 10.84  | 127.46      | 119.66   |
| 1   | A     | 419 | THR  | C-N-CA | 10.84  | 127.46      | 119.66   |
| 1   | A     | 492 | GLU  | N-CA-C | 10.82  | 123.17      | 110.41   |
| 1   | A     | 432 | GLU  | CA-C-N | 10.79  | 133.33      | 119.84   |
| 1   | A     | 432 | GLU  | C-N-CA | 10.79  | 133.33      | 119.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 391 | LEU  | N-CA-C | 10.61  | 122.98      | 109.72   |
| 2   | B     | 13  | LYS  | CA-C-N | 10.60  | 133.09      | 119.84   |
| 2   | B     | 13  | LYS  | C-N-CA | 10.60  | 133.09      | 119.84   |
| 2   | B     | 344 | GLU  | CA-C-N | 10.57  | 133.06      | 119.84   |
| 2   | B     | 344 | GLU  | C-N-CA | 10.57  | 133.06      | 119.84   |
| 1   | A     | 54  | ASN  | CA-C-N | 10.50  | 131.65      | 119.47   |
| 1   | A     | 54  | ASN  | C-N-CA | 10.50  | 131.65      | 119.47   |
| 2   | B     | 303 | LEU  | N-CA-C | -10.43 | 99.60       | 110.97   |
| 1   | A     | 13  | LYS  | CA-C-N | 10.18  | 132.57      | 119.84   |
| 1   | A     | 13  | LYS  | C-N-CA | 10.18  | 132.57      | 119.84   |
| 2   | B     | 96  | HIS  | CA-C-N | 10.07  | 132.62      | 120.23   |
| 2   | B     | 96  | HIS  | C-N-CA | 10.07  | 132.62      | 120.23   |
| 2   | B     | 233 | GLU  | N-CA-C | 9.43   | 124.68      | 107.99   |
| 2   | B     | 401 | TRP  | N-CA-C | 9.38   | 123.22      | 111.69   |
| 1   | A     | 289 | LEU  | N-CA-C | -9.35  | 102.38      | 113.88   |
| 2   | B     | 175 | ASN  | CA-C-N | 9.24   | 131.40      | 119.84   |
| 2   | B     | 175 | ASN  | C-N-CA | 9.24   | 131.40      | 119.84   |
| 1   | A     | 246 | LEU  | CA-C-N | 9.18   | 130.63      | 119.98   |
| 1   | A     | 246 | LEU  | C-N-CA | 9.18   | 130.63      | 119.98   |
| 1   | A     | 235 | HIS  | CA-C-N | 9.11   | 129.16      | 119.05   |
| 1   | A     | 235 | HIS  | C-N-CA | 9.11   | 129.16      | 119.05   |
| 2   | B     | 235 | HIS  | CA-C-N | 8.91   | 130.97      | 119.84   |
| 2   | B     | 235 | HIS  | C-N-CA | 8.91   | 130.97      | 119.84   |
| 1   | A     | 391 | LEU  | CA-C-N | 8.78   | 130.81      | 119.84   |
| 1   | A     | 391 | LEU  | C-N-CA | 8.78   | 130.81      | 119.84   |
| 2   | B     | 299 | ALA  | N-CA-C | -8.72  | 101.48      | 112.90   |
| 2   | B     | 268 | SER  | N-CA-C | -8.58  | 96.56       | 109.86   |
| 2   | B     | 115 | TYR  | N-CA-C | 8.37   | 121.33      | 111.71   |
| 1   | A     | 0   | SER  | CA-C-N | 8.36   | 128.41      | 119.89   |
| 1   | A     | 0   | SER  | C-N-CA | 8.36   | 128.41      | 119.89   |
| 1   | A     | 68  | SER  | N-CA-C | 8.09   | 121.21      | 110.53   |
| 1   | A     | 370 | GLU  | N-CA-C | -7.52  | 103.02      | 111.14   |
| 2   | B     | 312 | GLU  | C-N-CD | -7.45  | 94.47       | 125.00   |
| 2   | B     | 420 | PRO  | CA-C-N | 7.38   | 129.06      | 119.84   |
| 2   | B     | 420 | PRO  | C-N-CA | 7.38   | 129.06      | 119.84   |
| 1   | A     | 531 | VAL  | N-CA-C | 7.25   | 118.50      | 107.77   |
| 2   | B     | 420 | PRO  | C-N-CD | -6.90  | 96.70       | 125.00   |
| 1   | A     | 271 | TYR  | CA-C-N | 6.83   | 127.07      | 119.90   |
| 1   | A     | 271 | TYR  | C-N-CA | 6.83   | 127.07      | 119.90   |
| 1   | A     | 493 | VAL  | N-CA-C | 6.83   | 120.33      | 110.09   |
| 2   | B     | 195 | ILE  | N-CA-C | 6.79   | 117.29      | 110.23   |
| 1   | A     | 349 | LEU  | N-CA-C | -6.74  | 103.18      | 111.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 349 | LEU  | N-CA-C | -6.67 | 104.95      | 113.23   |
| 1   | A     | 93  | GLY  | N-CA-C | -6.61 | 102.30      | 111.09   |
| 1   | A     | 312 | GLU  | C-N-CD | -6.59 | 97.96       | 125.00   |
| 1   | A     | 147 | ASN  | N-CA-C | -6.55 | 105.02      | 114.12   |
| 1   | A     | 5   | ILE  | N-CA-C | 6.48  | 119.35      | 109.12   |
| 2   | B     | 32  | LYS  | N-CA-C | -6.42 | 103.57      | 111.40   |
| 1   | A     | 491 | LEU  | N-CA-C | 6.41  | 124.44      | 110.80   |
| 2   | B     | 117 | SER  | N-CA-C | -6.37 | 103.85      | 111.69   |
| 1   | A     | 344 | GLU  | CA-C-N | 6.37  | 127.80      | 119.84   |
| 1   | A     | 344 | GLU  | C-N-CA | 6.37  | 127.80      | 119.84   |
| 1   | A     | 18  | GLY  | CA-C-N | -6.30 | 114.14      | 120.31   |
| 1   | A     | 18  | GLY  | C-N-CA | -6.30 | 114.14      | 120.31   |
| 2   | B     | 258 | GLN  | N-CA-C | -6.27 | 103.73      | 111.75   |
| 1   | A     | 156 | SER  | CA-C-N | 6.26  | 126.45      | 119.32   |
| 1   | A     | 156 | SER  | C-N-CA | 6.26  | 126.45      | 119.32   |
| 1   | A     | 230 | MET  | N-CA-C | 6.24  | 124.10      | 110.80   |
| 2   | B     | 147 | ASN  | N-CA-C | -6.21 | 105.35      | 113.12   |
| 2   | B     | 415 | GLU  | N-CA-C | -6.19 | 99.63       | 109.23   |
| 1   | A     | 24  | TRP  | CA-C-N | 6.13  | 127.50      | 119.84   |
| 1   | A     | 24  | TRP  | C-N-CA | 6.13  | 127.50      | 119.84   |
| 1   | A     | 80  | LEU  | N-CA-C | -6.09 | 104.27      | 111.03   |
| 1   | A     | 239 | TRP  | N-CA-C | -6.07 | 99.92       | 108.96   |
| 2   | B     | 246 | LEU  | CA-C-N | -6.06 | 114.39      | 120.21   |
| 2   | B     | 246 | LEU  | C-N-CA | -6.06 | 114.39      | 120.21   |
| 1   | A     | 214 | LEU  | N-CA-C | 6.05  | 119.00      | 107.75   |
| 1   | A     | 489 | SER  | N-CA-C | 5.98  | 123.00      | 114.16   |
| 1   | A     | 143 | ARG  | N-CA-C | 5.94  | 118.58      | 108.90   |
| 1   | A     | 216 | THR  | CA-C-N | -5.91 | 112.46      | 119.84   |
| 1   | A     | 216 | THR  | C-N-CA | -5.91 | 112.46      | 119.84   |
| 1   | A     | 494 | ASN  | N-CA-C | -5.81 | 98.93       | 108.76   |
| 1   | A     | 94  | ILE  | C-N-CD | -5.80 | 101.23      | 125.00   |
| 2   | B     | 94  | ILE  | CA-C-N | -5.79 | 114.00      | 120.14   |
| 2   | B     | 94  | ILE  | C-N-CA | -5.79 | 114.00      | 120.14   |
| 2   | B     | 194 | GLU  | N-CA-C | -5.76 | 102.51      | 110.35   |
| 1   | A     | 388 | LYS  | N-CA-C | -5.73 | 99.90       | 109.24   |
| 2   | B     | 320 | ASP  | CA-C-N | 5.67  | 126.93      | 119.84   |
| 2   | B     | 320 | ASP  | C-N-CA | 5.67  | 126.93      | 119.84   |
| 2   | B     | 248 | GLU  | N-CA-C | -5.65 | 100.69      | 109.72   |
| 2   | B     | 192 | ASP  | N-CA-C | -5.62 | 106.31      | 112.72   |
| 1   | A     | 86  | ASP  | N-CA-C | -5.59 | 101.43      | 110.32   |
| 2   | B     | 85  | GLN  | N-CA-C | 5.54  | 119.54      | 112.34   |
| 2   | B     | 362 | THR  | N-CA-C | 5.53  | 117.54      | 108.52   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 496 | VAL  | N-CA-C | 5.50  | 115.78      | 107.75   |
| 2   | B     | 245 | VAL  | N-CA-C | 5.49  | 116.00      | 107.99   |
| 1   | A     | 46  | LYS  | N-CA-C | -5.43 | 105.46      | 111.71   |
| 1   | A     | 357 | MET  | N-CA-C | -5.41 | 102.08      | 109.71   |
| 1   | A     | 234 | LEU  | N-CA-C | 5.40  | 122.31      | 110.80   |
| 2   | B     | 246 | LEU  | N-CA-C | -5.39 | 103.28      | 110.07   |
| 2   | B     | 146 | TYR  | N-CA-C | 5.38  | 119.00      | 109.96   |
| 2   | B     | 52  | PRO  | N-CA-C | -5.28 | 107.54      | 114.03   |
| 1   | A     | 325 | LEU  | CA-C-N | -5.25 | 116.67      | 123.19   |
| 1   | A     | 325 | LEU  | C-N-CA | -5.25 | 116.67      | 123.19   |
| 2   | B     | 19  | PRO  | N-CA-C | -5.25 | 102.88      | 110.80   |
| 2   | B     | 254 | VAL  | N-CA-C | -5.25 | 104.77      | 110.23   |
| 1   | A     | 495 | ILE  | CA-C-N | -5.18 | 116.20      | 123.10   |
| 1   | A     | 495 | ILE  | C-N-CA | -5.18 | 116.20      | 123.10   |
| 1   | A     | 198 | HIS  | N-CA-C | -5.17 | 105.29      | 111.03   |
| 1   | A     | 251 | SER  | N-CA-C | 5.13  | 117.75      | 109.40   |
| 2   | B     | 118 | VAL  | C-N-CD | -5.10 | 104.10      | 125.00   |
| 1   | A     | 343 | GLN  | N-CA-C | -5.09 | 107.20      | 113.41   |
| 2   | B     | 333 | GLY  | N-CA-C | -5.09 | 103.47      | 111.00   |
| 1   | A     | 406 | TRP  | N-CA-C | 5.03  | 116.77      | 111.28   |
| 1   | A     | 175 | ASN  | CA-C-N | 5.03  | 124.81      | 119.28   |
| 1   | A     | 175 | ASN  | C-N-CA | 5.03  | 124.81      | 119.28   |
| 1   | A     | 248 | GLU  | N-CA-C | -5.03 | 101.77      | 109.76   |
| 2   | B     | 261 | VAL  | N-CA-C | -5.01 | 105.96      | 110.82   |
| 2   | B     | 391 | LEU  | CA-C-N | 5.01  | 129.50      | 120.88   |
| 2   | B     | 391 | LEU  | C-N-CA | 5.01  | 129.50      | 120.88   |
| 2   | B     | 293 | ILE  | CA-C-N | 5.01  | 125.00      | 119.89   |
| 2   | B     | 293 | ILE  | C-N-CA | 5.01  | 125.00      | 119.89   |
| 2   | B     | 419 | THR  | CA-C-N | 5.00  | 125.53      | 120.38   |
| 2   | B     | 419 | THR  | C-N-CA | 5.00  | 125.53      | 120.38   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4475  | 0        | 4514     | 629     | 1            |
| 2   | B     | 3351  | 0        | 3373     | 403     | 0            |
| 3   | A     | 28    | 0        | 12       | 16      | 0            |
| All | All   | 7854  | 0        | 7899     | 1005    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (1005) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:288:ALA:HB3  | 1:A:291:GLU:HB3  | 1.17                     | 1.17              |
| 1:A:318:TYR:CE2  | 3:A:601:R8D:H15  | 1.82                     | 1.14              |
| 1:A:469:LEU:HD21 | 1:A:480:GLN:HG2  | 1.32                     | 1.12              |
| 2:B:241:VAL:HG23 | 2:B:243:PRO:HD3  | 1.16                     | 1.08              |
| 1:A:122:GLU:HA   | 1:A:125:ARG:HD2  | 1.41                     | 1.02              |
| 1:A:271:TYR:HB3  | 1:A:274:ILE:HD11 | 1.42                     | 1.00              |
| 2:B:160:PHE:HE2  | 2:B:164:MET:HE2  | 1.25                     | 0.99              |
| 2:B:282:LEU:HD12 | 2:B:293:ILE:HD11 | 1.44                     | 0.96              |
| 1:A:175:ASN:HB3  | 1:A:178:ILE:HD13 | 1.43                     | 0.95              |
| 2:B:362:THR:HG23 | 2:B:366:LYS:HG2  | 1.48                     | 0.95              |
| 1:A:79:GLU:HG3   | 1:A:83:ARG:HE    | 1.30                     | 0.95              |
| 1:A:442:VAL:HG12 | 1:A:481:ALA:HB1  | 1.48                     | 0.94              |
| 2:B:298:GLU:HA   | 2:B:301:LEU:HG   | 1.49                     | 0.94              |
| 1:A:458:VAL:HG12 | 1:A:548:VAL:HG13 | 1.50                     | 0.94              |
| 1:A:406:TRP:CH2  | 1:A:407:GLN:HG3  | 2.03                     | 0.94              |
| 2:B:306:ASN:HA   | 2:B:309:ILE:HD12 | 1.50                     | 0.93              |
| 2:B:246:LEU:HD11 | 2:B:310:LEU:HD23 | 1.49                     | 0.93              |
| 1:A:380:ILE:HD11 | 1:A:386:THR:HG22 | 1.51                     | 0.92              |
| 2:B:50:ILE:HG21  | 2:B:145:GLN:HB3  | 1.52                     | 0.91              |
| 2:B:257:ILE:HG22 | 2:B:283:LEU:HD11 | 1.51                     | 0.91              |
| 1:A:475:GLN:HG3  | 1:A:501:TYR:CE2  | 2.06                     | 0.90              |
| 1:A:406:TRP:CH2  | 2:B:418:ASN:HA   | 2.07                     | 0.90              |
| 1:A:434:ILE:HG23 | 1:A:530:LYS:HD3  | 1.55                     | 0.90              |
| 1:A:64:LYS:NZ    | 1:A:69:THR:HA    | 1.87                     | 0.89              |
| 2:B:160:PHE:CE2  | 2:B:164:MET:HE2  | 2.07                     | 0.89              |
| 2:B:125:ARG:NH1  | 2:B:147:ASN:HA   | 1.87                     | 0.88              |
| 1:A:261:VAL:HG13 | 1:A:276:VAL:HG11 | 1.53                     | 0.88              |
| 2:B:253:THR:O    | 2:B:257:ILE:HD12 | 1.74                     | 0.88              |
| 1:A:181:TYR:HB2  | 1:A:188:TYR:HB2  | 1.55                     | 0.88              |
| 1:A:252:TRP:CD1  | 1:A:295:LEU:HD21 | 2.09                     | 0.88              |
| 1:A:469:LEU:CD2  | 1:A:480:GLN:HG2  | 2.04                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:241:VAL:CG2  | 2:B:243:PRO:HD3  | 2.03                     | 0.88              |
| 2:B:125:ARG:HB3  | 2:B:146:TYR:O    | 1.75                     | 0.87              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:CE3  | 2.10                     | 0.87              |
| 2:B:362:THR:CG2  | 2:B:367:GLN:HG3  | 2.05                     | 0.86              |
| 1:A:434:ILE:HG13 | 1:A:494:ASN:HD21 | 1.39                     | 0.86              |
| 1:A:107:THR:HG21 | 1:A:202:ILE:HD13 | 1.56                     | 0.86              |
| 2:B:12:LEU:HD23  | 2:B:17:ASP:HA    | 1.57                     | 0.85              |
| 1:A:288:ALA:CB   | 1:A:291:GLU:HB3  | 2.06                     | 0.85              |
| 2:B:246:LEU:HD12 | 2:B:307:ARG:HG3  | 1.58                     | 0.85              |
| 1:A:253:THR:HG22 | 1:A:292:VAL:HG22 | 1.56                     | 0.84              |
| 2:B:337:TRP:HE1  | 2:B:367:GLN:HE21 | 1.22                     | 0.84              |
| 1:A:175:ASN:CB   | 1:A:178:ILE:HD13 | 2.06                     | 0.84              |
| 1:A:448:ARG:HG2  | 1:A:448:ARG:HH11 | 1.41                     | 0.84              |
| 1:A:100:LEU:HD22 | 1:A:181:TYR:HE2  | 1.43                     | 0.84              |
| 1:A:85:GLN:O     | 1:A:154:LYS:HE2  | 1.78                     | 0.84              |
| 1:A:288:ALA:HB3  | 1:A:291:GLU:CB   | 2.05                     | 0.83              |
| 1:A:424:LYS:HE2  | 1:A:426:TRP:CZ2  | 2.13                     | 0.83              |
| 2:B:13:LYS:HB2   | 2:B:16:MET:HE3   | 1.59                     | 0.83              |
| 1:A:255:ASN:HB2  | 1:A:289:LEU:HD13 | 1.58                     | 0.83              |
| 1:A:1:PRO:O      | 1:A:2:ILE:HD13   | 1.78                     | 0.83              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:NZ   | 1.75                     | 0.83              |
| 2:B:87:PHE:CE2   | 2:B:92:LEU:HD12  | 2.12                     | 0.83              |
| 1:A:162:SER:HB2  | 2:B:52:PRO:HG3   | 1.61                     | 0.83              |
| 2:B:422:LEU:HB3  | 2:B:426:TRP:CZ2  | 2.13                     | 0.83              |
| 1:A:2:ILE:HD11   | 1:A:46:LYS:NZ    | 1.94                     | 0.83              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:NZ   | 2.27                     | 0.83              |
| 1:A:311:LYS:O    | 1:A:312:GLU:HB3  | 1.79                     | 0.83              |
| 1:A:122:GLU:HA   | 1:A:125:ARG:CD   | 2.08                     | 0.82              |
