



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:17 pm GMT

PDB ID : 1GLL
Title : ESCHERICHIA COLI GLYCEROL KINASE MUTANT WITH BOUND ATP
ANALOG SHOWING SUBSTANTIAL DOMAIN MOTION
Authors : Bystrom, C.E.; Pettigrew, D.W.; Branchaud, B.P.; Remington, S.J.
Deposited on : 1998-09-24
Resolution : 3.00 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.2 (RC1), CSD as538be (2017) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | trunk28620 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

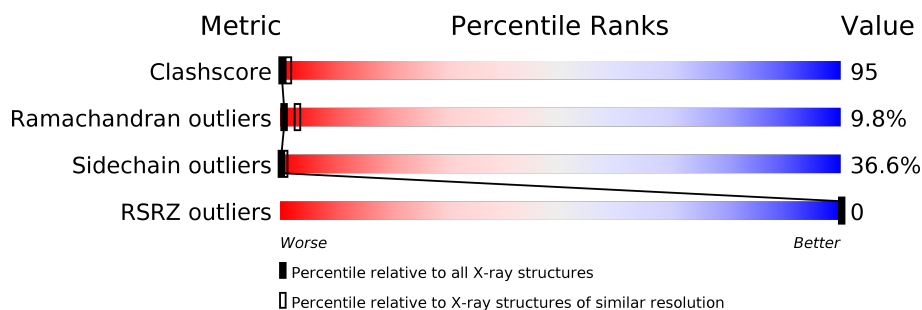
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

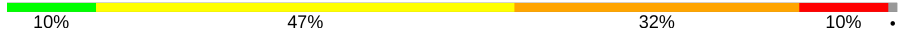
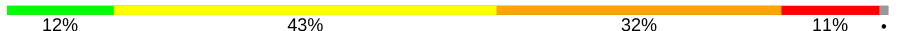
The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 112137 | 2037 (3.00-3.00) |
| Ramachandran outliers | 110173 | 1973 (3.00-3.00) |
| Sidechain outliers | 110143 | 1976 (3.00-3.00) |
| RSRZ outliers | 101464 | 1716 (3.00-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 | O | 501 |  |
| 1 | Y | 501 |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4 | GOL | O | 600 | - | - | X | - |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7896 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 GLYCEROL KINASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | Y | 494 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3910 | 2470 | 683 | 738 | 19 | | | |
| 1 | O | 494 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3910 | 2470 | 683 | 738 | 19 | | | |

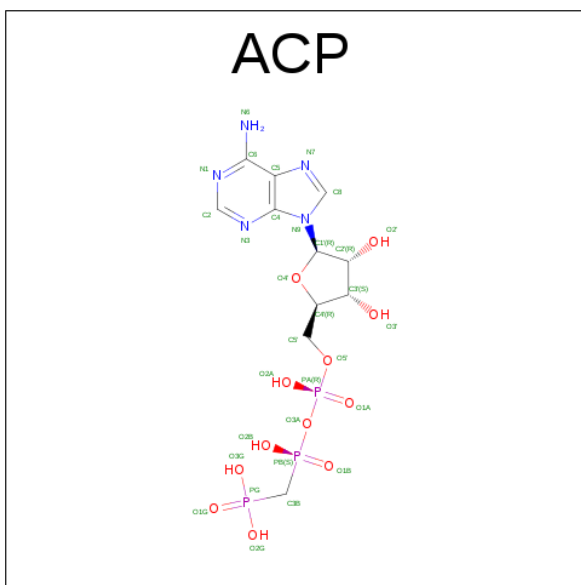
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| Y | 58 | TRP | SER | ENGINEERED | UNP P0A6F3 |
| O | 58 | TRP | SER | ENGINEERED | UNP P0A6F3 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

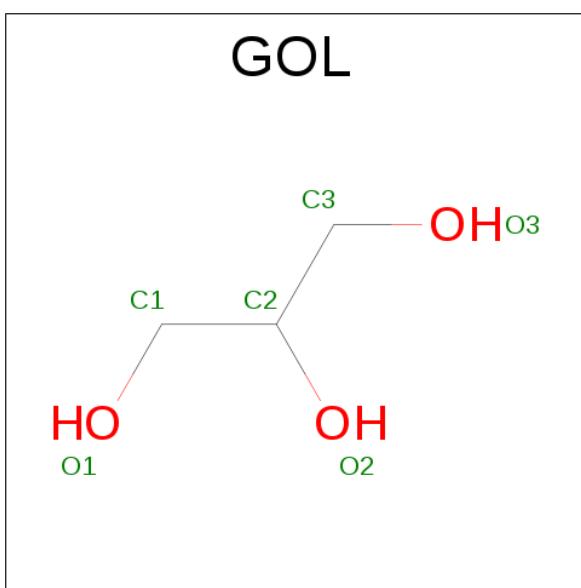
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | O | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3 | Y | 1 | Total 31 | C 11 | N 5 | O 12 | P 3 | 0 | 0 |
| 3 | O | 1 | Total 31 | C 11 | N 5 | O 12 | P 3 | 0 | 0 |

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

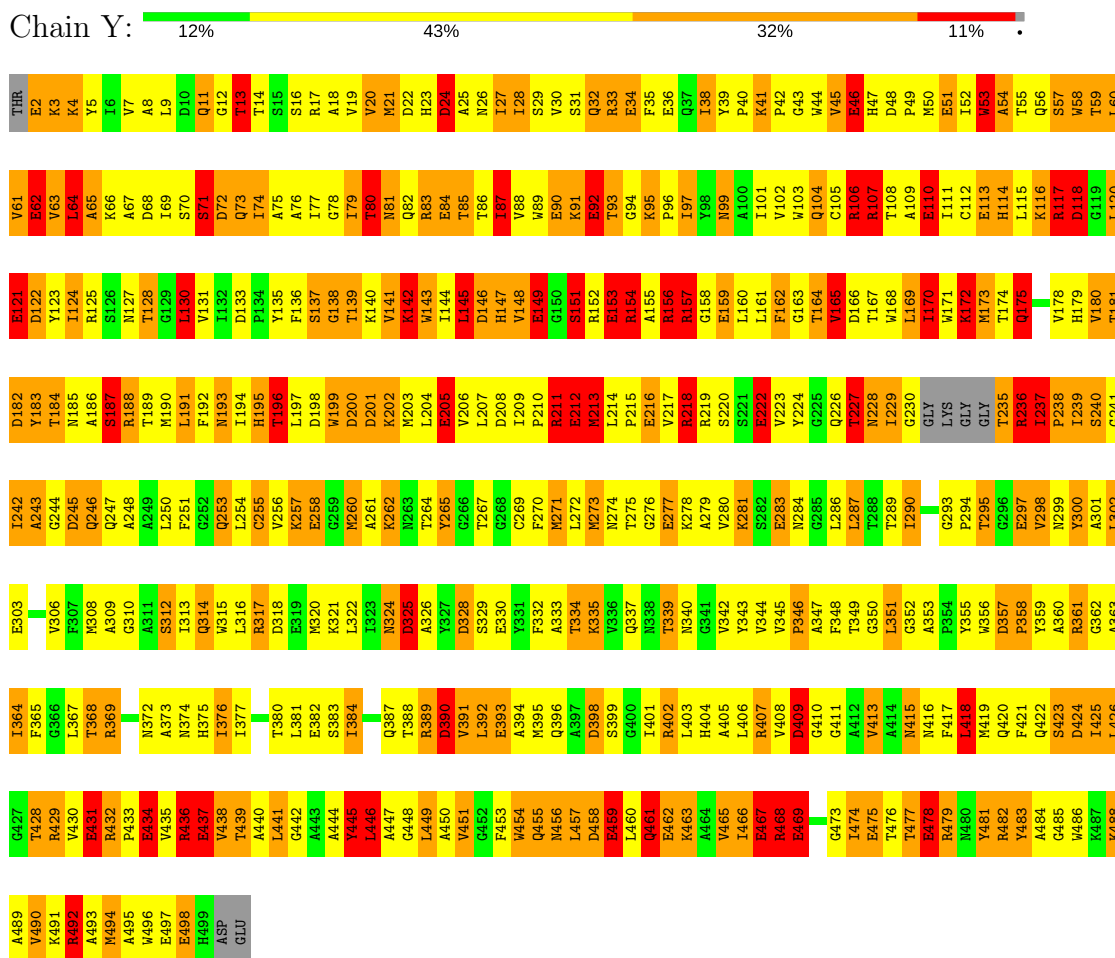


| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4 | Y | 1 | Total C O 6 3 3 | 0 | 0 |
| 4 | O | 1 | Total C O 6 3 3 | 0 | 0 |

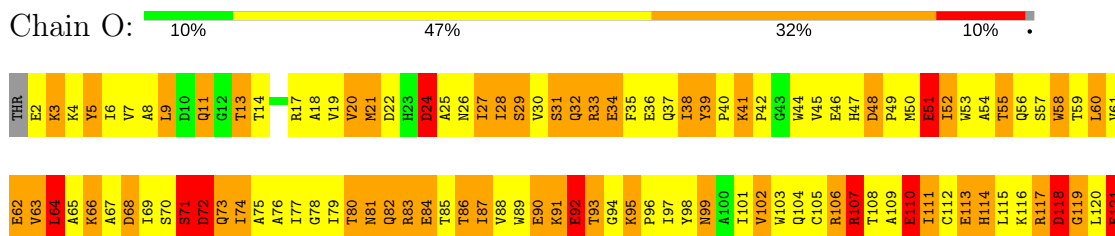
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: GLYCEROL KINASE



• Molecule 1: GLYCEROL KINASE