| 1:A:134:SER:CB   | 1:A:139:THR:HB   | 2.10                     | 0.82              |
| 2:B:298:GLU:CA   | 2:B:301:LEU:HG   | 2.08                     | 0.82              |
| 1:A:434:ILE:HD13 | 1:A:530:LYS:HB3  | 1.61                     | 0.81              |
| 1:A:64:LYS:HZ1   | 1:A:69:THR:HA    | 1.43                     | 0.81              |
| 1:A:100:LEU:O    | 1:A:318:TYR:HB3  | 1.80                     | 0.81              |
| 1:A:228:LEU:HB3  | 1:A:242:GLN:NE2  | 1.95                     | 0.81              |
| 2:B:13:LYS:CB    | 2:B:16:MET:HE3   | 2.11                     | 0.81              |
| 2:B:18:GLY:HA3   | 2:B:56:TYR:CE1   | 2.15                     | 0.81              |
| 1:A:125:ARG:HG2  | 1:A:146:TYR:O    | 1.81                     | 0.81              |
| 1:A:255:ASN:HB2  | 1:A:289:LEU:CD1  | 2.11                     | 0.81              |
| 2:B:125:ARG:HH11 | 2:B:147:ASN:HA   | 1.43                     | 0.80              |
| 1:A:486:LEU:HB3  | 1:A:524:GLN:HE21 | 1.45                     | 0.80              |
| 1:A:76:ASP:OD2   | 1:A:78:ARG:HG3   | 1.82                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:277:ARG:O    | 2:B:281:LYS:HG3  | 1.82                     | 0.79              |
| 2:B:420:PRO:HG2  | 2:B:423:VAL:CG2  | 2.12                     | 0.79              |
| 1:A:401:TRP:HA   | 1:A:404:GLU:OE2  | 1.82                     | 0.79              |
| 1:A:544:GLY:HA2  | 1:A:547:GLN:NE2  | 1.97                     | 0.79              |
| 2:B:362:THR:HG22 | 2:B:367:GLN:HG3  | 1.63                     | 0.79              |
| 1:A:258:GLN:HG3  | 1:A:283:LEU:HD11 | 1.64                     | 0.79              |
| 1:A:271:TYR:CE1  | 1:A:314:VAL:HG23 | 2.18                     | 0.79              |
| 1:A:460:ASN:ND2  | 2:B:288:ALA:HB2  | 1.97                     | 0.79              |
| 1:A:493:VAL:CG2  | 1:A:528:LYS:HE2  | 2.13                     | 0.79              |
| 2:B:241:VAL:HG23 | 2:B:243:PRO:CD   | 2.09                     | 0.78              |
| 1:A:21:VAL:CG2   | 1:A:59:PRO:HD3   | 2.13                     | 0.78              |
| 2:B:395:LYS:HG3  | 2:B:399:GLU:OE1  | 1.82                     | 0.78              |
| 2:B:246:LEU:HD11 | 2:B:310:LEU:CD2  | 2.13                     | 0.78              |
| 1:A:450:THR:OG1  | 1:A:452:LEU:HB2  | 1.83                     | 0.77              |
| 2:B:114:ALA:HB2  | 2:B:214:LEU:HD22 | 1.64                     | 0.77              |
| 2:B:114:ALA:CB   | 2:B:214:LEU:HD22 | 2.15                     | 0.77              |
| 2:B:335:GLY:HA3  | 2:B:356:ARG:HG2  | 1.67                     | 0.77              |
| 2:B:420:PRO:HG2  | 2:B:423:VAL:HG21 | 1.67                     | 0.77              |
| 1:A:2:ILE:HD11   | 1:A:46:LYS:CE    | 2.15                     | 0.77              |
| 1:A:271:TYR:CB   | 1:A:274:ILE:HD11 | 2.14                     | 0.77              |
| 1:A:424:LYS:HE2  | 1:A:426:TRP:CH2  | 2.20                     | 0.77              |
| 2:B:422:LEU:HB3  | 2:B:426:TRP:CE2  | 2.19                     | 0.76              |
| 1:A:318:TYR:CZ   | 3:A:601:R8D:H15  | 2.20                     | 0.76              |
| 1:A:95:PRO:HA    | 2:B:136:ASN:OD1  | 1.85                     | 0.76              |
| 1:A:454:LYS:HZ2  | 1:A:468:THR:HG23 | 1.50                     | 0.76              |
| 2:B:268:SER:O    | 2:B:270:ILE:HG22 | 1.85                     | 0.76              |
| 2:B:301:LEU:O    | 2:B:305:GLU:HG3  | 1.85                     | 0.76              |
| 2:B:104:LYS:HB2  | 2:B:192:ASP:HA   | 1.67                     | 0.76              |
| 1:A:3:SER:CB     | 1:A:5:ILE:HD12   | 2.14                     | 0.76              |
| 1:A:469:LEU:HD21 | 1:A:480:GLN:CG   | 2.15                     | 0.76              |
| 1:A:220:LYS:HE3  | 1:A:221:HIS:CE1  | 2.21                     | 0.76              |
| 1:A:356:ARG:CZ   | 1:A:358:ARG:HD2  | 2.16                     | 0.75              |
| 2:B:116:PHE:CZ   | 2:B:151:GLN:HG3  | 2.21                     | 0.75              |
| 1:A:460:ASN:HA   | 2:B:286:THR:OG1  | 1.87                     | 0.75              |
| 1:A:320:ASP:OD2  | 1:A:323:LYS:HE3  | 1.85                     | 0.75              |
| 2:B:303:LEU:O    | 2:B:307:ARG:HB2  | 1.85                     | 0.75              |
| 1:A:366:LYS:O    | 1:A:370:GLU:HG3  | 1.87                     | 0.74              |
| 1:A:522:ILE:O    | 1:A:526:ILE:HG13 | 1.87                     | 0.74              |
| 2:B:104:LYS:HD3  | 2:B:192:ASP:HB3  | 1.68                     | 0.74              |
| 1:A:328:GLU:HG2  | 1:A:390:LYS:HB2  | 1.67                     | 0.74              |
| 1:A:435:VAL:HG22 | 2:B:290:THR:OG1  | 1.87                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:64:LYS:HZ1   | 1:A:69:THR:HG23  | 1.51                     | 0.74              |
| 1:A:276:VAL:O    | 1:A:280:CYS:HB2  | 1.88                     | 0.74              |
| 1:A:520:GLN:O    | 1:A:523:GLU:HG3  | 1.87                     | 0.74              |
| 2:B:116:PHE:HA   | 2:B:148:VAL:HG21 | 1.68                     | 0.74              |
| 2:B:425:LEU:HD23 | 2:B:425:LEU:H    | 1.53                     | 0.74              |
| 1:A:3:SER:OG     | 1:A:5:ILE:HD12   | 1.86                     | 0.73              |
| 2:B:422:LEU:HD13 | 2:B:426:TRP:CZ2  | 2.23                     | 0.73              |
| 1:A:234:LEU:O    | 3:A:601:R8D:H21  | 1.89                     | 0.73              |
| 2:B:298:GLU:HA   | 2:B:301:LEU:CG   | 2.19                     | 0.73              |
| 1:A:244:ILE:HD12 | 1:A:267:ALA:HB2  | 1.69                     | 0.73              |
| 1:A:434:ILE:HG13 | 1:A:494:ASN:ND2  | 2.03                     | 0.73              |
| 1:A:21:VAL:HG22  | 1:A:59:PRO:HD3   | 1.69                     | 0.73              |
| 2:B:332:GLN:HA   | 2:B:332:GLN:OE1  | 1.87                     | 0.73              |
| 2:B:257:ILE:O    | 2:B:261:VAL:HG12 | 1.89                     | 0.73              |
| 1:A:34:LEU:HD21  | 1:A:62:ALA:HB2   | 1.71                     | 0.73              |
| 2:B:65:LYS:HE2   | 2:B:72:ARG:CZ    | 2.19                     | 0.73              |
| 2:B:243:PRO:HB3  | 2:B:311:LYS:HA   | 1.71                     | 0.73              |
| 1:A:105:SER:HB2  | 1:A:198:HIS:CE1  | 2.23                     | 0.72              |
| 2:B:246:LEU:CD1  | 2:B:310:LEU:HD23 | 2.19                     | 0.72              |
| 1:A:271:TYR:CD1  | 1:A:310:LEU:HD23 | 2.23                     | 0.72              |
| 1:A:454:LYS:NZ   | 1:A:468:THR:HG23 | 2.03                     | 0.72              |
| 2:B:27:THR:OG1   | 2:B:30:LYS:HD3   | 1.89                     | 0.72              |
| 2:B:114:ALA:CA   | 2:B:214:LEU:HD22 | 2.20                     | 0.72              |
| 1:A:27:THR:OG1   | 1:A:30:LYS:HG3   | 1.90                     | 0.72              |
| 2:B:33:ALA:O     | 2:B:37:ILE:HD12  | 1.90                     | 0.72              |
| 1:A:100:LEU:HD22 | 1:A:181:TYR:CE2  | 2.24                     | 0.72              |
| 1:A:437:ALA:HB1  | 1:A:492:GLU:O    | 1.90                     | 0.72              |
| 1:A:521:ILE:O    | 1:A:525:LEU:HG   | 1.90                     | 0.72              |
| 1:A:79:GLU:HG3   | 1:A:83:ARG:NE    | 2.02                     | 0.71              |
| 1:A:331:LYS:HE3  | 1:A:364:ASP:OD1  | 1.90                     | 0.71              |
| 1:A:211:ARG:O    | 1:A:211:ARG:HD3  | 1.90                     | 0.71              |
| 1:A:41:MET:HE2   | 1:A:47:ILE:HD13  | 1.72                     | 0.71              |
| 1:A:169:GLU:N    | 1:A:170:PRO:HD2  | 2.03                     | 0.71              |
| 1:A:270:ILE:O    | 1:A:272:PRO:HD3  | 1.89                     | 0.71              |
| 1:A:501:TYR:CZ   | 1:A:505:ILE:HD11 | 2.26                     | 0.71              |
| 1:A:356:ARG:NH2  | 1:A:358:ARG:HD2  | 2.05                     | 0.71              |
| 1:A:226:PRO:HG3  | 1:A:235:HIS:HD2  | 1.55                     | 0.70              |
| 1:A:502:ALA:O    | 1:A:506:ILE:HD12 | 1.91                     | 0.70              |
| 1:A:540:LYS:CB   | 1:A:542:ILE:HD13 | 2.21                     | 0.70              |
| 1:A:218:ASP:OD2  | 1:A:221:HIS:HB2  | 1.91                     | 0.70              |
| 2:B:72:ARG:HH12  | 2:B:409:THR:CG2  | 2.03                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:354:TYR:HB2  | 2:B:374:LYS:NZ   | 2.05                     | 0.70              |
| 1:A:108:VAL:HB   | 1:A:223:LYS:HG3  | 1.74                     | 0.70              |
| 2:B:301:LEU:N    | 2:B:301:LEU:HD23 | 2.07                     | 0.70              |
| 1:A:277:ARG:NH1  | 1:A:334:GLN:HB2  | 2.06                     | 0.70              |
| 1:A:58:THR:HG23  | 1:A:59:PRO:HD2   | 1.73                     | 0.70              |
| 1:A:206:ARG:CZ   | 1:A:218:ASP:HA   | 2.22                     | 0.70              |
| 1:A:57:ASN:ND2   | 1:A:131:THR:OG1  | 2.24                     | 0.70              |
| 1:A:41:MET:HB3   | 1:A:47:ILE:HG12  | 1.72                     | 0.70              |
| 1:A:54:ASN:O     | 1:A:143:ARG:NH2  | 2.25                     | 0.70              |
| 1:A:3:SER:HB3    | 1:A:5:ILE:HD12   | 1.71                     | 0.70              |
| 1:A:156:SER:N    | 1:A:157:PRO:HD2  | 2.07                     | 0.70              |
| 1:A:104:LYS:HG3  | 1:A:192:ASP:HA   | 1.74                     | 0.69              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:HZ2  | 1.39                     | 0.69              |
| 1:A:284:ARG:HH11 | 1:A:285:GLY:HA3  | 1.57                     | 0.69              |
| 1:A:171:PHE:CD2  | 1:A:205:LEU:HD23 | 2.26                     | 0.69              |
| 2:B:122:GLU:HA   | 2:B:125:ARG:HE   | 1.58                     | 0.69              |
| 2:B:283:LEU:HA   | 2:B:287:LYS:HE2  | 1.73                     | 0.69              |
| 1:A:424:LYS:HE2  | 1:A:426:TRP:CE2  | 2.26                     | 0.69              |
| 1:A:298:GLU:H    | 1:A:298:GLU:CD   | 2.01                     | 0.69              |
| 1:A:298:GLU:OE2  | 1:A:298:GLU:N    | 2.21                     | 0.69              |
| 2:B:87:PHE:CZ    | 2:B:92:LEU:HD12  | 2.27                     | 0.69              |
| 2:B:279:LEU:O    | 2:B:282:LEU:HB2  | 1.91                     | 0.69              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:CZ3  | 2.27                     | 0.69              |
| 1:A:162:SER:CB   | 2:B:52:PRO:HG3   | 2.23                     | 0.69              |
| 1:A:238:LYS:HB3  | 1:A:315:HIS:HD2  | 1.58                     | 0.69              |
| 2:B:116:PHE:HD2  | 2:B:148:VAL:CG2  | 2.06                     | 0.69              |
| 2:B:66:LYS:CA    | 2:B:407:GLN:HE22 | 2.04                     | 0.68              |
| 1:A:104:LYS:HG3  | 1:A:192:ASP:CA   | 2.23                     | 0.68              |
| 1:A:175:ASN:CA   | 1:A:178:ILE:HD13 | 2.23                     | 0.68              |
| 1:A:358:ARG:NH1  | 2:B:396:GLU:OE1  | 2.26                     | 0.68              |
| 1:A:516:GLU:O    | 1:A:520:GLN:HG2  | 1.93                     | 0.68              |
| 1:A:298:GLU:HA   | 1:A:301:LEU:HD12 | 1.74                     | 0.68              |
| 1:A:266:TRP:O    | 1:A:269:GLN:NE2  | 2.27                     | 0.68              |
| 2:B:260:LEU:HD13 | 2:B:260:LEU:O    | 1.93                     | 0.68              |
| 2:B:299:ALA:O    | 2:B:303:LEU:HD23 | 1.93                     | 0.68              |
| 1:A:317:VAL:HG23 | 1:A:318:TYR:N    | 2.08                     | 0.68              |
| 2:B:253:THR:HG23 | 2:B:289:LEU:O    | 1.94                     | 0.68              |
| 1:A:105:SER:HB2  | 1:A:198:HIS:ND1  | 2.08                     | 0.68              |
| 2:B:268:SER:C    | 2:B:269:GLN:HG3  | 2.18                     | 0.68              |
| 1:A:399:GLU:HG3  | 1:A:400:THR:N    | 2.09                     | 0.68              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:HD2  | 2.09                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:363:ASN:HA   | 1:A:511:ASP:OD2  | 1.93                     | 0.67              |
| 1:A:364:ASP:HB3  | 1:A:423:VAL:HG13 | 1.74                     | 0.67              |
| 1:A:244:ILE:CD1  | 1:A:267:ALA:HB2  | 2.25                     | 0.67              |
| 1:A:518:VAL:O    | 1:A:522:ILE:HD12 | 1.94                     | 0.67              |
| 2:B:362:THR:HG21 | 2:B:367:GLN:HG3  | 1.74                     | 0.67              |
| 1:A:20:LYS:HE2   | 1:A:55:PRO:HB2   | 1.76                     | 0.67              |
| 1:A:501:TYR:CE1  | 1:A:505:ILE:HD11 | 2.29                     | 0.67              |
| 2:B:175:ASN:ND2  | 2:B:201:LYS:HE3  | 2.09                     | 0.67              |
| 2:B:257:ILE:HG22 | 2:B:283:LEU:CD1  | 2.24                     | 0.67              |
| 2:B:278:GLN:HA   | 2:B:281:LYS:HD2  | 1.76                     | 0.67              |
| 1:A:175:ASN:N    | 1:A:176:PRO:HD3  | 2.08                     | 0.67              |
| 1:A:458:VAL:CG1  | 1:A:548:VAL:HG22 | 2.23                     | 0.67              |
| 2:B:298:GLU:C    | 2:B:301:LEU:HG   | 2.20                     | 0.67              |
| 1:A:434:ILE:CG1  | 1:A:494:ASN:HD21 | 2.08                     | 0.67              |
| 2:B:72:ARG:HH12  | 2:B:409:THR:HG22 | 1.59                     | 0.67              |
| 1:A:258:GLN:HG3  | 1:A:283:LEU:CD1  | 2.24                     | 0.67              |
| 1:A:538:ALA:O    | 1:A:539:HIS:HB2  | 1.95                     | 0.67              |
| 1:A:261:VAL:HG13 | 1:A:276:VAL:CG1  | 2.25                     | 0.67              |
| 1:A:538:ALA:HA   | 1:A:545:ASN:OD1  | 1.94                     | 0.66              |
| 2:B:64:LYS:NZ    | 2:B:69:THR:O     | 2.27                     | 0.66              |
| 1:A:399:GLU:O    | 1:A:403:THR:HB   | 1.95                     | 0.66              |
| 2:B:86:ASP:HA    | 2:B:90:VAL:CG2   | 2.24                     | 0.66              |
| 2:B:301:LEU:O    | 2:B:305:GLU:N    | 2.28                     | 0.66              |
| 1:A:107:THR:HB   | 1:A:202:ILE:HD11 | 1.78                     | 0.66              |
| 2:B:422:LEU:HA   | 2:B:425:LEU:HD21 | 1.76                     | 0.66              |
| 1:A:178:ILE:N    | 1:A:178:ILE:HD12 | 2.10                     | 0.66              |
| 2:B:278:GLN:O    | 2:B:281:LYS:HB2  | 1.96                     | 0.66              |
| 2:B:344:GLU:HB3  | 2:B:345:PRO:HD2  | 1.77                     | 0.66              |
| 2:B:266:TRP:HE1  | 2:B:346:PHE:HE2  | 1.42                     | 0.66              |
| 2:B:209:LEU:HD12 | 2:B:214:LEU:HD12 | 1.76                     | 0.66              |
| 2:B:302:GLU:O    | 2:B:306:ASN:HB2  | 1.96                     | 0.66              |
| 1:A:44:GLU:HB3   | 1:A:46:LYS:HE3   | 1.78                     | 0.65              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:HD2  | 1.61                     | 0.65              |
| 2:B:366:LYS:O    | 2:B:370:GLU:HG3  | 1.96                     | 0.65              |
| 1:A:77:PHE:CE2   | 1:A:150:PRO:HB2  | 2.32                     | 0.65              |
| 1:A:1:PRO:C      | 1:A:2:ILE:HD13   | 2.20                     | 0.65              |
| 1:A:13:LYS:O     | 1:A:16:MET:HB2   | 1.97                     | 0.65              |
| 2:B:253:THR:HG22 | 2:B:256:ASP:H    | 1.59                     | 0.65              |
| 1:A:403:THR:HG22 | 1:A:404:GLU:N    | 2.10                     | 0.65              |
| 1:A:486:LEU:CB   | 1:A:524:GLN:HE21 | 2.08                     | 0.65              |
| 1:A:490:GLY:O    | 1:A:492:GLU:N    | 2.28                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:66:LYS:H     | 2:B:407:GLN:NE2  | 1.95                     | 0.65              |
| 2:B:169:GLU:HB3  | 2:B:170:PRO:CD   | 2.26                     | 0.65              |
| 1:A:104:LYS:HG3  | 1:A:192:ASP:C    | 2.22                     | 0.65              |
| 1:A:395:LYS:HD3  | 1:A:414:TRP:CH2  | 2.32                     | 0.65              |
| 1:A:400:THR:HG22 | 1:A:401:TRP:N    | 2.10                     | 0.65              |
| 2:B:261:VAL:O    | 2:B:265:ASN:HB3  | 1.96                     | 0.65              |
| 1:A:91:GLN:HE21  | 2:B:137:ASN:HB3  | 1.62                     | 0.64              |
| 2:B:396:GLU:O    | 2:B:400:THR:HG22 | 1.97                     | 0.64              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:CH2  | 2.32                     | 0.64              |
| 1:A:104:LYS:CG   | 1:A:192:ASP:HA   | 2.27                     | 0.64              |
| 1:A:365:VAL:O    | 1:A:369:THR:HG23 | 1.97                     | 0.64              |
| 2:B:282:LEU:CD1  | 2:B:293:ILE:HD11 | 2.25                     | 0.64              |
| 2:B:293:ILE:HD12 | 2:B:294:PRO:O    | 1.97                     | 0.64              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:CZ2  | 2.33                     | 0.64              |
| 1:A:443:ASP:HB2  | 1:A:548:VAL:HB   | 1.80                     | 0.64              |
| 1:A:458:VAL:CG1  | 1:A:548:VAL:HG13 | 2.25                     | 0.64              |
| 2:B:142:ILE:HG22 | 2:B:144:TYR:CE2  | 2.33                     | 0.64              |
| 2:B:195:ILE:HD12 | 2:B:195:ILE:O    | 1.97                     | 0.64              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:HZ1  | 1.95                     | 0.64              |
| 2:B:92:LEU:HB3   | 2:B:158:ALA:HB1  | 1.80                     | 0.64              |
| 2:B:282:LEU:O    | 2:B:287:LYS:NZ   | 2.30                     | 0.64              |
| 2:B:301:LEU:C    | 2:B:305:GLU:HG3  | 2.22                     | 0.64              |
| 2:B:246:LEU:HD12 | 2:B:307:ARG:CG   | 2.27                     | 0.64              |
| 2:B:66:LYS:HA    | 2:B:407:GLN:HE22 | 1.63                     | 0.64              |
| 2:B:118:VAL:O    | 2:B:148:VAL:HB   | 1.98                     | 0.64              |
| 2:B:283:LEU:HA   | 2:B:287:LYS:CE   | 2.28                     | 0.64              |
| 1:A:79:GLU:CG    | 1:A:83:ARG:HH21  | 2.11                     | 0.63              |
| 1:A:2:ILE:HD11   | 1:A:46:LYS:HE2   | 1.80                     | 0.63              |
| 1:A:464:GLN:HG2  | 1:A:465:LYS:H    | 1.63                     | 0.63              |
| 1:A:540:LYS:O    | 1:A:542:ILE:N    | 2.30                     | 0.63              |
| 2:B:65:LYS:HB2   | 2:B:65:LYS:NZ    | 2.13                     | 0.63              |
| 2:B:82:LYS:HE3   | 2:B:413:GLU:OE2  | 1.97                     | 0.63              |
| 2:B:180:ILE:HG13 | 2:B:189:VAL:HG13 | 1.80                     | 0.63              |
| 1:A:434:ILE:CG2  | 1:A:530:LYS:HD3  | 2.27                     | 0.63              |
| 1:A:458:VAL:CG2  | 2:B:286:THR:HG21 | 2.29                     | 0.63              |
| 1:A:540:LYS:HB3  | 1:A:542:ILE:HD13 | 1.79                     | 0.63              |
| 2:B:162:SER:O    | 2:B:166:LYS:HE2  | 1.97                     | 0.63              |
| 1:A:65:LYS:HB3   | 1:A:65:LYS:HZ3   | 1.63                     | 0.63              |
| 1:A:171:PHE:O    | 1:A:175:ASN:HB2  | 1.99                     | 0.63              |
| 1:A:500:GLN:HG2  | 2:B:421:PRO:HG2  | 1.79                     | 0.63              |
| 2:B:306:ASN:HD22 | 2:B:309:ILE:HD12 | 1.63                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:388:LYS:HE3  | 2:B:415:GLU:HG3  | 1.79                     | 0.63              |
| 1:A:59:PRO:HG2   | 1:A:76:ASP:HB3   | 1.81                     | 0.63              |
| 2:B:116:PHE:HZ   | 2:B:151:GLN:HG3  | 1.61                     | 0.63              |
| 2:B:125:ARG:HD2  | 2:B:146:TYR:O    | 1.98                     | 0.63              |
| 1:A:296:THR:HG23 | 1:A:299:ALA:H    | 1.63                     | 0.63              |
| 1:A:491:LEU:HB3  | 1:A:529:GLU:HB2  | 1.80                     | 0.63              |
| 2:B:268:SER:O    | 2:B:269:GLN:HG3  | 1.99                     | 0.63              |
| 1:A:1:PRO:HB2    | 1:A:213:GLY:HA2  | 1.80                     | 0.63              |
| 2:B:111:VAL:HG21 | 2:B:187:LEU:HD22 | 1.79                     | 0.62              |
| 2:B:284:ARG:HH11 | 2:B:284:ARG:HB2  | 1.63                     | 0.62              |
| 2:B:267:ALA:O    | 2:B:271:TYR:HB2  | 1.99                     | 0.62              |
| 1:A:12:LEU:HD23  | 1:A:124:PHE:CE1  | 2.35                     | 0.62              |
| 1:A:458:VAL:HG12 | 1:A:548:VAL:CG1  | 2.28                     | 0.62              |
| 1:A:544:GLY:O    | 1:A:547:GLN:HB2  | 2.00                     | 0.62              |
| 2:B:255:ASN:O    | 2:B:259:LYS:HG3  | 1.98                     | 0.62              |
| 1:A:466:VAL:HG12 | 1:A:467:VAL:H    | 1.64                     | 0.62              |
| 2:B:169:GLU:HB3  | 2:B:170:PRO:HD3  | 1.80                     | 0.62              |
| 1:A:500:GLN:HG3  | 2:B:422:LEU:CD1  | 2.28                     | 0.62              |
| 1:A:448:ARG:HH11 | 1:A:448:ARG:CG   | 2.12                     | 0.62              |
| 1:A:23:GLN:OE1   | 1:A:60:VAL:HG23  | 1.99                     | 0.62              |
| 1:A:195:ILE:O    | 1:A:198:HIS:HB3  | 1.99                     | 0.62              |
| 1:A:406:TRP:HZ2  | 2:B:418:ASN:OD1  | 1.82                     | 0.62              |
| 1:A:460:ASN:HD21 | 2:B:288:ALA:HB2  | 1.64                     | 0.62              |
| 1:A:466:VAL:HG12 | 1:A:467:VAL:N    | 2.14                     | 0.62              |
| 2:B:174:GLN:C    | 2:B:176:PRO:HD3  | 2.25                     | 0.62              |
| 2:B:354:TYR:HD2  | 2:B:374:LYS:HE3  | 1.64                     | 0.62              |
| 2:B:388:LYS:HE3  | 2:B:415:GLU:CG   | 2.29                     | 0.62              |
| 1:A:307:ARG:O    | 1:A:311:LYS:HD2  | 1.98                     | 0.61              |
| 1:A:346:PHE:N    | 1:A:346:PHE:CD1  | 2.66                     | 0.61              |
| 1:A:440:PHE:CZ   | 1:A:489:SER:HB3  | 2.35                     | 0.61              |
| 2:B:154:LYS:HA   | 2:B:184:MET:HE3  | 1.81                     | 0.61              |
| 1:A:106:VAL:HG13 | 1:A:227:PHE:HE2  | 1.63                     | 0.61              |
| 2:B:114:ALA:HA   | 2:B:214:LEU:HD22 | 1.80                     | 0.61              |
| 1:A:21:VAL:HG21  | 1:A:59:PRO:HD3   | 1.82                     | 0.61              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:CD   | 2.12                     | 0.61              |
| 1:A:500:GLN:HG3  | 2:B:422:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:399:GLU:HA   | 1:A:402:TRP:HE3  | 1.65                     | 0.61              |
| 2:B:254:VAL:HB   | 2:B:289:LEU:HA   | 1.82                     | 0.61              |
| 1:A:406:TRP:CZ2  | 2:B:418:ASN:HA   | 2.36                     | 0.61              |
| 1:A:440:PHE:CE1  | 1:A:489:SER:HB3  | 2.35                     | 0.61              |
| 2:B:120:LEU:HD22 | 2:B:121:ASP:N    | 2.14                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:297:GLU:O    | 1:A:301:LEU:HG   | 2.01                     | 0.61              |
| 2:B:122:GLU:HA   | 2:B:125:ARG:NE   | 2.15                     | 0.61              |
| 1:A:380:ILE:HD11 | 1:A:386:THR:CG2  | 2.26                     | 0.60              |
| 1:A:195:ILE:HG23 | 1:A:199:ARG:NE   | 2.16                     | 0.60              |
| 1:A:101:LYS:HE2  | 1:A:321:PRO:HG3  | 1.82                     | 0.60              |
| 2:B:270:ILE:HG23 | 2:B:271:TYR:H    | 1.66                     | 0.60              |
| 2:B:369:THR:HG21 | 2:B:405:TYR:HB2  | 1.82                     | 0.60              |
| 1:A:199:ARG:HG3  | 1:A:219:LYS:HE3  | 1.83                     | 0.60              |
| 1:A:277:ARG:HH11 | 1:A:334:GLN:HE21 | 1.48                     | 0.60              |
| 1:A:479:LEU:CD2  | 1:A:501:TYR:HE2  | 2.14                     | 0.60              |
| 1:A:58:THR:HG23  | 1:A:76:ASP:O     | 2.02                     | 0.60              |
| 1:A:318:TYR:CZ   | 3:A:601:R8D:C15  | 2.84                     | 0.60              |
| 2:B:319:TYR:OH   | 2:B:385:LYS:HD3  | 2.01                     | 0.60              |
| 1:A:295:LEU:HD23 | 1:A:295:LEU:H    | 1.66                     | 0.60              |
| 1:A:41:MET:HE1   | 1:A:73:LYS:HZ1   | 1.65                     | 0.60              |
| 1:A:497:THR:O    | 1:A:535:TRP:HA   | 2.01                     | 0.60              |
| 1:A:2:ILE:HD11   | 1:A:46:LYS:HZ1   | 1.66                     | 0.59              |
| 2:B:72:ARG:HG3   | 2:B:73:LYS:N     | 2.17                     | 0.59              |
| 2:B:205:LEU:O    | 2:B:209:LEU:HD22 | 2.01                     | 0.59              |
| 1:A:540:LYS:HB3  | 1:A:542:ILE:CD1  | 2.33                     | 0.59              |
| 1:A:177:ASP:OD2  | 1:A:177:ASP:N    | 2.36                     | 0.59              |
| 1:A:208:HIS:O    | 1:A:212:TRP:HD1  | 1.84                     | 0.59              |
| 1:A:235:HIS:HB3  | 1:A:236:PRO:HD2  | 1.85                     | 0.59              |
| 2:B:66:LYS:N     | 2:B:407:GLN:NE2  | 2.50                     | 0.59              |
| 1:A:301:LEU:O    | 1:A:304:ALA:HB3  | 2.02                     | 0.59              |
| 2:B:354:TYR:HB2  | 2:B:374:LYS:HZ2  | 1.67                     | 0.59              |
| 1:A:330:GLN:HE22 | 1:A:340:GLN:HE22 | 1.49                     | 0.59              |
| 1:A:401:TRP:HB2  | 1:A:425:LEU:HD21 | 1.84                     | 0.59              |
| 1:A:500:GLN:HG2  | 2:B:421:PRO:CG   | 2.32                     | 0.59              |
| 1:A:400:THR:O    | 1:A:404:GLU:HG3  | 2.03                     | 0.59              |
| 1:A:520:GLN:HA   | 1:A:523:GLU:CG   | 2.32                     | 0.59              |
| 1:A:325:LEU:HD11 | 1:A:383:TRP:CD2  | 2.38                     | 0.59              |
| 2:B:297:GLU:HA   | 2:B:300:GLU:HB2  | 1.83                     | 0.59              |
| 2:B:382:ILE:HG22 | 2:B:383:TRP:CD2  | 2.38                     | 0.59              |
| 1:A:194:GLU:O    | 1:A:197:GLN:HG2  | 2.03                     | 0.59              |
| 1:A:278:GLN:HG3  | 1:A:298:GLU:CB   | 2.33                     | 0.59              |
| 1:A:325:LEU:O    | 1:A:326:ILE:HD13 | 2.03                     | 0.59              |
| 2:B:175:ASN:HB3  | 2:B:178:ILE:HG13 | 1.83                     | 0.59              |
| 1:A:3:SER:HB3    | 1:A:5:ILE:CD1    | 2.33                     | 0.59              |
| 2:B:283:LEU:HD23 | 2:B:287:LYS:HE3  | 1.85                     | 0.59              |
| 1:A:64:LYS:HZ1   | 1:A:69:THR:CA    | 2.16                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:420:PRO:HA   | 1:A:421:PRO:C    | 2.27                     | 0.58              |
| 1:A:449:GLU:O    | 1:A:451:LYS:HE2  | 2.03                     | 0.58              |
| 1:A:3:SER:OG     | 1:A:5:ILE:HG23   | 2.03                     | 0.58              |
| 1:A:70:LYS:HE2   | 1:A:71:TRP:O     | 2.02                     | 0.58              |
| 1:A:324:ASP:HB3  | 1:A:388:LYS:CE   | 2.33                     | 0.58              |
| 1:A:491:LEU:H    | 1:A:491:LEU:CD1  | 2.16                     | 0.58              |
| 1:A:245:VAL:HG22 | 1:A:245:VAL:O    | 2.04                     | 0.58              |
| 2:B:267:ALA:O    | 2:B:270:ILE:HG23 | 2.03                     | 0.58              |
| 1:A:199:ARG:HG2  | 1:A:199:ARG:HH11 | 1.68                     | 0.58              |
| 1:A:122:GLU:CA   | 1:A:125:ARG:HD2  | 2.27                     | 0.58              |
| 1:A:312:GLU:HG2  | 1:A:313:PRO:N    | 2.19                     | 0.58              |
| 2:B:382:ILE:HG22 | 2:B:383:TRP:CG   | 2.39                     | 0.58              |
| 2:B:305:GLU:O    | 2:B:309:ILE:HG13 | 2.04                     | 0.58              |
| 1:A:175:ASN:C    | 1:A:178:ILE:HD13 | 2.29                     | 0.58              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:HE3  | 1.67                     | 0.57              |
| 1:A:107:THR:HG21 | 1:A:202:ILE:CD1  | 2.30                     | 0.57              |
| 1:A:333:GLY:O    | 1:A:335:GLY:N    | 2.37                     | 0.57              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:HA   | 2.39                     | 0.57              |
| 1:A:454:LYS:HA   | 1:A:467:VAL:O    | 2.04                     | 0.57              |
| 1:A:101:LYS:CD   | 1:A:321:PRO:HG3  | 2.35                     | 0.57              |
| 1:A:209:LEU:HD13 | 1:A:216:THR:HG21 | 1.85                     | 0.57              |
| 1:A:432:GLU:OE1  | 1:A:432:GLU:HA   | 2.04                     | 0.57              |
| 1:A:535:TRP:CZ3  | 1:A:537:PRO:HD3  | 2.38                     | 0.57              |