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A489 | A490 | A491 | A492 | A493 | A494 | A495 | A496 | E497 | E498 | H499 | ASP | GLU | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G427 | T428 | R429 | V430 | E431 | R432 | P433 | E434 | V435 | R436 | E437 | V438 | T439 | A440 | L441 | G442 | A443 | A444 | Y445 | L446 | A447 | G448 | L449 | A450 | V451 | G452 | F453 | W454 | Q455 | N456 | L457 | D458 | E459 | L460 | Q461 | E462 | K463 | A464 | V465 | I466 | E467 | R468 | E469 | F470 | | I474 | E475 | T476 | T477 | E478 | N479 | N480 | Y481 | R482 | Y483 | A484 | G485 | W486 | K487 | K488 | |
| A363 | I364 | F365 | | T368 | B369 | | N372 | A373 | N374 | H375 | I376 | I377 | R378 | A379 | T380 | L381 | A382 | S383 | T384 | A385 | Y386 | Q387 | T388 | B389 | D390 | V391 | L392 | E393 | A394 | K395 | Q396 | A397 | D398 | | I401 | R402 | L403 | H404 | A405 | L406 | R407 | V408 | D409 | G410 | | V413 | A414 | N415 | W416 | F417 | L418 | M419 | Q420 | F421 | Q422 | S423 | D424 | I425 | L426 | |
| L302 | E303 | | V306 | M308 | A309 | Q310 | A311 | I312 | I313 | G252 | Q253 | L254 | C255 | V256 | K257 | E258 | G259 | N260 | K261 | N262 | T263 | T264 | Y265 | G266 | T267 | G268 | C269 | F270 | N271 | L272 | N273 | K334 | K335 | V336 | Q337 | N338 | T339 | N340 | G341 | V342 | Y343 | E283 | N284 | G285 | L286 | L287 | T288 | G289 | L290 | A291 | C292 | P293 | Y355 | W356 | D357 | P358 | Y359 | A360 | R361 | G362 |
| T242 | A243 | G244 | D245 | Q246 | Q247 | A248 | A249 | L250 | F251 | G252 | Q253 | L254 | C255 | V256 | K257 | E258 | G259 | N260 | K261 | N262 | T263 | T264 | Y265 | G266 | T267 | G268 | C269 | F270 | N271 | L272 | N273 | K334 | K335 | V336 | Q337 | N338 | T339 | N340 | G341 | V342 | Y343 | E283 | N284 | G285 | L286 | L287 | T288 | G289 | L290 | A291 | C292 | P293 | Y355 | W356 | D357 | P358 | Y359 | A360 | R361 | G362 |
| D182 | Y183 | T184 | N185 | A186 | N187 | R188 | T189 | M190 | F191 | I192 | N193 | I194 | H195 | T196 | L197 | D198 | W199 | D200 | D201 | K202 | M203 | L204 | E205 | V206 | L207 | D208 | I209 | P210 | R211 | E212 | N213 | L214 | P215 | E216 | V217 | R218 | R219 | S220 | S221 | F222 | Y223 | Y224 | G225 | Q226 | T227 | N228 | I229 | G230 | GLY | LYS | GLY | GLY | T235 | Q175 | R236 | I237 | P238 | I239 | S240 | G241 |