| 2:B:175:ASN:N    | 2:B:176:PRO:HD3  | 2.18                     | 0.57              |
| 1:A:122:GLU:HA   | 1:A:125:ARG:NE   | 2.19                     | 0.57              |
| 1:A:244:ILE:HD12 | 1:A:267:ALA:CB   | 2.35                     | 0.57              |
| 2:B:322:SER:O    | 2:B:323:LYS:HG2  | 2.04                     | 0.57              |
| 1:A:460:ASN:HB2  | 2:B:286:THR:O    | 2.05                     | 0.57              |
| 2:B:13:LYS:O     | 2:B:16:MET:HG2   | 2.04                     | 0.57              |
| 2:B:114:ALA:HA   | 2:B:214:LEU:CD2  | 2.35                     | 0.57              |
| 2:B:271:TYR:O    | 2:B:274:ILE:HG12 | 2.04                     | 0.57              |
| 2:B:293:ILE:HG13 | 2:B:293:ILE:O    | 2.02                     | 0.57              |
| 2:B:400:THR:HG1  | 2:B:401:TRP:CD1  | 2.22                     | 0.57              |
| 1:A:12:LEU:HD23  | 1:A:124:PHE:HE1  | 1.69                     | 0.57              |
| 1:A:64:LYS:HE2   | 1:A:69:THR:C     | 2.29                     | 0.57              |
| 1:A:168:LEU:C    | 1:A:170:PRO:HD2  | 2.29                     | 0.57              |
| 1:A:380:ILE:CD1  | 1:A:386:THR:HG22 | 2.32                     | 0.57              |
| 1:A:540:LYS:HB2  | 1:A:542:ILE:HD13 | 1.86                     | 0.57              |
| 1:A:443:ASP:CB   | 1:A:548:VAL:HB   | 2.33                     | 0.57              |
| 2:B:374:LYS:O    | 2:B:378:GLU:HG3  | 2.04                     | 0.57              |
| 1:A:227:PHE:HB2  | 1:A:234:LEU:HB2  | 1.85                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:487:GLN:HA   | 1:A:524:GLN:HE22 | 1.69                     | 0.57              |
| 2:B:284:ARG:HB2  | 2:B:284:ARG:NH1  | 2.19                     | 0.57              |
| 1:A:41:MET:HE1   | 1:A:73:LYS:NZ    | 2.19                     | 0.57              |
| 1:A:228:LEU:HB3  | 1:A:242:GLN:HE22 | 1.66                     | 0.57              |
| 1:A:65:LYS:HD3   | 1:A:70:LYS:HG2   | 1.86                     | 0.56              |
| 1:A:324:ASP:CG   | 1:A:388:LYS:HE2  | 2.30                     | 0.56              |
| 1:A:64:LYS:HZ1   | 1:A:69:THR:CG2   | 2.18                     | 0.56              |
| 1:A:324:ASP:OD2  | 1:A:388:LYS:NZ   | 2.34                     | 0.56              |
| 1:A:395:LYS:HD2  | 1:A:414:TRP:CZ2  | 2.39                     | 0.56              |
| 1:A:455:ALA:HB3  | 1:A:469:LEU:HD11 | 1.86                     | 0.56              |
| 2:B:98:ALA:O     | 2:B:101:LYS:NZ   | 2.31                     | 0.56              |
| 1:A:209:LEU:CD1  | 1:A:216:THR:HG21 | 2.35                     | 0.56              |
| 1:A:332:GLN:HG3  | 1:A:338:THR:HG22 | 1.86                     | 0.56              |
| 2:B:194:GLU:OE1  | 2:B:197:GLN:N    | 2.36                     | 0.56              |
| 2:B:270:ILE:O    | 2:B:272:PRO:HD3  | 2.06                     | 0.56              |
| 2:B:284:ARG:N    | 2:B:287:LYS:HE2  | 2.21                     | 0.56              |
| 2:B:314:VAL:HB   | 2:B:317:VAL:HG23 | 1.87                     | 0.56              |
| 1:A:34:LEU:CD2   | 1:A:62:ALA:HB2   | 2.33                     | 0.56              |
| 1:A:339:TYR:CG   | 1:A:375:ILE:CD1  | 2.88                     | 0.56              |
| 2:B:153:TRP:CZ2  | 2:B:155:GLY:HA3  | 2.41                     | 0.56              |
| 2:B:63:ILE:HD13  | 2:B:74:LEU:HD13  | 1.86                     | 0.56              |
| 2:B:378:GLU:O    | 2:B:382:ILE:HD12 | 2.06                     | 0.56              |
| 1:A:91:GLN:NE2   | 2:B:137:ASN:HB3  | 2.20                     | 0.56              |
| 1:A:395:LYS:CD   | 1:A:414:TRP:CZ2  | 2.88                     | 0.56              |
| 1:A:425:LEU:HD23 | 1:A:428:GLN:NE2  | 2.20                     | 0.56              |
| 2:B:5:ILE:HG23   | 2:B:6:GLU:OE1    | 2.06                     | 0.56              |
| 1:A:332:GLN:HG3  | 1:A:338:THR:CG2  | 2.35                     | 0.56              |
| 2:B:373:GLN:HE22 | 2:B:407:GLN:H    | 1.53                     | 0.56              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:CE   | 2.17                     | 0.56              |
| 2:B:425:LEU:HA   | 2:B:428:GLN:HB2  | 1.87                     | 0.56              |
| 1:A:424:LYS:HE2  | 1:A:426:TRP:CZ3  | 2.40                     | 0.55              |
| 1:A:238:LYS:HD2  | 1:A:315:HIS:CD2  | 2.42                     | 0.55              |
| 1:A:478:GLU:OE1  | 1:A:499:SER:HB2  | 2.07                     | 0.55              |
| 1:A:114:ALA:HB1  | 1:A:160:PHE:CE1  | 2.42                     | 0.55              |
| 2:B:115:TYR:HB3  | 2:B:149:LEU:HB2  | 1.88                     | 0.55              |
| 2:B:116:PHE:HD2  | 2:B:148:VAL:HG21 | 1.69                     | 0.55              |
| 1:A:277:ARG:CZ   | 1:A:334:GLN:HB2  | 2.37                     | 0.55              |
| 2:B:247:PRO:O    | 2:B:307:ARG:NH1  | 2.30                     | 0.55              |
| 1:A:89:GLU:HB3   | 1:A:92:LEU:HD11  | 1.88                     | 0.55              |
| 1:A:135:ILE:O    | 1:A:136:ASN:HB2  | 2.06                     | 0.55              |
| 2:B:393:ILE:HD11 | 2:B:397:THR:HG22 | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:65:LYS:HD3   | 1:A:70:LYS:CG    | 2.36                     | 0.55              |
| 1:A:164:MET:O    | 1:A:168:LEU:HD12 | 2.06                     | 0.55              |
| 2:B:96:HIS:HE1   | 2:B:381:VAL:O    | 1.89                     | 0.55              |
| 2:B:422:LEU:HB3  | 2:B:426:TRP:CH2  | 2.41                     | 0.55              |
| 1:A:325:LEU:C    | 1:A:326:ILE:HD13 | 2.32                     | 0.55              |
| 2:B:312:GLU:HB3  | 2:B:313:PRO:HD2  | 1.89                     | 0.55              |
| 2:B:369:THR:HG22 | 2:B:370:GLU:N    | 2.22                     | 0.55              |
| 2:B:253:THR:HG23 | 2:B:254:VAL:N    | 2.21                     | 0.54              |
| 2:B:116:PHE:HA   | 2:B:148:VAL:CG2  | 2.36                     | 0.54              |
| 2:B:24:TRP:H     | 2:B:24:TRP:CD1   | 2.25                     | 0.54              |
| 2:B:330:GLN:HE22 | 2:B:340:GLN:HE22 | 1.54                     | 0.54              |
| 1:A:173:LYS:HA   | 1:A:173:LYS:CE   | 2.37                     | 0.54              |
| 2:B:13:LYS:HB3   | 2:B:16:MET:HE3   | 1.89                     | 0.54              |
| 2:B:122:GLU:HG2  | 2:B:125:ARG:NH2  | 2.23                     | 0.54              |
| 2:B:301:LEU:O    | 2:B:304:ALA:HB3  | 2.07                     | 0.54              |
| 1:A:433:PRO:HG3  | 2:B:255:ASN:ND2  | 2.22                     | 0.54              |
| 1:A:101:LYS:HD2  | 1:A:321:PRO:HG3  | 1.89                     | 0.54              |
| 2:B:284:ARG:H    | 2:B:287:LYS:CE   | 2.20                     | 0.54              |
| 2:B:285:GLY:O    | 2:B:287:LYS:HG2  | 2.07                     | 0.54              |
| 1:A:52:PRO:HD2   | 1:A:53:GLU:OE2   | 2.07                     | 0.54              |
| 1:A:220:LYS:HE3  | 1:A:221:HIS:ND1  | 2.23                     | 0.54              |
| 1:A:442:VAL:CG2  | 1:A:495:ILE:HG23 | 2.37                     | 0.54              |
| 2:B:183:TYR:CD2  | 2:B:184:MET:HG3  | 2.43                     | 0.54              |
| 2:B:247:PRO:C    | 2:B:307:ARG:HH12 | 2.14                     | 0.54              |
| 2:B:425:LEU:HG   | 2:B:426:TRP:N    | 2.23                     | 0.54              |
| 2:B:278:GLN:O    | 2:B:282:LEU:HD23 | 2.07                     | 0.54              |
| 1:A:219:LYS:O    | 1:A:220:LYS:HD2  | 2.07                     | 0.54              |
| 1:A:369:THR:HG21 | 1:A:398:TRP:CH2  | 2.43                     | 0.54              |
| 2:B:79:GLU:O     | 2:B:83:ARG:HG2   | 2.08                     | 0.54              |
| 1:A:164:MET:SD   | 1:A:168:LEU:HD11 | 2.48                     | 0.53              |
| 1:A:464:GLN:HG2  | 1:A:465:LYS:N    | 2.23                     | 0.53              |
| 2:B:253:THR:CG2  | 2:B:255:ASN:HB3  | 2.38                     | 0.53              |
| 2:B:254:VAL:HG21 | 2:B:288:ALA:O    | 2.08                     | 0.53              |
| 2:B:270:ILE:HG23 | 2:B:271:TYR:N    | 2.22                     | 0.53              |
| 1:A:226:PRO:HG3  | 1:A:235:HIS:CD2  | 2.41                     | 0.53              |
| 1:A:283:LEU:N    | 1:A:283:LEU:HD23 | 2.21                     | 0.53              |
| 2:B:276:VAL:HG22 | 2:B:279:LEU:HB2  | 1.91                     | 0.53              |
| 2:B:80:LEU:O     | 2:B:80:LEU:HD22  | 2.08                     | 0.53              |
| 1:A:355:ALA:O    | 1:A:356:ARG:O    | 2.26                     | 0.53              |
| 1:A:520:GLN:HA   | 1:A:523:GLU:HG3  | 1.91                     | 0.53              |
| 1:A:406:TRP:CZ3  | 1:A:407:GLN:HG3  | 2.43                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:430:GLU:CD   | 1:A:530:LYS:HG2  | 2.34                     | 0.53              |
| 2:B:270:ILE:HG13 | 2:B:346:PHE:O    | 2.08                     | 0.53              |
| 2:B:354:TYR:HB2  | 2:B:374:LYS:HZ1  | 1.74                     | 0.53              |
| 1:A:219:LYS:C    | 1:A:221:HIS:H    | 2.16                     | 0.53              |
| 2:B:263:LYS:O    | 2:B:266:TRP:HE3  | 1.90                     | 0.53              |
| 1:A:69:THR:O     | 1:A:69:THR:HG22  | 2.08                     | 0.53              |
| 1:A:238:LYS:CB   | 1:A:315:HIS:HD2  | 2.22                     | 0.53              |
| 1:A:402:TRP:CG   | 1:A:403:THR:N    | 2.75                     | 0.53              |
| 1:A:271:TYR:CZ   | 1:A:314:VAL:HG23 | 2.44                     | 0.53              |
| 1:A:317:VAL:CG2  | 1:A:318:TYR:N    | 2.72                     | 0.53              |
| 2:B:298:GLU:O    | 2:B:301:LEU:HG   | 2.08                     | 0.53              |
| 1:A:38:CYS:HB3   | 1:A:144:TYR:CE2  | 2.44                     | 0.53              |
| 1:A:42:GLU:OE2   | 1:A:49:LYS:HE3   | 2.08                     | 0.53              |
| 1:A:330:GLN:NE2  | 1:A:340:GLN:HE22 | 2.07                     | 0.53              |
| 2:B:88:TRP:CZ3   | 2:B:89:GLU:HB2   | 2.44                     | 0.53              |
| 2:B:330:GLN:NE2  | 2:B:340:GLN:HE22 | 2.07                     | 0.53              |
| 1:A:228:LEU:HB3  | 1:A:242:GLN:HE21 | 1.73                     | 0.52              |
| 1:A:278:GLN:N    | 1:A:302:GLU:OE1  | 2.42                     | 0.52              |
| 1:A:291:GLU:O    | 1:A:291:GLU:HG3  | 2.09                     | 0.52              |
| 2:B:284:ARG:H    | 2:B:287:LYS:HE2  | 1.74                     | 0.52              |
| 2:B:354:TYR:CB   | 2:B:374:LYS:HZ1  | 2.22                     | 0.52              |
| 1:A:13:LYS:HB2   | 1:A:16:MET:SD    | 2.49                     | 0.52              |
| 1:A:295:LEU:HD23 | 1:A:295:LEU:N    | 2.24                     | 0.52              |
| 1:A:320:ASP:C    | 1:A:322:SER:H    | 2.17                     | 0.52              |
| 1:A:65:LYS:HZ2   | 1:A:68:SER:CB    | 2.22                     | 0.52              |
| 1:A:241:VAL:HG12 | 1:A:266:TRP:NE1  | 2.24                     | 0.52              |
| 1:A:276:VAL:O    | 1:A:276:VAL:HG12 | 2.09                     | 0.52              |
| 1:A:311:LYS:O    | 1:A:312:GLU:OE2  | 2.28                     | 0.52              |
| 1:A:458:VAL:HG13 | 1:A:548:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:475:GLN:HG3  | 1:A:501:TYR:CZ   | 2.44                     | 0.52              |
| 2:B:116:PHE:HZ   | 2:B:151:GLN:CG   | 2.21                     | 0.52              |
| 1:A:171:PHE:CE2  | 1:A:205:LEU:HD23 | 2.45                     | 0.52              |
| 1:A:230:MET:HE3  | 1:A:230:MET:H    | 1.74                     | 0.52              |
| 1:A:236:PRO:HA   | 3:A:601:R8D:C17  | 2.39                     | 0.52              |
| 1:A:246:LEU:N    | 1:A:246:LEU:HD23 | 2.24                     | 0.52              |
| 1:A:296:THR:HG23 | 1:A:299:ALA:CB   | 2.39                     | 0.52              |
| 1:A:320:ASP:O    | 1:A:343:GLN:NE2  | 2.42                     | 0.52              |
| 1:A:2:ILE:HG22   | 1:A:2:ILE:O      | 2.09                     | 0.52              |
| 1:A:135:ILE:O    | 1:A:138:GLU:OE2  | 2.27                     | 0.52              |
| 1:A:546:GLU:HG2  | 1:A:547:GLN:HE21 | 1.72                     | 0.52              |
| 2:B:88:TRP:CE3   | 2:B:89:GLU:HB2   | 2.43                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:60:VAL:HG13  | 1:A:75:VAL:HG22  | 1.92                     | 0.52              |
| 1:A:438:GLU:O    | 1:A:494:ASN:HB2  | 2.10                     | 0.52              |
| 1:A:5:ILE:HD11   | 1:A:119:PRO:HG2  | 1.92                     | 0.52              |
| 1:A:230:MET:HA   | 1:A:230:MET:HE2  | 1.90                     | 0.52              |
| 1:A:403:THR:CG2  | 1:A:404:GLU:N    | 2.73                     | 0.52              |
| 2:B:131:THR:OG1  | 2:B:143:ARG:HD2  | 2.08                     | 0.52              |
| 1:A:53:GLU:HG2   | 1:A:54:ASN:N     | 2.24                     | 0.52              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:CA   | 2.93                     | 0.52              |
| 1:A:411:ILE:HG22 | 1:A:412:PRO:O    | 2.10                     | 0.52              |
| 1:A:429:LEU:HD21 | 1:A:506:ILE:HG22 | 1.92                     | 0.52              |
| 1:A:493:VAL:HG21 | 1:A:528:LYS:HE2  | 1.90                     | 0.52              |
| 1:A:459:THR:CG2  | 1:A:463:ARG:HB3  | 2.40                     | 0.52              |
| 2:B:261:VAL:O    | 2:B:265:ASN:N    | 2.26                     | 0.52              |
| 2:B:266:TRP:NE1  | 2:B:346:PHE:CE2  | 2.77                     | 0.52              |
| 1:A:252:TRP:CG   | 1:A:295:LEU:HD21 | 2.45                     | 0.52              |
| 1:A:438:GLU:HG3  | 1:A:461:ARG:HG3  | 1.91                     | 0.52              |
| 2:B:131:THR:HG22 | 2:B:132:ILE:N    | 2.24                     | 0.52              |
| 2:B:271:TYR:HB3  | 2:B:274:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:188:TYR:CD2  | 3:A:601:R8D:C25  | 2.93                     | 0.51              |
| 1:A:235:HIS:HB3  | 1:A:236:PRO:CD   | 2.40                     | 0.51              |
| 2:B:297:GLU:N    | 2:B:298:GLU:OE2  | 2.43                     | 0.51              |
| 1:A:65:LYS:CD    | 1:A:70:LYS:HG2   | 2.39                     | 0.51              |
| 1:A:79:GLU:OE1   | 1:A:82:LYS:HE2   | 2.10                     | 0.51              |
| 2:B:175:ASN:HD21 | 2:B:201:LYS:NZ   | 2.09                     | 0.51              |
| 2:B:183:TYR:CE2  | 2:B:184:MET:HG3  | 2.46                     | 0.51              |
| 2:B:379:SER:OG   | 2:B:387:PRO:HD3  | 2.09                     | 0.51              |
| 1:A:17:ASP:O     | 1:A:83:ARG:HD3   | 2.09                     | 0.51              |
| 1:A:65:LYS:HD2   | 1:A:72:ARG:HD2   | 1.92                     | 0.51              |
| 1:A:289:LEU:HD13 | 1:A:289:LEU:O    | 2.09                     | 0.51              |
| 1:A:527:LYS:O    | 1:A:528:LYS:O    | 2.28                     | 0.51              |
| 2:B:306:ASN:O    | 2:B:309:ILE:N    | 2.43                     | 0.51              |
| 1:A:94:ILE:HB    | 1:A:95:PRO:HD2   | 1.93                     | 0.51              |
| 1:A:330:GLN:HE22 | 1:A:340:GLN:NE2  | 2.08                     | 0.51              |
| 2:B:120:LEU:HD22 | 2:B:121:ASP:H    | 1.74                     | 0.51              |
| 1:A:134:SER:HB2  | 1:A:139:THR:HB   | 1.90                     | 0.51              |
| 1:A:181:TYR:HD2  | 3:A:601:R8D:H5   | 1.76                     | 0.51              |
| 1:A:284:ARG:NH1  | 1:A:285:GLY:HA3  | 2.23                     | 0.51              |
| 1:A:296:THR:CG2  | 1:A:299:ALA:HB2  | 2.40                     | 0.51              |
| 1:A:458:VAL:O    | 1:A:458:VAL:HG22 | 2.10                     | 0.51              |
| 1:A:459:THR:HG21 | 1:A:463:ARG:HB3  | 1.92                     | 0.51              |
| 1:A:210:LEU:C    | 1:A:212:TRP:H    | 2.18                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:278:GLN:HG3  | 1:A:298:GLU:HB3  | 1.93                     | 0.51              |
| 1:A:311:LYS:O    | 1:A:312:GLU:CB   | 2.56                     | 0.51              |
| 1:A:346:PHE:N    | 1:A:346:PHE:HD1  | 2.08                     | 0.51              |
| 2:B:266:TRP:NE1  | 2:B:346:PHE:HE2  | 2.08                     | 0.51              |
| 1:A:127:TYR:C    | 1:A:129:ALA:H    | 2.19                     | 0.51              |
| 1:A:173:LYS:HA   | 1:A:173:LYS:HE3  | 1.92                     | 0.51              |
| 2:B:354:TYR:HA   | 2:B:374:LYS:HZ1  | 1.76                     | 0.51              |
| 1:A:254:VAL:HG21 | 1:A:288:ALA:O    | 2.11                     | 0.51              |
| 1:A:137:ASN:O    | 1:A:138:GLU:O    | 2.28                     | 0.50              |
| 1:A:120:LEU:HD21 | 1:A:128:THR:HG21 | 1.93                     | 0.50              |
| 1:A:206:ARG:NH2  | 1:A:218:ASP:N    | 2.58                     | 0.50              |
| 1:A:330:GLN:NE2  | 1:A:338:THR:HG23 | 2.26                     | 0.50              |
| 2:B:18:GLY:HA3   | 2:B:56:TYR:CD1   | 2.47                     | 0.50              |
| 2:B:87:PHE:O     | 2:B:91:GLN:HB3   | 2.12                     | 0.50              |
| 1:A:324:ASP:O    | 1:A:343:GLN:HG2  | 2.11                     | 0.50              |
| 2:B:66:LYS:O     | 2:B:67:ASP:HB2   | 2.09                     | 0.50              |
| 2:B:195:ILE:HG23 | 2:B:196:GLY:N    | 2.26                     | 0.50              |
| 2:B:306:ASN:O    | 2:B:310:LEU:N    | 2.35                     | 0.50              |
| 1:A:402:TRP:CD1  | 1:A:402:TRP:C    | 2.85                     | 0.50              |
| 2:B:88:TRP:CZ2   | 2:B:154:LYS:HD3  | 2.47                     | 0.50              |
| 2:B:142:ILE:CG2  | 2:B:144:TYR:CE2  | 2.95                     | 0.50              |
| 1:A:2:ILE:CD1    | 1:A:46:LYS:HE2   | 2.41                     | 0.50              |
| 1:A:228:LEU:N    | 1:A:228:LEU:CD1  | 2.74                     | 0.50              |
| 1:A:393:ILE:O    | 1:A:416:PHE:HD1  | 1.95                     | 0.50              |
| 1:A:432:GLU:OE1  | 1:A:433:PRO:HD3  | 2.12                     | 0.50              |
| 1:A:231:GLY:O    | 1:A:242:GLN:N    | 2.45                     | 0.50              |
| 1:A:391:LEU:HB3  | 1:A:392:PRO:HD2  | 1.93                     | 0.50              |
| 2:B:50:ILE:CG2   | 2:B:145:GLN:HB3  | 2.32                     | 0.50              |
| 1:A:233:GLU:O    | 1:A:234:LEU:HD23 | 2.12                     | 0.50              |
| 1:A:448:ARG:HG2  | 1:A:448:ARG:NH1  | 2.21                     | 0.50              |
| 1:A:35:VAL:O     | 1:A:39:THR:HG23  | 2.12                     | 0.50              |
| 1:A:101:LYS:CE   | 1:A:321:PRO:HG3  | 2.41                     | 0.50              |
| 1:A:324:ASP:HB3  | 1:A:388:LYS:HE2  | 1.93                     | 0.50              |
| 2:B:254:VAL:O    | 2:B:257:ILE:N    | 2.37                     | 0.50              |
| 2:B:154:LYS:HA   | 2:B:184:MET:CE   | 2.41                     | 0.49              |
| 2:B:160:PHE:HE2  | 2:B:164:MET:CE   | 2.11                     | 0.49              |
| 1:A:101:LYS:HD3  | 1:A:321:PRO:HD3  | 1.93                     | 0.49              |
| 1:A:418:ASN:C    | 1:A:420:PRO:HD3  | 2.36                     | 0.49              |
| 2:B:125:ARG:NH1  | 2:B:147:ASN:HD22 | 2.11                     | 0.49              |
| 1:A:200:THR:HG22 | 1:A:201:LYS:N    | 2.26                     | 0.49              |
| 2:B:196:GLY:HA2  | 2:B:199:ARG:HG3  | 1.93                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:276:VAL:HG22 | 2:B:279:LEU:CB   | 2.42                     | 0.49              |
| 2:B:320:ASP:O    | 2:B:343:GLN:NE2  | 2.45                     | 0.49              |
| 2:B:342:TYR:HB3  | 2:B:348:ASN:HA   | 1.93                     | 0.49              |
| 1:A:65:LYS:HB3   | 1:A:65:LYS:NZ    | 2.28                     | 0.49              |
| 1:A:66:LYS:O     | 1:A:67:ASP:HB3   | 2.12                     | 0.49              |
| 1:A:167:ILE:O    | 1:A:208:HIS:NE2  | 2.38                     | 0.49              |
| 1:A:174:GLN:O    | 1:A:175:ASN:OD1  | 2.31                     | 0.49              |
| 2:B:159:ILE:HG22 | 2:B:160:PHE:N    | 2.27                     | 0.49              |
| 2:B:422:LEU:O    | 2:B:425:LEU:HD23 | 2.13                     | 0.49              |
| 1:A:278:GLN:HB3  | 1:A:299:ALA:HA   | 1.94                     | 0.49              |
| 1:A:511:ASP:OD2  | 1:A:512:GLN:HG2  | 2.11                     | 0.49              |
| 2:B:79:GLU:HG3   | 2:B:83:ARG:HE    | 1.78                     | 0.49              |
| 2:B:422:LEU:CB   | 2:B:426:TRP:CH2  | 2.96                     | 0.49              |
| 1:A:13:LYS:HG3   | 1:A:84:THR:O     | 2.12                     | 0.49              |
| 1:A:100:LEU:CD2  | 1:A:181:TYR:CE2  | 2.95                     | 0.49              |
| 1:A:278:GLN:HB2  | 1:A:302:GLU:CD   | 2.38                     | 0.49              |
| 1:A:477:THR:O    | 1:A:480:GLN:HB3  | 2.13                     | 0.49              |
| 2:B:66:LYS:N     | 2:B:407:GLN:HE22 | 2.11                     | 0.49              |
| 2:B:74:LEU:HD21  | 2:B:411:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:79:GLU:HG2   | 1:A:83:ARG:HH21  | 1.78                     | 0.49              |
| 1:A:5:ILE:HD11   | 1:A:119:PRO:CG   | 2.43                     | 0.48              |
| 2:B:66:LYS:CA    | 2:B:407:GLN:NE2  | 2.75                     | 0.48              |
| 2:B:154:LYS:HG3  | 2:B:184:MET:CE   | 2.42                     | 0.48              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:CE   | 2.76                     | 0.48              |
| 1:A:195:ILE:CG2  | 1:A:199:ARG:NE   | 2.76                     | 0.48              |
| 1:A:209:LEU:HB3  | 1:A:214:LEU:HB2  | 1.94                     | 0.48              |
| 1:A:361:HIS:HB3  | 1:A:513:SER:HB2  | 1.93                     | 0.48              |
| 2:B:172:ARG:HH21 | 2:B:180:ILE:HB   | 1.78                     | 0.48              |
| 1:A:77:PHE:HE2   | 1:A:150:PRO:HB2  | 1.77                     | 0.48              |
| 1:A:101:LYS:O    | 3:A:601:R8D:H11  | 2.13                     | 0.48              |
| 1:A:120:LEU:O    | 1:A:125:ARG:NE   | 2.43                     | 0.48              |
| 1:A:339:TYR:CD1  | 1:A:375:ILE:CD1  | 2.96                     | 0.48              |
| 1:A:442:VAL:HG11 | 1:A:481:ALA:C    | 2.37                     | 0.48              |
| 2:B:85:GLN:O     | 2:B:85:GLN:HG2   | 2.13                     | 0.48              |
| 2:B:254:VAL:HG13 | 2:B:283:LEU:HD21 | 1.94                     | 0.48              |
| 1:A:399:GLU:CG   | 1:A:400:THR:N    | 2.77                     | 0.48              |
| 1:A:47:ILE:HG22  | 1:A:146:TYR:HA   | 1.96                     | 0.48              |
| 1:A:125:ARG:NH1  | 1:A:147:ASN:HD22 | 2.12                     | 0.48              |
| 1:A:199:ARG:H    | 1:A:199:ARG:HD2  | 1.79                     | 0.48              |
| 1:A:339:TYR:CD1  | 1:A:375:ILE:HD11 | 2.49                     | 0.48              |
| 1:A:424:LYS:HE2  | 1:A:426:TRP:CD2  | 2.49                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:63:ILE:CD1   | 2:B:74:LEU:HD13  | 2.43                     | 0.48              |
| 2:B:204:GLU:O    | 2:B:207:GLN:HB2  | 2.14                     | 0.48              |
| 1:A:63:ILE:CG1   | 1:A:74:LEU:CD1   | 2.91                     | 0.48              |
| 1:A:202:ILE:O    | 1:A:206:ARG:HG3  | 2.13                     | 0.48              |
| 2:B:254:VAL:HG13 | 2:B:283:LEU:CD2  | 2.44                     | 0.48              |
| 1:A:230:MET:CE   | 1:A:230:MET:CA   | 2.91                     | 0.48              |
| 1:A:411:ILE:CG2  | 1:A:414:TRP:CD1  | 2.96                     | 0.48              |
| 1:A:491:LEU:CD1  | 1:A:491:LEU:N    | 2.76                     | 0.48              |
| 1:A:517:LEU:HA   | 1:A:520:GLN:HG3  | 1.95                     | 0.48              |
| 2:B:72:ARG:NH1   | 2:B:409:THR:HG22 | 2.29                     | 0.48              |
| 1:A:188:TYR:CE2  | 3:A:601:R8D:C25  | 2.96                     | 0.48              |
| 1:A:427:TYR:O    | 1:A:428:GLN:HG2  | 2.14                     | 0.48              |
| 1:A:443:ASP:O    | 1:A:481:ALA:HB2  | 2.14                     | 0.48              |
| 1:A:476:LYS:O    | 1:A:480:GLN:HB2  | 2.14                     | 0.48              |
| 1:A:116:PHE:HD1  | 1:A:148:VAL:CG2  | 2.27                     | 0.47              |
| 1:A:318:TYR:CD2  | 3:A:601:R8D:H15  | 2.42                     | 0.47              |
| 2:B:387:PRO:HG2  | 2:B:389:PHE:CE1  | 2.49                     | 0.47              |
| 1:A:349:LEU:HA   | 1:A:349:LEU:HD12 | 1.59                     | 0.47              |
| 2:B:234:LEU:O    | 2:B:236:PRO:HD3  | 2.14                     | 0.47              |
| 1:A:226:PRO:O    | 1:A:228:LEU:HD13 | 2.13                     | 0.47              |
| 1:A:378:GLU:O    | 1:A:382:ILE:HG13 | 2.14                     | 0.47              |
| 2:B:7:THR:CG2    | 2:B:119:PRO:HB2  | 2.45                     | 0.47              |
| 2:B:283:LEU:HD23 | 2:B:287:LYS:CE   | 2.43                     | 0.47              |
| 1:A:479:LEU:HD22 | 1:A:501:TYR:HE2  | 1.77                     | 0.47              |
| 2:B:96:HIS:HA    | 2:B:97:PRO:HD2   | 1.47                     | 0.47              |
| 2:B:211:ARG:N    | 2:B:211:ARG:CD   | 2.76                     | 0.47              |
| 2:B:393:ILE:CG2  | 2:B:398:TRP:HB2  | 2.44                     | 0.47              |
| 1:A:283:LEU:HD22 | 1:A:283:LEU:HA   | 1.62                     | 0.47              |
| 1:A:435:VAL:HG22 | 2:B:290:THR:CB   | 2.44                     | 0.47              |
| 1:A:175:ASN:N    | 1:A:176:PRO:CD   | 2.76                     | 0.47              |
| 2:B:10:VAL:HB    | 2:B:124:PHE:CD1  | 2.50                     | 0.47              |
| 2:B:195:ILE:CG2  | 2:B:196:GLY:N    | 2.77                     | 0.47              |
| 2:B:396:GLU:O    | 2:B:400:THR:CG2  | 2.63                     | 0.47              |
| 2:B:420:PRO:CG   | 2:B:423:VAL:HG21 | 2.43                     | 0.47              |
| 1:A:225:PRO:HA   | 1:A:226:PRO:C    | 2.40                     | 0.47              |
| 1:A:320:ASP:OD1  | 1:A:322:SER:OG   | 2.28                     | 0.47              |
| 1:A:398:TRP:CZ2  | 1:A:411:ILE:HD12 | 2.49                     | 0.47              |
| 2:B:105:SER:O    | 2:B:190:GLY:HA2  | 2.15                     | 0.47              |
| 2:B:195:ILE:O    | 2:B:199:ARG:HG2  | 2.13                     | 0.47              |
| 2:B:214:LEU:H    | 2:B:214:LEU:HD23 | 1.79                     | 0.47              |
| 2:B:279:LEU:HD23 | 2:B:302:GLU:OE1  | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:286:THR:OG1  | 2:B:286:THR:O    | 2.32                     | 0.47              |
| 1:A:215:THR:O    | 1:A:215:THR:OG1  | 2.32                     | 0.47              |
| 2:B:164:MET:O    | 2:B:164:MET:HG3  | 2.14                     | 0.47              |
| 2:B:271:TYR:HE2  | 2:B:314:VAL:HA   | 1.79                     | 0.47              |
| 1:A:220:LYS:HD3  | 1:A:221:HIS:CG   | 2.50                     | 0.47              |
| 1:A:474:ASN:O    | 1:A:475:GLN:C    | 2.56                     | 0.47              |
| 2:B:194:GLU:HB3  | 2:B:197:GLN:HB2  | 1.97                     | 0.47              |
| 2:B:244:ILE:HD13 | 2:B:266:TRP:CH2  | 2.50                     | 0.47              |
| 1:A:13:LYS:HE2   | 1:A:84:THR:O     | 2.15                     | 0.47              |
| 1:A:509:GLN:N    | 1:A:510:PRO:HD3  | 2.30                     | 0.47              |
| 2:B:44:GLU:O     | 2:B:46:LYS:HE2   | 2.15                     | 0.47              |
| 2:B:214:LEU:HD23 | 2:B:214:LEU:N    | 2.30                     | 0.47              |
| 1:A:234:LEU:HD23 | 1:A:234:LEU:HA   | 1.65                     | 0.46              |
| 1:A:458:VAL:HG11 | 1:A:548:VAL:HG22 | 1.95                     | 0.46              |
| 2:B:148:VAL:HG23 | 2:B:149:LEU:N    | 2.29                     | 0.46              |
| 1:A:475:GLN:CG   | 1:A:501:TYR:CZ   | 2.98                     | 0.46              |
| 2:B:50:ILE:HD12  | 2:B:54:ASN:HB3   | 1.96                     | 0.46              |
| 1:A:175:ASN:HB3  | 1:A:178:ILE:CD1  | 2.31                     | 0.46              |
| 1:A:287:LYS:HB2  | 1:A:291:GLU:OE2  | 2.14                     | 0.46              |
| 1:A:466:VAL:CG1  | 1:A:467:VAL:H    | 2.27                     | 0.46              |