| D122 | Y123 | I124 | N125 | S126 | N127 | T128 | G129 | L130 | V131 | I132 | D133 | P134 | Y135 | F136 | S137 | G138 | T139 | K140 | V141 | K142 | W143 | I144 | E145 | D146 | H147 | V148 | E149 | G150 | S151 | E152 | E153 | R154 | A155 | R156 | V157 | G158 | E159 | L160 | L161 | F162 | G163 | T164 | V165 | D166 | T167 | W168 | L169 | I170 | W171 | K172 | M173 | T174 | Q175 | G176 | R177 | V178 | H179 | V180 | T181 | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 99.77Å 201.15Å 114.34Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.00 18.03 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 95.0 (20.00-3.00) 82.7 (18.03-3.00) | Depositor EDS |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 93.19 (at 2.97Å) | Xtriage |
| Refinement program | TNT V. 5-F | Depositor |
| R, R_{free} | 0.176 , (Not available) 0.166 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 53.7 | Xtriage |
| Anisotropy | 0.286 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.21 , 157.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 7896 | wwPDB-VP |
| Average B, all atoms (Å ²) | 55.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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 | O | 1.27 | 37/3991 (0.9%) | 1.68 | 72/5412 (1.3%) |
| 1 | Y | 1.38 | 35/3991 (0.9%) | 1.76 | 90/5412 (1.7%) |
| All | All | 1.33 | 72/7982 (0.9%) | 1.72 | 162/10824 (1.5%) |

All (72) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | O | 478 | GLU | CD-OE2 | 9.70 | 1.36 | 1.25 |
| 1 | Y | 153 | GLU | CD-OE1 | 9.27 | 1.35 | 1.25 |
| 1 | O | 258 | GLU | CD-OE2 | 9.23 | 1.35 | 1.25 |
| 1 | Y | 34 | GLU | CD-OE1 | 9.09 | 1.35 | 1.25 |
| 1 | Y | 478 | GLU | CD-OE2 | 9.08 | 1.35 | 1.25 |
| 1 | Y | 84 | GLU | CD-OE1 | 9.01 | 1.35 | 1.25 |
| 1 | Y | 110 | GLU | CD-OE2 | 8.68 | 1.35 | 1.25 |
| 1 | O | 153 | GLU | CD-OE1 | 8.55 | 1.35 | 1.25 |
| 1 | Y | 36 | GLU | CD-OE2 | 8.55 | 1.35 | 1.25 |
| 1 | Y | 216 | GLU | CD-OE2 | 8.53 | 1.35 | 1.25 |
| 1 | Y | 462 | GLU | CD-OE2 | 8.52 | 1.35 | 1.25 |
| 1 | Y | 149 | GLU | CD-OE1 | 8.26 | 1.34 | 1.25 |
| 1 | Y | 283 | GLU | CD-OE1 | 8.24 | 1.34 | 1.25 |
| 1 | O | 475 | GLU | CD-OE2 | 8.14 | 1.34 | 1.25 |
| 1 | Y | 92 | GLU | CD-OE1 | 7.97 | 1.34 | 1.25 |
| 1 | Y | 382 | GLU | CD-OE2 | 7.88 | 1.34 | 1.25 |
| 1 | O | 462 | GLU | CD-OE2 | 7.83 | 1.34 | 1.25 |
| 1 | Y | 475 | GLU | CD-OE2 | 7.73 | 1.34 | 1.25 |
| 1 | O | 459 | GLU | CD-OE2 | 7.71 | 1.34 | 1.25 |
| 1 | Y | 90 | GLU | CD-OE2 | 7.41 | 1.33 | 1.25 |
| 1 | Y | 205 | GLU | CD-OE1 | 7.40 | 1.33 | 1.25 |
| 1 | O | 497 | GLU | CD-OE1 | 7.40 | 1.33 | 1.25 |
| 1 | O | 36 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | O | 92 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | O | 34 | GLU | CD-OE1 | 7.21 | 1.33 | 1.25 |
| 1 | Y | 2 | GLU | CD-OE2 | 7.18 | 1.33 | 1.25 |
| 1 | O | 431 | GLU | CD-OE1 | 7.14 | 1.33 | 1.25 |
| 1 | O | 149 | GLU | CD-OE2 | 7.14 | 1.33 | 1.25 |
| 1 | Y | 297 | GLU | CD-OE2 | 7.13 | 1.33 | 1.25 |
| 1 | O | 469 | GLU | CD-OE2 | 7.11 | 1.33 | 1.25 |
| 1 | O | 283 | GLU | CD-OE1 | 7.09 | 1.33 | 1.25 |
| 1 | Y | 277 | GLU | CD-OE1 | 7.06 | 1.33 | 1.25 |
| 1 | O | 393 | GLU | CD-OE1 | 6.97 | 1.33 | 1.25 |
| 1 | O | 159 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | Y | 498 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | O | 113 | GLU | CD-OE2 | 6.68 | 1.33 | 1.25 |
| 1 | O | 90 | GLU | CD-OE2 | 6.66 | 1.32 | 1.25 |
| 1 | O | 121 | GLU | CD-OE2 | 6.63 | 1.32 | 1.25 |
| 1 | Y | 431 | GLU | CD-OE1 | 6.61 | 1.32 | 1.25 |
| 1 | O | 498 | GLU | CD-OE2 | 6.57 | 1.32 | 1.25 |
| 1 | O | 382 | GLU | CD-OE2 | 6.53 | 1.32 | 1.25 |
| 1 | Y | 393 | GLU | CD-OE1 | 6.51 | 1.32 | 1.25 |
| 1 | O | 319 | GLU | CD-OE2 | 6.51 | 1.32 | 1.25 |
| 1 | O | 277 | GLU | CD-OE1 | 6.45 | 1.32 | 1.25 |
| 1 | O | 222 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 1 | Y | 212 | GLU | CD-OE2 | 6.38 | 1.32 | 1.25 |
| 1 | O | 62 | GLU | CD-OE1 | 6.37 | 1.32 | 1.25 |
| 1 | Y | 51 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 1 | O | 2 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | O | 437 | GLU | CD-OE1 | 6.01 | 1.32 | 1.25 |
| 1 | Y | 469 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | O | 110 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | O | 330 | GLU | CD-OE1 | 5.97 | 1.32 | 1.25 |
| 1 | O | 51 | GLU | CD-OE1 | 5.96 | 1.32 | 1.25 |
| 1 | Y | 62 | GLU | CD-OE1 | 5.93 | 1.32 | 1.25 |
| 1 | O | 84 | GLU | CD-OE1 | 5.85 | 1.32 | 1.25 |
| 1 | O | 205 | GLU | CD-OE1 | 5.85 | 1.32 | 1.25 |
| 1 | O | 216 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | O | 212 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | Y | 159 | GLU | CD-OE2 | 5.69 | 1.31 | 1.25 |
| 1 | Y | 437 | GLU | CD-OE1 | 5.67 | 1.31 | 1.25 |
| 1 | Y | 459 | GLU | CD-OE1 | 5.62 | 1.31 | 1.25 |
| 1 | Y | 434 | GLU | CD-OE1 | 5.58 | 1.31 | 1.25 |
| 1 | Y | 113 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | O | 467 | GLU | CD-OE2 | 5.50 | 1.31 | 1.25 |