| 1:A:466:VAL:O    | 1:A:467:VAL:HG23 | 2.15                     | 0.46              |
| 2:B:195:ILE:HD13 | 2:B:195:ILE:HA   | 1.80                     | 0.46              |
| 2:B:344:GLU:O    | 2:B:347:LYS:HB2  | 2.15                     | 0.46              |
| 1:A:188:TYR:CD2  | 3:A:601:R8D:C2   | 2.98                     | 0.46              |
| 1:A:500:GLN:CG   | 2:B:422:LEU:HG   | 2.45                     | 0.46              |
| 2:B:138:GLU:HB3  | 2:B:139:THR:HG23 | 1.97                     | 0.46              |
| 2:B:284:ARG:NH1  | 2:B:284:ARG:CB   | 2.79                     | 0.46              |
| 1:A:54:ASN:HA    | 1:A:55:PRO:HD3   | 1.73                     | 0.46              |
| 1:A:183:TYR:HB3  | 1:A:188:TYR:HE1  | 1.80                     | 0.46              |
| 1:A:210:LEU:C    | 1:A:212:TRP:N    | 2.73                     | 0.46              |
| 1:A:246:LEU:HD11 | 1:A:310:LEU:CD1  | 2.45                     | 0.46              |
| 2:B:13:LYS:HA    | 2:B:14:PRO:HD2   | 1.48                     | 0.46              |
| 2:B:271:TYR:HD2  | 2:B:272:PRO:HD2  | 1.81                     | 0.46              |
| 2:B:422:LEU:CD1  | 2:B:426:TRP:CH2  | 2.99                     | 0.46              |
| 2:B:254:VAL:CG1  | 2:B:283:LEU:HD21 | 2.46                     | 0.46              |
| 2:B:382:ILE:CG2  | 2:B:383:TRP:CD2  | 2.99                     | 0.46              |
| 1:A:64:LYS:HZ3   | 1:A:69:THR:HA    | 1.79                     | 0.46              |
| 1:A:435:VAL:HA   | 2:B:290:THR:HG21 | 1.97                     | 0.46              |
| 2:B:164:MET:HA   | 2:B:167:ILE:HD12 | 1.98                     | 0.46              |
| 2:B:320:ASP:OD1  | 2:B:321:PRO:HD2  | 2.16                     | 0.46              |
| 1:A:325:LEU:HD22 | 1:A:341:ILE:CG2  | 2.46                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:72:ARG:HH12  | 2:B:409:THR:HG21 | 1.78                     | 0.46              |
| 2:B:425:LEU:C    | 2:B:427:TYR:N    | 2.70                     | 0.46              |
| 1:A:448:ARG:CG   | 1:A:448:ARG:NH1  | 2.75                     | 0.46              |
| 2:B:330:GLN:CD   | 2:B:340:GLN:HE22 | 2.24                     | 0.46              |
| 1:A:115:TYR:HB2  | 1:A:151:GLN:NE2  | 2.30                     | 0.46              |
| 1:A:134:SER:OG   | 1:A:139:THR:HB   | 2.16                     | 0.46              |
| 1:A:178:ILE:N    | 1:A:178:ILE:CD1  | 2.79                     | 0.46              |
| 1:A:199:ARG:HG2  | 1:A:199:ARG:NH1  | 2.31                     | 0.46              |
| 1:A:418:ASN:O    | 1:A:420:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:425:LEU:HD12 | 1:A:425:LEU:HA   | 1.54                     | 0.46              |
| 1:A:442:VAL:HG21 | 1:A:495:ILE:HG23 | 1.97                     | 0.46              |
| 2:B:118:VAL:HA   | 2:B:119:PRO:HD2  | 1.67                     | 0.46              |
| 1:A:2:ILE:CD1    | 1:A:46:LYS:NZ    | 2.73                     | 0.45              |
| 1:A:65:LYS:NZ    | 1:A:68:SER:CB    | 2.78                     | 0.45              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:CD   | 2.77                     | 0.45              |
| 1:A:30:LYS:CE    | 1:A:61:PHE:CE1   | 2.98                     | 0.45              |
| 1:A:277:ARG:HB2  | 1:A:336:GLN:NE2  | 2.32                     | 0.45              |
| 1:A:327:ALA:O    | 1:A:389:PHE:HA   | 2.16                     | 0.45              |
| 1:A:540:LYS:CD   | 1:A:540:LYS:N    | 2.80                     | 0.45              |
| 2:B:7:THR:HG22   | 2:B:119:PRO:HB2  | 1.96                     | 0.45              |
| 2:B:183:TYR:OH   | 2:B:386:THR:HG23 | 2.16                     | 0.45              |
| 2:B:301:LEU:O    | 2:B:304:ALA:N    | 2.49                     | 0.45              |
| 1:A:0:SER:HB2    | 1:A:1:PRO:CD     | 2.46                     | 0.45              |
| 1:A:103:ASN:O    | 3:A:601:R8D:N19  | 2.46                     | 0.45              |
| 1:A:325:LEU:HD22 | 1:A:341:ILE:HG21 | 1.98                     | 0.45              |
| 2:B:154:LYS:CG   | 2:B:184:MET:HE3  | 2.46                     | 0.45              |
| 1:A:70:LYS:O     | 1:A:70:LYS:HG3   | 2.12                     | 0.45              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:N    | 2.84                     | 0.45              |
| 1:A:411:ILE:HG22 | 1:A:414:TRP:CD1  | 2.51                     | 0.45              |
| 2:B:312:GLU:CB   | 2:B:313:PRO:HD2  | 2.43                     | 0.45              |
| 1:A:26:LEU:HB2   | 1:A:133:PRO:HG2  | 1.99                     | 0.45              |
| 1:A:63:ILE:HG12  | 1:A:74:LEU:HD11  | 1.98                     | 0.45              |
| 2:B:21:VAL:HB    | 2:B:59:PRO:HD3   | 1.98                     | 0.45              |
| 1:A:65:LYS:NZ    | 1:A:68:SER:HB2   | 2.31                     | 0.45              |
| 1:A:195:ILE:O    | 1:A:199:ARG:HD2  | 2.16                     | 0.45              |
| 1:A:289:LEU:HD13 | 1:A:289:LEU:C    | 2.41                     | 0.45              |
| 1:A:339:TYR:O    | 1:A:340:GLN:HG3  | 2.15                     | 0.45              |
| 1:A:519:ASN:O    | 1:A:522:ILE:HB   | 2.17                     | 0.45              |
| 2:B:382:ILE:HG21 | 2:B:383:TRP:CE2  | 2.51                     | 0.45              |
| 1:A:64:LYS:NZ    | 1:A:69:THR:HG23  | 2.27                     | 0.45              |
| 1:A:84:THR:HG22  | 1:A:85:GLN:N     | 2.31                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:286:THR:HG23 | 1:A:287:LYS:O    | 2.17                     | 0.45              |
| 1:A:340:GLN:HA   | 1:A:351:THR:HA   | 1.99                     | 0.45              |
| 2:B:242:GLN:HB2  | 2:B:352:GLY:HA2  | 1.99                     | 0.45              |
| 1:A:255:ASN:HB2  | 1:A:289:LEU:HD11 | 1.97                     | 0.45              |
| 1:A:422:LEU:HD12 | 1:A:422:LEU:HA   | 1.54                     | 0.45              |
| 1:A:253:THR:O    | 1:A:257:ILE:HG12 | 2.17                     | 0.45              |
| 1:A:324:ASP:CB   | 1:A:388:LYS:HE2  | 2.47                     | 0.45              |
| 1:A:442:VAL:HG13 | 1:A:457:TYR:HB3  | 1.98                     | 0.45              |
| 1:A:491:LEU:O    | 1:A:492:GLU:HG3  | 2.17                     | 0.45              |
| 2:B:116:PHE:CD2  | 2:B:148:VAL:HG21 | 2.50                     | 0.45              |
| 1:A:209:LEU:HD13 | 1:A:216:THR:CG2  | 2.45                     | 0.45              |
| 1:A:220:LYS:CE   | 1:A:221:HIS:CE1  | 2.98                     | 0.45              |
| 1:A:239:TRP:C    | 1:A:240:THR:HG22 | 2.41                     | 0.45              |
| 1:A:522:ILE:HG23 | 1:A:526:ILE:HD11 | 1.99                     | 0.45              |
| 2:B:60:VAL:CG2   | 2:B:73:LYS:HD2   | 2.47                     | 0.45              |
| 1:A:63:ILE:HG12  | 1:A:74:LEU:CD1   | 2.47                     | 0.44              |
| 1:A:244:ILE:HG22 | 1:A:246:LEU:CD2  | 2.46                     | 0.44              |
| 1:A:319:TYR:CE1  | 1:A:343:GLN:NE2  | 2.85                     | 0.44              |
| 2:B:6:GLU:CD     | 2:B:6:GLU:H      | 2.24                     | 0.44              |
| 2:B:125:ARG:H    | 2:B:125:ARG:HG2  | 1.50                     | 0.44              |
| 1:A:41:MET:HE2   | 1:A:47:ILE:CD1   | 2.44                     | 0.44              |
| 2:B:12:LEU:HD22  | 2:B:127:TYR:CZ   | 2.53                     | 0.44              |
| 2:B:65:LYS:NZ    | 2:B:65:LYS:CB    | 2.79                     | 0.44              |
| 2:B:89:GLU:O     | 2:B:89:GLU:HG2   | 2.17                     | 0.44              |
| 2:B:116:PHE:CZ   | 2:B:151:GLN:CG   | 2.95                     | 0.44              |
| 2:B:255:ASN:HA   | 2:B:258:GLN:HG3  | 1.98                     | 0.44              |
| 2:B:298:GLU:CD   | 2:B:298:GLU:N    | 2.74                     | 0.44              |
| 1:A:246:LEU:HD11 | 1:A:310:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:401:TRP:O    | 1:A:402:TRP:C    | 2.60                     | 0.44              |
| 1:A:406:TRP:CD2  | 1:A:407:GLN:N    | 2.85                     | 0.44              |
| 1:A:486:LEU:O    | 1:A:528:LYS:NZ   | 2.49                     | 0.44              |
| 2:B:28:GLU:HA    | 2:B:135:ILE:HD11 | 1.99                     | 0.44              |
| 2:B:66:LYS:HE2   | 2:B:67:ASP:OD2   | 2.16                     | 0.44              |
| 2:B:195:ILE:HD12 | 2:B:195:ILE:C    | 2.40                     | 0.44              |
| 1:A:324:ASP:CB   | 1:A:388:LYS:CE   | 2.95                     | 0.44              |
| 1:A:425:LEU:HD23 | 1:A:428:GLN:HE22 | 1.82                     | 0.44              |
| 1:A:466:VAL:CG1  | 1:A:467:VAL:N    | 2.80                     | 0.44              |
| 2:B:314:VAL:HB   | 2:B:317:VAL:CG2  | 2.46                     | 0.44              |
| 1:A:181:TYR:CD2  | 3:A:601:R8D:H5   | 2.51                     | 0.44              |
| 1:A:490:GLY:O    | 1:A:528:LYS:HE3  | 2.18                     | 0.44              |
| 1:A:542:ILE:O    | 1:A:543:GLY:C    | 2.60                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:422:LEU:HD13 | 2:B:426:TRP:CH2  | 2.52                     | 0.44              |
| 1:A:236:PRO:HA   | 3:A:601:R8D:C18  | 2.48                     | 0.44              |
| 1:A:486:LEU:C    | 1:A:524:GLN:NE2  | 2.75                     | 0.44              |
| 1:A:228:LEU:CB   | 1:A:242:GLN:HE21 | 2.30                     | 0.44              |
| 1:A:253:THR:HG22 | 1:A:292:VAL:CG2  | 2.40                     | 0.44              |
| 1:A:326:ILE:HD12 | 1:A:388:LYS:HB2  | 2.00                     | 0.44              |
| 1:A:434:ILE:CB   | 1:A:494:ASN:HD21 | 2.30                     | 0.44              |
| 1:A:106:VAL:HG12 | 3:A:601:R8D:N24  | 2.33                     | 0.44              |
| 1:A:326:ILE:HD11 | 1:A:388:LYS:HE3  | 2.00                     | 0.44              |
| 1:A:406:TRP:CZ3  | 1:A:407:GLN:CG   | 3.01                     | 0.44              |
| 2:B:276:VAL:CG2  | 2:B:279:LEU:HB2  | 2.48                     | 0.44              |
| 1:A:19:PRO:C     | 1:A:20:LYS:HG2   | 2.42                     | 0.43              |
| 1:A:92:LEU:HA    | 1:A:92:LEU:HD13  | 1.63                     | 0.43              |
| 2:B:153:TRP:CE2  | 2:B:155:GLY:HA3  | 2.54                     | 0.43              |
| 2:B:253:THR:HG22 | 2:B:255:ASN:HB3  | 2.00                     | 0.43              |
| 1:A:54:ASN:HB3   | 1:A:143:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:63:ILE:CG1   | 1:A:74:LEU:HD11  | 2.47                     | 0.43              |
| 1:A:360:ALA:HA   | 1:A:514:GLU:CD   | 2.43                     | 0.43              |
| 1:A:440:PHE:CE1  | 1:A:489:SER:CB   | 3.01                     | 0.43              |
| 2:B:259:LYS:HB3  | 2:B:259:LYS:HE3  | 1.60                     | 0.43              |
| 1:A:142:ILE:C    | 1:A:143:ARG:HG2  | 2.43                     | 0.43              |
| 1:A:30:LYS:HE2   | 1:A:61:PHE:CZ    | 2.53                     | 0.43              |
| 1:A:174:GLN:H    | 1:A:174:GLN:HG2  | 1.57                     | 0.43              |
| 1:A:457:TYR:CE2  | 1:A:465:LYS:HB3  | 2.53                     | 0.43              |
| 1:A:53:GLU:H     | 1:A:53:GLU:CD    | 2.27                     | 0.43              |
| 1:A:63:ILE:HG13  | 1:A:74:LEU:HD12  | 2.00                     | 0.43              |
| 1:A:175:ASN:O    | 1:A:178:ILE:HD13 | 2.18                     | 0.43              |
| 1:A:393:ILE:HG12 | 1:A:394:GLN:N    | 2.33                     | 0.43              |
| 1:A:472:THR:HB   | 1:A:473:THR:H    | 1.55                     | 0.43              |
| 2:B:80:LEU:HD22  | 2:B:84:THR:HG23  | 1.99                     | 0.43              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:HH2  | 1.82                     | 0.43              |
| 1:A:270:ILE:HA   | 1:A:351:THR:HG23 | 1.99                     | 0.43              |
| 1:A:430:GLU:HG2  | 1:A:531:VAL:C    | 2.43                     | 0.43              |
| 2:B:8:VAL:HA     | 2:B:9:PRO:HD2    | 1.61                     | 0.43              |
| 2:B:115:TYR:N    | 2:B:115:TYR:CD1  | 2.83                     | 0.43              |
| 1:A:160:PHE:CD2  | 1:A:160:PHE:C    | 2.97                     | 0.43              |
| 1:A:150:PRO:HG2  | 1:A:153:TRP:CB   | 2.49                     | 0.43              |
| 1:A:230:MET:HA   | 1:A:230:MET:CE   | 2.49                     | 0.43              |
| 1:A:246:LEU:HA   | 1:A:247:PRO:HD2  | 1.51                     | 0.43              |
| 1:A:320:ASP:C    | 1:A:322:SER:N    | 2.75                     | 0.43              |
| 1:A:179:VAL:HG12 | 1:A:190:GLY:O    | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:459:THR:HG23 | 1:A:463:ARG:O    | 2.19                     | 0.43              |
| 2:B:9:PRO:HA     | 2:B:121:ASP:OD1  | 2.18                     | 0.43              |
| 2:B:312:GLU:HA   | 2:B:313:PRO:HD3  | 1.71                     | 0.43              |
| 1:A:375:ILE:O    | 1:A:378:GLU:HB3  | 2.19                     | 0.43              |
| 1:A:120:LEU:CD2  | 1:A:128:THR:HG21 | 2.49                     | 0.42              |
| 1:A:175:ASN:CG   | 1:A:201:LYS:HZ1  | 2.27                     | 0.42              |
| 2:B:100:LEU:CD2  | 2:B:181:TYR:HB3  | 2.49                     | 0.42              |
| 2:B:175:ASN:HD21 | 2:B:201:LYS:HE3  | 1.82                     | 0.42              |
| 2:B:279:LEU:HD21 | 2:B:303:LEU:CD2  | 2.49                     | 0.42              |
| 2:B:422:LEU:CB   | 2:B:426:TRP:CZ2  | 2.95                     | 0.42              |
| 1:A:479:LEU:CD2  | 1:A:501:TYR:CE2  | 2.99                     | 0.42              |
| 2:B:382:ILE:CG2  | 2:B:383:TRP:CE2  | 3.02                     | 0.42              |
| 2:B:398:TRP:CG   | 2:B:416:PHE:HE1  | 2.37                     | 0.42              |
| 1:A:107:THR:CB   | 1:A:202:ILE:HD11 | 2.48                     | 0.42              |
| 1:A:432:GLU:HA   | 1:A:433:PRO:HD3  | 1.79                     | 0.42              |
| 1:A:449:GLU:C    | 1:A:451:LYS:HE2  | 2.43                     | 0.42              |
| 1:A:464:GLN:CG   | 1:A:465:LYS:N    | 2.83                     | 0.42              |
| 1:A:500:GLN:CD   | 2:B:422:LEU:HD12 | 2.44                     | 0.42              |
| 1:A:500:GLN:OE1  | 2:B:422:LEU:HG   | 2.19                     | 0.42              |