| 1 | Y | 222 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | O | 297 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | Y | 467 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | Y | 46 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | Y | 121 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 1 | Y | 258 | GLU | CD-OE2 | 5.19 | 1.31 | 1.25 |
| 1 | O | 434 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |

All (162) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | Y | 237 | ILE | C-N-CD | -15.74 | 85.98 | 120.60 |
| 1 | Y | 83 | ARG | C-N-CA | -10.97 | 94.28 | 121.70 |
| 1 | Y | 200 | ASP | CB-CG-OD2 | -10.81 | 108.57 | 118.30 |
| 1 | Y | 492 | ARG | NE-CZ-NH1 | 10.66 | 125.63 | 120.30 |
| 1 | O | 468 | ARG | NE-CZ-NH1 | 9.89 | 125.25 | 120.30 |
| 1 | O | 378 | ARG | NE-CZ-NH1 | 9.25 | 124.92 | 120.30 |
| 1 | O | 492 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 1 | O | 122 | ASP | CB-CG-OD2 | -8.61 | 110.55 | 118.30 |
| 1 | Y | 328 | ASP | CB-CG-OD1 | -8.56 | 110.60 | 118.30 |
| 1 | Y | 361 | ARG | NE-CZ-NH2 | -8.48 | 116.06 | 120.30 |
| 1 | Y | 107 | ARG | NE-CZ-NH1 | 8.48 | 124.54 | 120.30 |
| 1 | Y | 424 | ASP | CB-CG-OD2 | -8.44 | 110.71 | 118.30 |
| 1 | Y | 245 | ASP | CB-CG-OD2 | -8.33 | 110.81 | 118.30 |
| 1 | O | 398 | ASP | CB-CG-OD1 | -8.29 | 110.84 | 118.30 |
| 1 | Y | 83 | ARG | NE-CZ-NH1 | -8.22 | 116.19 | 120.30 |
| 1 | O | 211 | ARG | NE-CZ-NH1 | 8.04 | 124.32 | 120.30 |
| 1 | O | 198 | ASP | CB-CG-OD2 | -8.04 | 111.07 | 118.30 |
| 1 | Y | 334 | THR | CA-CB-CG2 | -7.87 | 101.38 | 112.40 |
| 1 | Y | 80 | THR | CA-CB-CG2 | -7.82 | 101.45 | 112.40 |
| 1 | O | 458 | ASP | CB-CG-OD2 | -7.79 | 111.29 | 118.30 |
| 1 | Y | 117 | ARG | NE-CZ-NH1 | 7.77 | 124.19 | 120.30 |
| 1 | O | 198 | ASP | CB-CG-OD1 | 7.71 | 125.24 | 118.30 |
| 1 | Y | 107 | ARG | NE-CZ-NH2 | -7.60 | 116.50 | 120.30 |
| 1 | O | 107 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |
| 1 | Y | 198 | ASP | CB-CG-OD1 | 7.54 | 125.09 | 118.30 |
| 1 | Y | 436 | ARG | NE-CZ-NH1 | 7.47 | 124.04 | 120.30 |
| 1 | O | 133 | ASP | CB-CG-OD2 | -7.45 | 111.60 | 118.30 |
| 1 | Y | 72 | ASP | CB-CG-OD2 | -7.37 | 111.67 | 118.30 |
| 1 | Y | 409 | ASP | CB-CG-OD2 | -7.27 | 111.76 | 118.30 |
| 1 | Y | 390 | ASP | N-CA-CB | 7.23 | 123.62 | 110.60 |
| 1 | Y | 236 | ARG | NE-CZ-NH1 | 7.22 | 123.91 | 120.30 |
| 1 | O | 125 | ARG | NE-CZ-NH2 | 7.21 | 123.91 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | O | 378 | ARG | NE-CZ-NH2 | -7.17 | 116.72 | 120.30 |
| 1 | Y | 328 | ASP | CB-CG-OD2 | 7.16 | 124.75 | 118.30 |
| 1 | Y | 265 | TYR | CB-CG-CD2 | -7.14 | 116.72 | 121.00 |
| 1 | Y | 157 | ARG | NE-CZ-NH2 | -7.08 | 116.76 | 120.30 |
| 1 | Y | 357 | ASP | CB-CG-OD1 | 7.01 | 124.61 | 118.30 |
| 1 | O | 357 | ASP | CB-CG-OD1 | 6.96 | 124.56 | 118.30 |
| 1 | O | 398 | ASP | CB-CG-OD2 | 6.89 | 124.50 | 118.30 |
| 1 | O | 146 | ASP | CB-CG-OD2 | -6.84 | 112.14 | 118.30 |
| 1 | O | 318 | ASP | CB-CG-OD2 | -6.84 | 112.14 | 118.30 |
| 1 | O | 118 | ASP | CB-CG-OD2 | -6.79 | 112.19 | 118.30 |
| 1 | Y | 398 | ASP | CB-CG-OD1 | -6.73 | 112.24 | 118.30 |
| 1 | Y | 156 | ARG | NE-CZ-NH2 | -6.71 | 116.95 | 120.30 |
| 1 | O | 325 | ASP | CB-CG-OD2 | -6.70 | 112.27 | 118.30 |
| 1 | Y | 64 | LEU | N-CA-CB | 6.67 | 123.75 | 110.40 |
| 1 | O | 317 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 1 | O | 188 | ARG | NE-CZ-NH1 | 6.65 | 123.63 | 120.30 |
| 1 | O | 182 | ASP | CB-CG-OD2 | -6.64 | 112.33 | 118.30 |
| 1 | O | 458 | ASP | CB-CG-OD1 | 6.61 | 124.25 | 118.30 |
| 1 | Y | 80 | THR | N-CA-CB | 6.58 | 122.81 | 110.30 |
| 1 | O | 156 | ARG | NE-CZ-NH1 | 6.49 | 123.54 | 120.30 |
| 1 | O | 476 | THR | CA-CB-CG2 | -6.43 | 103.40 | 112.40 |
| 1 | O | 24 | ASP | CB-CG-OD2 | 6.36 | 124.03 | 118.30 |
| 1 | Y | 122 | ASP | CB-CG-OD2 | -6.34 | 112.59 | 118.30 |
| 1 | Y | 156 | ARG | NE-CZ-NH1 | 6.33 | 123.47 | 120.30 |
| 1 | Y | 325 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | Y | 458 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 1 | Y | 106 | ARG | NE-CZ-NH2 | -6.28 | 117.16 | 120.30 |
| 1 | O | 200 | ASP | CB-CG-OD2 | -6.25 | 112.67 | 118.30 |
| 1 | Y | 68 | ASP | CB-CG-OD1 | -6.20 | 112.72 | 118.30 |
| 1 | O | 479 | ARG | NE-CZ-NH1 | 6.19 | 123.40 | 120.30 |
| 1 | Y | 83 | ARG | O-C-N | -6.18 | 112.81 | 122.70 |
| 1 | Y | 24 | ASP | CB-CG-OD1 | -6.17 | 112.75 | 118.30 |
| 1 | Y | 182 | ASP | CB-CG-OD2 | -6.13 | 112.78 | 118.30 |
| 1 | Y | 361 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | Y | 227 | THR | CA-CB-CG2 | -6.04 | 103.94 | 112.40 |
| 1 | Y | 62 | GLU | N-CA-CB | 5.98 | 121.37 | 110.60 |
| 1 | Y | 357 | ASP | CB-CG-OD2 | -5.96 | 112.93 | 118.30 |
| 1 | O | 20 | VAL | CB-CA-C | -5.95 | 100.11 | 111.40 |
| 1 | Y | 20 | VAL | CB-CA-C | -5.94 | 100.11 | 111.40 |
| 1 | O | 357 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | O | 83 | ARG | N-CA-C | 5.87 | 126.84 | 111.00 |
| 1 | O | 68 | ASP | CB-CG-OD2 | 5.85 | 123.57 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | O | 107 | ARG | NE-CZ-NH2 | -5.85 | 117.37 | 120.30 |