| 2:B:320:ASP:HA   | 2:B:321:PRO:HD3  | 1.92                     | 0.42              |
| 2:B:393:ILE:HG12 | 2:B:394:GLN:H    | 1.83                     | 0.42              |
| 1:A:54:ASN:OD1   | 1:A:55:PRO:HD2   | 2.19                     | 0.42              |
| 1:A:94:ILE:O     | 1:A:95:PRO:C     | 2.60                     | 0.42              |
| 1:A:134:SER:OG   | 1:A:139:THR:O    | 2.37                     | 0.42              |
| 1:A:296:THR:HG23 | 1:A:299:ALA:HB2  | 1.99                     | 0.42              |
| 1:A:452:LEU:HD22 | 1:A:452:LEU:HA   | 1.73                     | 0.42              |
| 2:B:28:GLU:HG2   | 2:B:32:LYS:HE2   | 2.00                     | 0.42              |
| 2:B:295:LEU:HD23 | 2:B:300:GLU:OE1  | 2.19                     | 0.42              |
| 2:B:354:TYR:CB   | 2:B:374:LYS:NZ   | 2.79                     | 0.42              |
| 1:A:72:ARG:HE    | 1:A:72:ARG:HB3   | 1.54                     | 0.42              |
| 1:A:296:THR:CG2  | 1:A:299:ALA:CB   | 2.98                     | 0.42              |
| 1:A:65:LYS:CG    | 1:A:72:ARG:HD2   | 2.48                     | 0.42              |
| 1:A:303:LEU:O    | 1:A:307:ARG:HG3  | 2.20                     | 0.42              |
| 1:A:342:TYR:CD1  | 1:A:342:TYR:C    | 2.97                     | 0.42              |
| 1:A:491:LEU:N    | 1:A:491:LEU:HD12 | 2.34                     | 0.42              |
| 2:B:337:TRP:NE1  | 2:B:367:GLN:HE21 | 2.02                     | 0.42              |
| 2:B:345:PRO:C    | 2:B:347:LYS:H    | 2.28                     | 0.42              |
| 2:B:395:LYS:O    | 2:B:399:GLU:N    | 2.48                     | 0.42              |
| 1:A:424:LYS:CE   | 1:A:426:TRP:CE2  | 3.00                     | 0.42              |
| 1:A:442:VAL:HG21 | 1:A:495:ILE:CG2  | 2.49                     | 0.42              |
| 1:A:473:THR:OG1  | 1:A:476:LYS:HD3  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:180:ILE:CG1  | 2:B:189:VAL:HG13 | 2.49                     | 0.42              |
| 2:B:376:THR:HB   | 2:B:410:TRP:CH2  | 2.55                     | 0.42              |
| 1:A:8:VAL:HG21   | 2:B:52:PRO:HG2   | 2.02                     | 0.42              |
| 1:A:195:ILE:CG2  | 1:A:199:ARG:CZ   | 2.97                     | 0.42              |
| 1:A:288:ALA:HB3  | 1:A:291:GLU:H    | 1.85                     | 0.42              |
| 2:B:87:PHE:CZ    | 2:B:92:LEU:CD1   | 2.99                     | 0.42              |
| 2:B:339:TYR:CD1  | 2:B:339:TYR:C    | 2.98                     | 0.42              |
| 2:B:373:GLN:NE2  | 2:B:408:ALA:H    | 2.18                     | 0.42              |
| 1:A:96:HIS:N     | 2:B:136:ASN:OD1  | 2.46                     | 0.42              |
| 1:A:319:TYR:CZ   | 1:A:321:PRO:HA   | 2.55                     | 0.42              |
| 1:A:373:GLN:N    | 1:A:373:GLN:HE21 | 2.18                     | 0.42              |
| 1:A:457:TYR:CD1  | 1:A:457:TYR:C    | 2.97                     | 0.42              |
| 1:A:475:GLN:HG3  | 1:A:501:TYR:CD2  | 2.51                     | 0.42              |
| 2:B:46:LYS:H     | 2:B:46:LYS:HG2   | 1.54                     | 0.42              |
| 2:B:72:ARG:NH1   | 2:B:72:ARG:HG2   | 2.35                     | 0.42              |
| 2:B:175:ASN:HD21 | 2:B:201:LYS:CE   | 2.32                     | 0.42              |
| 2:B:376:THR:HG23 | 2:B:386:THR:HB   | 2.01                     | 0.42              |
| 1:A:205:LEU:HD23 | 1:A:205:LEU:HA   | 1.89                     | 0.42              |
| 1:A:228:LEU:CB   | 1:A:242:GLN:NE2  | 2.76                     | 0.42              |
| 1:A:19:PRO:HB3   | 1:A:79:GLU:HB3   | 2.00                     | 0.41              |
| 1:A:66:LYS:O     | 1:A:67:ASP:CB    | 2.68                     | 0.41              |
| 1:A:220:LYS:HD3  | 1:A:221:HIS:N    | 2.35                     | 0.41              |
| 1:A:223:LYS:H    | 1:A:223:LYS:HG2  | 1.48                     | 0.41              |
| 1:A:235:HIS:CB   | 1:A:236:PRO:CD   | 2.94                     | 0.41              |
| 2:B:320:ASP:OD1  | 2:B:322:SER:OG   | 2.29                     | 0.41              |
| 1:A:163:SER:O    | 1:A:166:LYS:N    | 2.53                     | 0.41              |
| 1:A:249:LYS:HB2  | 1:A:249:LYS:HE2  | 1.69                     | 0.41              |
| 1:A:424:LYS:HE2  | 1:A:426:TRP:CE3  | 2.55                     | 0.41              |
| 1:A:520:GLN:C    | 1:A:523:GLU:HG3  | 2.45                     | 0.41              |
| 2:B:18:GLY:CA    | 2:B:56:TYR:CE1   | 2.98                     | 0.41              |
| 2:B:83:ARG:HG2   | 2:B:83:ARG:H     | 1.44                     | 0.41              |
| 2:B:253:THR:CG2  | 2:B:255:ASN:CB   | 2.97                     | 0.41              |
| 2:B:306:ASN:HD22 | 2:B:309:ILE:CD1  | 2.32                     | 0.41              |
| 2:B:331:LYS:HB2  | 2:B:337:TRP:CZ3  | 2.55                     | 0.41              |
| 2:B:354:TYR:CA   | 2:B:374:LYS:HZ1  | 2.33                     | 0.41              |
| 2:B:373:GLN:NE2  | 2:B:407:GLN:H    | 2.19                     | 0.41              |
| 2:B:422:LEU:CD1  | 2:B:426:TRP:CZ2  | 2.99                     | 0.41              |
| 1:A:30:LYS:CD    | 1:A:61:PHE:CE1   | 3.03                     | 0.41              |
| 1:A:63:ILE:CG1   | 1:A:74:LEU:HD12  | 2.50                     | 0.41              |
| 1:A:197:GLN:HA   | 1:A:200:THR:HB   | 2.03                     | 0.41              |
| 1:A:373:GLN:CA   | 1:A:373:GLN:NE2  | 2.83                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:432:GLU:HG3  | 1:A:433:PRO:HD2  | 2.02                     | 0.41              |
| 1:A:191:SER:OG   | 1:A:198:HIS:CD2  | 2.74                     | 0.41              |
| 2:B:80:LEU:HD13  | 2:B:153:TRP:CD1  | 2.55                     | 0.41              |
| 2:B:349:LEU:HB3  | 2:B:383:TRP:CZ2  | 2.55                     | 0.41              |
| 2:B:391:LEU:HA   | 2:B:392:PRO:HD3  | 1.68                     | 0.41              |
| 2:B:393:ILE:HG21 | 2:B:398:TRP:HB2  | 2.01                     | 0.41              |
| 1:A:164:MET:O    | 1:A:164:MET:SD   | 2.79                     | 0.41              |
| 1:A:211:ARG:HD3  | 1:A:211:ARG:C    | 2.45                     | 0.41              |
| 1:A:320:ASP:O    | 1:A:322:SER:N    | 2.53                     | 0.41              |
| 1:A:479:LEU:HD21 | 1:A:501:TYR:CE2  | 2.55                     | 0.41              |
| 2:B:80:LEU:HA    | 2:B:80:LEU:HD23  | 1.80                     | 0.41              |
| 2:B:329:ILE:HA   | 2:B:338:THR:O    | 2.20                     | 0.41              |
| 1:A:206:ARG:NH2  | 1:A:217:PRO:C    | 2.78                     | 0.41              |
| 2:B:122:GLU:HG2  | 2:B:125:ARG:HH21 | 1.86                     | 0.41              |
| 2:B:310:LEU:HD12 | 2:B:310:LEU:HA   | 1.71                     | 0.41              |
| 1:A:171:PHE:CD1  | 1:A:171:PHE:C    | 2.98                     | 0.41              |
| 1:A:287:LYS:O    | 1:A:288:ALA:O    | 2.38                     | 0.41              |
| 1:A:411:ILE:HA   | 1:A:412:PRO:HD2  | 1.87                     | 0.41              |
| 2:B:13:LYS:HD2   | 2:B:85:GLN:N     | 2.36                     | 0.41              |
| 2:B:376:THR:CG2  | 2:B:386:THR:HB   | 2.51                     | 0.41              |
| 1:A:164:MET:HE2  | 1:A:214:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:406:TRP:CE3  | 1:A:406:TRP:C    | 2.99                     | 0.41              |
| 2:B:63:ILE:HD13  | 2:B:74:LEU:HB2   | 2.03                     | 0.41              |
| 2:B:125:ARG:O    | 2:B:145:GLN:HG3  | 2.20                     | 0.41              |
| 2:B:150:PRO:HD2  | 2:B:153:TRP:HE3  | 1.86                     | 0.41              |
| 2:B:246:LEU:CD1  | 2:B:307:ARG:HG3  | 2.39                     | 0.41              |
| 1:A:0:SER:CB     | 1:A:1:PRO:CD     | 2.98                     | 0.41              |
| 1:A:10:VAL:HG13  | 1:A:87:PHE:CZ    | 2.56                     | 0.41              |
| 1:A:107:THR:CG2  | 1:A:202:ILE:CD1  | 2.97                     | 0.41              |
| 1:A:171:PHE:O    | 1:A:171:PHE:CD1  | 2.74                     | 0.41              |
| 1:A:175:ASN:CG   | 1:A:201:LYS:NZ   | 2.78                     | 0.41              |
| 1:A:356:ARG:NH2  | 1:A:358:ARG:CD   | 2.79                     | 0.41              |
| 1:A:411:ILE:HG21 | 1:A:414:TRP:CD1  | 2.56                     | 0.41              |
| 2:B:64:LYS:O     | 2:B:65:LYS:HB2   | 2.20                     | 0.41              |
| 2:B:168:LEU:HA   | 2:B:168:LEU:HD23 | 1.74                     | 0.41              |
| 2:B:252:TRP:HB3  | 2:B:257:ILE:HD11 | 2.02                     | 0.41              |
| 2:B:260:LEU:CD1  | 2:B:264:LEU:CD1  | 2.98                     | 0.41              |
| 2:B:344:GLU:CB   | 2:B:345:PRO:HD2  | 2.38                     | 0.41              |
| 2:B:369:THR:O    | 2:B:373:GLN:HG3  | 2.21                     | 0.41              |
| 2:B:382:ILE:HG22 | 2:B:383:TRP:CD1  | 2.56                     | 0.41              |
| 1:A:63:ILE:HD12  | 1:A:72:ARG:HG3   | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:395:LYS:CD   | 1:A:414:TRP:CH2  | 3.02                     | 0.41              |
| 2:B:128:THR:OG1  | 2:B:146:TYR:HB2  | 2.21                     | 0.41              |
| 2:B:416:PHE:C    | 2:B:417:VAL:HG13 | 2.46                     | 0.41              |
| 1:A:169:GLU:N    | 1:A:170:PRO:CD   | 2.77                     | 0.40              |
| 2:B:257:ILE:C    | 2:B:259:LYS:N    | 2.78                     | 0.40              |
| 2:B:268:SER:C    | 2:B:270:ILE:N    | 2.78                     | 0.40              |
| 2:B:393:ILE:HD11 | 2:B:397:THR:CG2  | 2.50                     | 0.40              |
| 1:A:64:LYS:HB3   | 1:A:65:LYS:H     | 1.62                     | 0.40              |
| 1:A:231:GLY:O    | 1:A:242:GLN:HB2  | 2.22                     | 0.40              |
| 1:A:245:VAL:O    | 1:A:247:PRO:HD3  | 2.21                     | 0.40              |
| 1:A:282:LEU:HD21 | 1:A:296:THR:HG22 | 2.03                     | 0.40              |
| 2:B:203:GLU:OE1  | 2:B:206:ARG:NH1  | 2.54                     | 0.40              |
| 2:B:271:TYR:CE2  | 2:B:314:VAL:HA   | 2.56                     | 0.40              |
| 1:A:179:VAL:O    | 1:A:179:VAL:HG13 | 2.20                     | 0.40              |
| 2:B:46:LYS:HA    | 2:B:148:VAL:HG13 | 2.02                     | 0.40              |
| 2:B:209:LEU:HB3  | 2:B:214:LEU:O    | 2.21                     | 0.40              |
| 2:B:320:ASP:CG   | 2:B:323:LYS:HG3  | 2.46                     | 0.40              |
| 1:A:4:PRO:HG2    | 1:A:212:TRP:CE3  | 2.56                     | 0.40              |
| 1:A:64:LYS:HD3   | 1:A:64:LYS:HA    | 1.69                     | 0.40              |
| 1:A:124:PHE:O    | 1:A:127:TYR:HD1  | 2.05                     | 0.40              |
| 1:A:155:GLY:O    | 1:A:159:ILE:HD12 | 2.22                     | 0.40              |
| 1:A:187:LEU:HA   | 1:A:187:LEU:HD23 | 1.61                     | 0.40              |
| 1:A:235:HIS:O    | 3:A:601:R8D:C21  | 2.69                     | 0.40              |
| 2:B:260:LEU:CD1  | 2:B:264:LEU:HD11 | 2.51                     | 0.40              |
| 2:B:296:THR:OG1  | 2:B:298:GLU:OE1  | 2.29                     | 0.40              |
| 1:A:96:HIS:HB3   | 1:A:382:ILE:HD13 | 2.03                     | 0.40              |
| 1:A:369:THR:HG21 | 1:A:398:TRP:HH2  | 1.87                     | 0.40              |
| 2:B:64:LYS:O     | 2:B:65:LYS:CB    | 2.70                     | 0.40              |
| 2:B:195:ILE:O    | 2:B:199:ARG:CG   | 2.70                     | 0.40              |
| 2:B:271:TYR:HA   | 2:B:272:PRO:HD2  | 1.81                     | 0.40              |
| 2:B:328:GLU:O    | 2:B:339:TYR:HA   | 2.21                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:448:ARG:NH2 | 1:A:448:ARG:NH2[3_555] | 1.54                     | 0.66              |

## 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     | 547/563 (97%)  | 427 (78%) | 91 (17%)  | 29 (5%)  | 1           | 10 |
| 2   | B     | 399/443 (90%)  | 338 (85%) | 44 (11%)  | 17 (4%)  | 2           | 13 |
| All | All   | 946/1006 (94%) | 765 (81%) | 135 (14%) | 46 (5%)  | 1           | 11 |

All (46) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 90  | VAL  |
| 1   | A     | 138 | GLU  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 230 | MET  |
| 1   | A     | 286 | THR  |
| 1   | A     | 288 | ALA  |
| 1   | A     | 312 | GLU  |
| 1   | A     | 313 | PRO  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 345 | PRO  |
| 1   | A     | 356 | ARG  |
| 1   | A     | 491 | LEU  |
| 1   | A     | 528 | LYS  |
| 2   | B     | 241 | VAL  |
| 2   | B     | 345 | PRO  |
| 1   | A     | 64  | LYS  |
| 1   | A     | 136 | ASN  |
| 1   | A     | 243 | PRO  |
| 1   | A     | 541 | GLY  |
| 1   | A     | 543 | GLY  |
| 2   | B     | 14  | PRO  |
| 2   | B     | 160 | PHE  |
| 2   | B     | 270 | ILE  |
| 2   | B     | 282 | LEU  |
| 2   | B     | 304 | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 313 | PRO  |
| 1   | A     | 3   | SER  |
| 1   | A     | 78  | ARG  |
| 1   | A     | 163 | SER  |
| 2   | B     | 66  | LYS  |
| 2   | B     | 125 | ARG  |
| 2   | B     | 137 | ASN  |
| 2   | B     | 240 | THR  |
| 2   | B     | 251 | SER  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 164 | MET  |
| 1   | A     | 547 | GLN  |
| 2   | B     | 402 | TRP  |
| 1   | A     | 139 | THR  |
| 2   | B     | 276 | VAL  |
| 1   | A     | 346 | PHE  |
| 2   | B     | 161 | GLN  |
| 2   | B     | 237 | ASP  |
| 1   | A     | 490 | GLY  |
| 1   | A     | 95  | PRO  |
| 1   | A     | 276 | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 491/503 (98%) | 322 (66%) | 169 (34%) | 0           | 0 |
| 2   | B     | 369/403 (92%) | 251 (68%) | 118 (32%) | 0           | 1 |
| All | All   | 860/906 (95%) | 573 (67%) | 287 (33%) | 0           | 0 |

All (287) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | SER  |
| 1   | A     | 5   | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | GLU  |
| 1   | A     | 7   | THR  |
| 1   | A     | 10  | VAL  |
| 1   | A     | 21  | VAL  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 26  | LEU  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 36  | GLU  |