| 1 | Y | 481 | TYR | CB-CG-CD1 | -5.83 | 117.50 | 121.00 |
| 1 | Y | 200 | ASP | CB-CG-OD1 | 5.83 | 123.54 | 118.30 |
| 1 | Y | 255 | CYS | CA-CB-SG | -5.82 | 103.53 | 114.00 |
| 1 | Y | 104 | GLN | N-CA-CB | -5.81 | 100.15 | 110.60 |
| 1 | O | 106 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | O | 48 | ASP | CB-CG-OD1 | -5.80 | 113.08 | 118.30 |
| 1 | O | 118 | ASP | CB-CG-OD1 | 5.80 | 123.52 | 118.30 |
| 1 | O | 407 | ARG | NE-CZ-NH1 | 5.77 | 123.19 | 120.30 |
| 1 | O | 342 | VAL | CA-CB-CG2 | -5.75 | 102.27 | 110.90 |
| 1 | O | 83 | ARG | C-N-CA | -5.71 | 107.42 | 121.70 |
| 1 | Y | 20 | VAL | N-CA-CB | 5.70 | 124.04 | 111.50 |
| 1 | O | 58 | TRP | CA-C-N | -5.70 | 104.66 | 117.20 |
| 1 | Y | 183 | TYR | CA-CB-CG | -5.68 | 102.61 | 113.40 |
| 1 | O | 288 | THR | CA-CB-CG2 | -5.67 | 104.46 | 112.40 |
| 1 | Y | 201 | ASP | CB-CG-OD1 | 5.65 | 123.39 | 118.30 |
| 1 | Y | 72 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | O | 200 | ASP | CB-CG-OD1 | 5.64 | 123.37 | 118.30 |
| 1 | Y | 445 | TYR | CB-CG-CD1 | 5.61 | 124.36 | 121.00 |
| 1 | O | 166 | ASP | CB-CG-OD1 | 5.57 | 123.32 | 118.30 |
| 1 | O | 68 | ASP | CB-CG-OD1 | -5.57 | 113.29 | 118.30 |
| 1 | Y | 436 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | Y | 481 | TYR | CA-CB-CG | -5.56 | 102.84 | 113.40 |
| 1 | O | 409 | ASP | CB-CG-OD2 | -5.54 | 113.31 | 118.30 |
| 1 | O | 468 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 1 | Y | 114 | HIS | CA-CB-CG | -5.51 | 104.23 | 113.60 |
| 1 | O | 237 | ILE | C-N-CD | -5.50 | 108.50 | 120.60 |
| 1 | O | 38 | ILE | CB-CA-C | -5.46 | 100.69 | 111.60 |
| 1 | Y | 201 | ASP | CB-CG-OD2 | -5.45 | 113.39 | 118.30 |
| 1 | O | 156 | ARG | NE-CZ-NH2 | -5.45 | 117.58 | 120.30 |
| 1 | Y | 130 | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 1 | Y | 117 | ARG | CB-CA-C | -5.40 | 99.60 | 110.40 |
| 1 | Y | 118 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | O | 268 | GLY | N-CA-C | -5.40 | 99.60 | 113.10 |
| 1 | O | 211 | ARG | NE-CZ-NH2 | -5.39 | 117.61 | 120.30 |
| 1 | O | 423 | SER | N-CA-CB | 5.38 | 118.58 | 110.50 |
| 1 | O | 265 | TYR | CB-CG-CD2 | -5.38 | 117.77 | 121.00 |
| 1 | O | 201 | ASP | CB-CG-OD2 | -5.36 | 113.48 | 118.30 |
| 1 | O | 494 | MET | N-CA-CB | 5.35 | 120.24 | 110.60 |
| 1 | O | 72 | ASP | CB-CG-OD2 | -5.35 | 113.48 | 118.30 |
| 1 | Y | 380 | THR | CA-CB-CG2 | -5.33 | 104.94 | 112.40 |