| 1   | A     | 40  | GLU  |
| 1   | A     | 42  | GLU  |
| 1   | A     | 44  | GLU  |
| 1   | A     | 46  | LYS  |
| 1   | A     | 58  | THR  |
| 1   | A     | 60  | VAL  |
| 1   | A     | 63  | ILE  |
| 1   | A     | 64  | LYS  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 68  | SER  |
| 1   | A     | 70  | LYS  |
| 1   | A     | 72  | ARG  |
| 1   | A     | 73  | LYS  |
| 1   | A     | 82  | LYS  |
| 1   | A     | 92  | LEU  |
| 1   | A     | 101 | LYS  |
| 1   | A     | 105 | SER  |
| 1   | A     | 107 | THR  |
| 1   | A     | 111 | VAL  |
| 1   | A     | 113 | ASP  |
| 1   | A     | 118 | VAL  |
| 1   | A     | 122 | GLU  |
| 1   | A     | 123 | ASP  |
| 1   | A     | 126 | LYS  |
| 1   | A     | 132 | ILE  |
| 1   | A     | 134 | SER  |
| 1   | A     | 135 | ILE  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 138 | GLU  |
| 1   | A     | 151 | GLN  |
| 1   | A     | 159 | ILE  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 162 | SER  |
| 1   | A     | 164 | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 166 | LYS  |
| 1   | A     | 172 | ARG  |
| 1   | A     | 173 | LYS  |
| 1   | A     | 174 | GLN  |
| 1   | A     | 177 | ASP  |
| 1   | A     | 178 | ILE  |
| 1   | A     | 193 | LEU  |
| 1   | A     | 197 | GLN  |
| 1   | A     | 200 | THR  |
| 1   | A     | 205 | LEU  |
| 1   | A     | 207 | GLN  |
| 1   | A     | 210 | LEU  |
| 1   | A     | 215 | THR  |
| 1   | A     | 220 | LYS  |
| 1   | A     | 221 | HIS  |
| 1   | A     | 223 | LYS  |
| 1   | A     | 230 | MET  |
| 1   | A     | 233 | GLU  |
| 1   | A     | 237 | ASP  |
| 1   | A     | 238 | LYS  |
| 1   | A     | 240 | THR  |
| 1   | A     | 241 | VAL  |
| 1   | A     | 244 | ILE  |
| 1   | A     | 245 | VAL  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 248 | GLU  |
| 1   | A     | 249 | LYS  |
| 1   | A     | 251 | SER  |
| 1   | A     | 254 | VAL  |
| 1   | A     | 257 | ILE  |
| 1   | A     | 259 | LYS  |
| 1   | A     | 260 | LEU  |
| 1   | A     | 269 | GLN  |
| 1   | A     | 274 | ILE  |
| 1   | A     | 275 | LYS  |
| 1   | A     | 277 | ARG  |
| 1   | A     | 278 | GLN  |
| 1   | A     | 279 | LEU  |
| 1   | A     | 280 | CYS  |
| 1   | A     | 283 | LEU  |
| 1   | A     | 284 | ARG  |
| 1   | A     | 286 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 289 | LEU  |
| 1   | A     | 290 | THR  |
| 1   | A     | 291 | GLU  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 296 | THR  |
| 1   | A     | 297 | GLU  |
| 1   | A     | 300 | GLU  |
| 1   | A     | 303 | LEU  |
| 1   | A     | 305 | GLU  |
| 1   | A     | 308 | GLU  |
| 1   | A     | 309 | ILE  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 312 | GLU  |
| 1   | A     | 314 | VAL  |
| 1   | A     | 317 | VAL  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 336 | GLN  |
| 1   | A     | 344 | GLU  |
| 1   | A     | 345 | PRO  |
| 1   | A     | 346 | PHE  |
| 1   | A     | 349 | LEU  |
| 1   | A     | 350 | LYS  |
| 1   | A     | 351 | THR  |
| 1   | A     | 353 | LYS  |
| 1   | A     | 356 | ARG  |
| 1   | A     | 357 | MET  |
| 1   | A     | 358 | ARG  |
| 1   | A     | 361 | HIS  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 369 | THR  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 375 | ILE  |
| 1   | A     | 379 | SER  |
| 1   | A     | 380 | ILE  |
| 1   | A     | 382 | ILE  |
| 1   | A     | 390 | LYS  |
| 1   | A     | 393 | ILE  |
| 1   | A     | 395 | LYS  |
| 1   | A     | 400 | THR  |
| 1   | A     | 402 | TRP  |
| 1   | A     | 403 | THR  |
| 1   | A     | 404 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 407 | GLN  |
| 1   | A     | 409 | THR  |
| 1   | A     | 422 | LEU  |
| 1   | A     | 424 | LYS  |
| 1   | A     | 425 | LEU  |
| 1   | A     | 429 | LEU  |
| 1   | A     | 430 | GLU  |
| 1   | A     | 432 | GLU  |
| 1   | A     | 434 | ILE  |
| 1   | A     | 435 | VAL  |
| 1   | A     | 442 | VAL  |
| 1   | A     | 448 | ARG  |
| 1   | A     | 451 | LYS  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 454 | LYS  |
| 1   | A     | 458 | VAL  |
| 1   | A     | 459 | THR  |
| 1   | A     | 470 | THR  |
| 1   | A     | 471 | ASP  |
| 1   | A     | 475 | GLN  |
| 1   | A     | 479 | LEU  |
| 1   | A     | 491 | LEU  |
| 1   | A     | 493 | VAL  |
| 1   | A     | 494 | ASN  |
| 1   | A     | 495 | ILE  |
| 1   | A     | 496 | VAL  |
| 1   | A     | 497 | THR  |
| 1   | A     | 500 | GLN  |
| 1   | A     | 503 | LEU  |
| 1   | A     | 512 | GLN  |
| 1   | A     | 519 | ASN  |
| 1   | A     | 520 | GLN  |
| 1   | A     | 522 | ILE  |
| 1   | A     | 523 | GLU  |
| 1   | A     | 526 | ILE  |
| 1   | A     | 528 | LYS  |
| 1   | A     | 530 | LYS  |
| 1   | A     | 536 | VAL  |
| 1   | A     | 540 | LYS  |
| 1   | A     | 547 | GLN  |
| 1   | A     | 548 | VAL  |
| 2   | B     | 6   | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 8   | VAL  |
| 2   | B     | 10  | VAL  |
| 2   | B     | 11  | LYS  |
| 2   | B     | 12  | LEU  |
| 2   | B     | 26  | LEU  |
| 2   | B     | 29  | GLU  |
| 2   | B     | 30  | LYS  |
| 2   | B     | 35  | VAL  |
| 2   | B     | 40  | GLU  |
| 2   | B     | 44  | GLU  |
| 2   | B     | 46  | LYS  |
| 2   | B     | 48  | SER  |
| 2   | B     | 63  | ILE  |
| 2   | B     | 64  | LYS  |
| 2   | B     | 65  | LYS  |
| 2   | B     | 66  | LYS  |
| 2   | B     | 67  | ASP  |
| 2   | B     | 68  | SER  |
| 2   | B     | 72  | ARG  |
| 2   | B     | 73  | LYS  |
| 2   | B     | 80  | LEU  |
| 2   | B     | 90  | VAL  |
| 2   | B     | 91  | GLN  |
| 2   | B     | 100 | LEU  |
| 2   | B     | 101 | LYS  |
| 2   | B     | 102 | LYS  |
| 2   | B     | 104 | LYS  |
| 2   | B     | 111 | VAL  |
| 2   | B     | 120 | LEU  |
| 2   | B     | 122 | GLU  |
| 2   | B     | 125 | ARG  |
| 2   | B     | 126 | LYS  |
| 2   | B     | 132 | ILE  |
| 2   | B     | 134 | SER  |
| 2   | B     | 138 | GLU  |
| 2   | B     | 145 | GLN  |
| 2   | B     | 148 | VAL  |
| 2   | B     | 163 | SER  |
| 2   | B     | 165 | THR  |
| 2   | B     | 173 | LYS  |
| 2   | B     | 178 | ILE  |
| 2   | B     | 182 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 184 | MET  |
| 2   | B     | 187 | LEU  |
| 2   | B     | 189 | VAL  |
| 2   | B     | 195 | ILE  |
| 2   | B     | 199 | ARG  |
| 2   | B     | 201 | LYS  |
| 2   | B     | 202 | ILE  |
| 2   | B     | 205 | LEU  |
| 2   | B     | 209 | LEU  |
| 2   | B     | 211 | ARG  |
| 2   | B     | 214 | LEU  |
| 2   | B     | 234 | LEU  |
| 2   | B     | 240 | THR  |
| 2   | B     | 245 | VAL  |
| 2   | B     | 246 | LEU  |
| 2   | B     | 248 | GLU  |
| 2   | B     | 249 | LYS  |
| 2   | B     | 251 | SER  |
| 2   | B     | 253 | THR  |
| 2   | B     | 256 | ASP  |
| 2   | B     | 257 | ILE  |
| 2   | B     | 258 | GLN  |
| 2   | B     | 259 | LYS  |
| 2   | B     | 260 | LEU  |
| 2   | B     | 261 | VAL  |
| 2   | B     | 265 | ASN  |
| 2   | B     | 266 | TRP  |
| 2   | B     | 268 | SER  |
| 2   | B     | 269 | GLN  |
| 2   | B     | 271 | TYR  |
| 2   | B     | 275 | LYS  |
| 2   | B     | 276 | VAL  |
| 2   | B     | 277 | ARG  |
| 2   | B     | 279 | LEU  |
| 2   | B     | 286 | THR  |
| 2   | B     | 287 | LYS  |
| 2   | B     | 289 | LEU  |
| 2   | B     | 290 | THR  |
| 2   | B     | 291 | GLU  |
| 2   | B     | 293 | ILE  |
| 2   | B     | 295 | LEU  |
| 2   | B     | 297 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 298 | GLU  |
| 2   | B     | 300 | GLU  |
| 2   | B     | 301 | LEU  |
| 2   | B     | 302 | GLU  |
| 2   | B     | 303 | LEU  |
| 2   | B     | 305 | GLU  |
| 2   | B     | 308 | GLU  |
| 2   | B     | 310 | LEU  |
| 2   | B     | 311 | LYS  |
| 2   | B     | 314 | VAL  |
| 2   | B     | 334 | GLN  |
| 2   | B     | 336 | GLN  |
| 2   | B     | 347 | LYS  |
| 2   | B     | 349 | LEU  |
| 2   | B     | 353 | LYS  |
| 2   | B     | 356 | ARG  |
| 2   | B     | 362 | THR  |
| 2   | B     | 366 | LYS  |
| 2   | B     | 369 | THR  |
| 2   | B     | 374 | LYS  |
| 2   | B     | 376 | THR  |
| 2   | B     | 380 | ILE  |
| 2   | B     | 381 | VAL  |
| 2   | B     | 382 | ILE  |
| 2   | B     | 390 | LYS  |
| 2   | B     | 393 | ILE  |
| 2   | B     | 394 | GLN  |
| 2   | B     | 395 | LYS  |
| 2   | B     | 399 | GLU  |
| 2   | B     | 400 | THR  |
| 2   | B     | 403 | THR  |
| 2   | B     | 407 | GLN  |
| 2   | B     | 419 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | ASN  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 151 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 175 | ASN  |
| 1   | A     | 197 | GLN  |
| 1   | A     | 198 | HIS  |
| 1   | A     | 242 | GLN  |
| 1   | A     | 258 | GLN  |
| 1   | A     | 315 | HIS  |
| 1   | A     | 330 | GLN  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 340 | GLN  |
| 1   | A     | 460 | ASN  |
| 1   | A     | 474 | ASN  |
| 1   | A     | 480 | GLN  |
| 1   | A     | 494 | ASN  |
| 1   | A     | 512 | GLN  |
| 1   | A     | 519 | ASN  |
| 1   | A     | 524 | GLN  |
| 2   | B     | 147 | ASN  |
| 2   | B     | 161 | GLN  |
| 2   | B     | 175 | ASN  |
| 2   | B     | 182 | GLN  |
| 2   | B     | 255 | ASN  |
| 2   | B     | 258 | GLN  |
| 2   | B     | 269 | GLN  |
| 2   | B     | 306 | ASN  |
| 2   | B     | 330 | GLN  |
| 2   | B     | 336 | GLN  |
| 2   | B     | 340 | GLN  |
| 2   | B     | 367 | GLN  |
| 2   | B     | 373 | GLN  |
| 2   | B     | 394 | GLN  |
| 2   | B     | 407 | GLN  |
| 2   | B     | 428 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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 | $\# Z  > 2$ |
| 3   | R8D  | A     | 601 | -    | 30,31,31     | 2.90 | 16 (53%)    | 41,43,43    | 3.70 | 21 (51%)    |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | R8D  | A     | 601 | -    | -       | 6/11/11/11 | 0/4/4/4 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | A     | 601 | R8D  | C2-C25   | -6.46 | 1.30        | 1.44     |
| 3   | A     | 601 | R8D  | C18-N19  | 5.18  | 1.39        | 1.35     |
| 3   | A     | 601 | R8D  | C18-N24  | 5.06  | 1.42        | 1.35     |
| 3   | A     | 601 | R8D  | C5-C4    | -4.48 | 1.31        | 1.39     |
| 3   | A     | 601 | R8D  | C25-N26  | 4.09  | 1.23        | 1.14     |
| 3   | A     | 601 | R8D  | C6-CL27  | -3.90 | 1.65        | 1.74     |
| 3   | A     | 601 | R8D  | O7-C4    | -3.84 | 1.31        | 1.39     |
| 3   | A     | 601 | R8D  | C17-C16  | 3.54  | 1.53        | 1.45     |
| 3   | A     | 601 | R8D  | C16-N20  | 3.52  | 1.36        | 1.29     |
| 3   | A     | 601 | R8D  | C13-CL28 | 3.39  | 1.81        | 1.73     |
| 3   | A     | 601 | R8D  | N19-N20  | 3.01  | 1.43        | 1.36     |
| 3   | A     | 601 | R8D  | C22-C21  | 3.00  | 1.44        | 1.38     |
| 3   | A     | 601 | R8D  | O7-C8    | -2.76 | 1.33        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | A     | 601 | R8D  | C8-C13 | -2.70 | 1.34        | 1.39     |
| 3   | A     | 601 | R8D  | C5-C6  | -2.52 | 1.34        | 1.38     |
| 3   | A     | 601 | R8D  | C9-C10 | 2.42  | 1.43        | 1.39     |

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms        | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------------|-------|-------------|----------|
| 3   | A     | 601 | R8D  | N19-C18-N24  | 10.68 | 135.22      | 125.83   |
| 3   | A     | 601 | R8D  | C1-C6-C5     | 8.34  | 131.76      | 121.64   |
| 3   | A     | 601 | R8D  | C5-C6-CL27   | -6.76 | 110.69      | 119.17   |
| 3   | A     | 601 | R8D  | C17-C18-N24  | -6.32 | 118.66      | 126.31   |
| 3   | A     | 601 | R8D  | O7-C8-C13    | -6.02 | 106.05      | 119.51   |
| 3   | A     | 601 | R8D  | C18-C17-C16  | 5.66  | 108.08      | 105.02   |
| 3   | A     | 601 | R8D  | C4-C5-C6     | -5.54 | 111.80      | 118.08   |
| 3   | A     | 601 | R8D  | C8-C13-CL28  | -4.68 | 114.09      | 119.44   |
| 3   | A     | 601 | R8D  | C2-C1-C6     | -4.54 | 114.78      | 118.89   |
| 3   | A     | 601 | R8D  | C9-C8-C13    | 4.34  | 125.14      | 119.29   |
| 3   | A     | 601 | R8D  | C8-O7-C4     | 3.99  | 127.61      | 117.95   |
| 3   | A     | 601 | R8D  | C2-C3-C4     | 3.90  | 123.99      | 119.30   |
| 3   | A     | 601 | R8D  | C23-N24-C18  | 3.74  | 124.02      | 116.74   |
| 3   | A     | 601 | R8D  | C12-C13-CL28 | 3.41  | 125.13      | 118.42   |
| 3   | A     | 601 | R8D  | C8-C9-C10    | -3.32 | 113.44      | 119.13   |
| 3   | A     | 601 | R8D  | C22-C23-N24  | -3.20 | 118.35      | 123.42   |
| 3   | A     | 601 | R8D  | O14-C15-C16  | 3.20  | 117.47      | 109.50   |
| 3   | A     | 601 | R8D  | C1-C2-C3     | -2.76 | 115.44      | 119.70   |
| 3   | A     | 601 | R8D  | O7-C8-C9     | 2.47  | 128.78      | 121.63   |
| 3   | A     | 601 | R8D  | C15-C16-N20  | 2.13  | 125.47      | 120.93   |
| 3   | A     | 601 | R8D  | C1-C2-C25    | 2.02  | 122.28      | 119.55   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

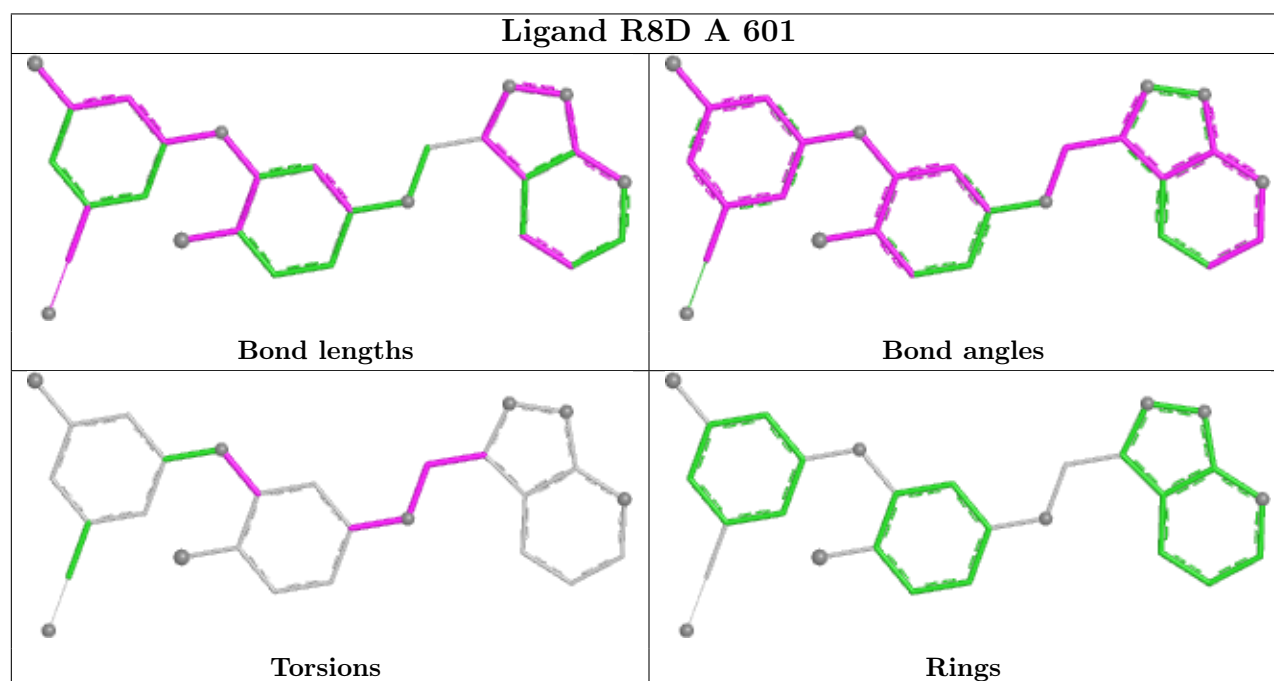
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 601 | R8D  | O14-C15-C16-C17 |
| 3   | A     | 601 | R8D  | C11-C10-O14-C15 |
| 3   | A     | 601 | R8D  | C9-C10-O14-C15  |
| 3   | A     | 601 | R8D  | C13-C8-O7-C4    |
| 3   | A     | 601 | R8D  | O14-C15-C16-N20 |
| 3   | A     | 601 | R8D  | C16-C15-O14-C10 |

There are no ring outliers.

1 monomer is involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 601 | R8D  | 16      | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | A     | 549/563 (97%)  | -0.12  | 2 (0%) 88 78 | 26, 58, 95, 145       | 0     |
| 2   | B     | 405/443 (91%)  | -0.08  | 3 (0%) 84 69 | 23, 51, 107, 124      | 0     |
| All | All   | 954/1006 (94%) | -0.10  | 5 (0%) 87 75 | 23, 56, 105, 145      | 0     |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 543 | GLY  | 3.1  |
| 2   | B     | 266 | TRP  | 2.4  |
| 2   | B     | 215 | THR  | 2.3  |
| 2   | B     | 90  | VAL  | 2.3  |
| 1   | A     | 291 | GLU  | 2.2  |

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

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

### 6.3 Carbohydrates [i](#)

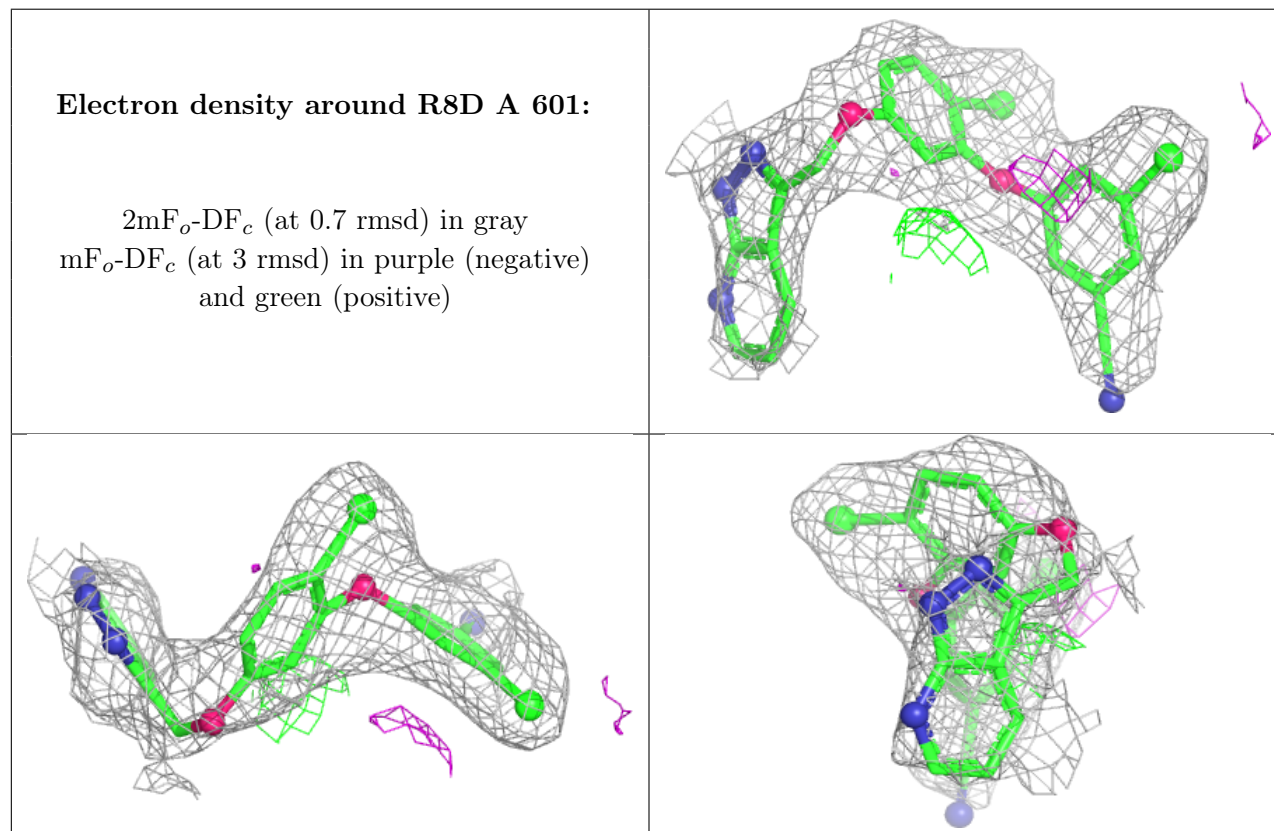
There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | R8D  | A     | 601 | 28/28 | 0.92 | 0.10 | 64,69,79,79                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.