| 1 | Y | 492 | ARG | NE-CZ-NH2 | -5.33 | 117.64 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | Y | 458 | ASP | CB-CG-OD2 | -5.32 | 113.51 | 118.30 |
| 1 | O | 300 | TYR | N-CA-CB | 5.32 | 120.17 | 110.60 |
| 1 | Y | 184 | THR | CA-CB-CG2 | -5.31 | 104.96 | 112.40 |
| 1 | Y | 45 | VAL | CA-CB-CG1 | -5.31 | 102.93 | 110.90 |
| 1 | Y | 211 | ARG | NE-CZ-NH1 | 5.31 | 122.95 | 120.30 |
| 1 | O | 267 | THR | CA-CB-CG2 | -5.29 | 104.99 | 112.40 |
| 1 | Y | 409 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | Y | 413 | VAL | CA-CB-CG1 | -5.28 | 102.99 | 110.90 |
| 1 | Y | 55 | THR | N-CA-CB | 5.25 | 120.28 | 110.30 |
| 1 | Y | 125 | ARG | NE-CZ-NH2 | 5.24 | 122.92 | 120.30 |
| 1 | Y | 333 | ALA | CB-CA-C | 5.24 | 117.97 | 110.10 |
| 1 | Y | 24 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 1 | Y | 390 | ASP | CB-CA-C | -5.21 | 99.97 | 110.40 |
| 1 | Y | 218 | ARG | NE-CZ-NH2 | 5.21 | 122.90 | 120.30 |
| 1 | O | 13 | THR | CA-CB-CG2 | -5.21 | 105.11 | 112.40 |
| 1 | O | 445 | TYR | N-CA-CB | 5.20 | 119.95 | 110.60 |
| 1 | Y | 85 | THR | N-CA-CB | -5.20 | 100.43 | 110.30 |
| 1 | O | 24 | ASP | CB-CG-OD1 | -5.18 | 113.64 | 118.30 |
| 1 | Y | 13 | THR | CA-CB-CG2 | -5.18 | 105.15 | 112.40 |
| 1 | O | 478 | GLU | CG-CD-OE1 | 5.18 | 128.65 | 118.30 |
| 1 | O | 359 | TYR | CA-CB-CG | -5.17 | 103.57 | 113.40 |
| 1 | O | 429 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 1 | Y | 333 | ALA | N-CA-CB | -5.13 | 102.91 | 110.10 |
| 1 | O | 227 | THR | CA-CB-CG2 | -5.13 | 105.22 | 112.40 |
| 1 | Y | 339 | THR | CA-CB-CG2 | -5.13 | 105.22 | 112.40 |
| 1 | Y | 468 | ARG | NE-CZ-NH2 | -5.13 | 117.74 | 120.30 |
| 1 | Y | 243 | ALA | N-CA-CB | 5.12 | 117.27 | 110.10 |
| 1 | Y | 465 | VAL | CA-CB-CG1 | -5.12 | 103.23 | 110.90 |
| 1 | Y | 154 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 1 | Y | 84 | GLU | O-C-N | 5.10 | 130.85 | 122.70 |
| 1 | O | 201 | ASP | CB-CG-OD1 | 5.09 | 122.88 | 118.30 |
| 1 | Y | 83 | ARG | N-CA-C | 5.08 | 124.73 | 111.00 |
| 1 | O | 72 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | O | 130 | LEU | CA-CB-CG | -5.08 | 103.62 | 115.30 |
| 1 | Y | 87 | ILE | CB-CA-C | -5.07 | 101.47 | 111.60 |
| 1 | O | 39 | TYR | CB-CG-CD2 | 5.07 | 124.04 | 121.00 |
| 1 | Y | 390 | ASP | CA-CB-CG | 5.06 | 124.53 | 113.40 |
| 1 | Y | 300 | TYR | CB-CG-CD1 | -5.05 | 117.97 | 121.00 |
| 1 | Y | 117 | ARG | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 1 | O | 492 | ARG | CD-NE-CZ | 5.05 | 130.67 | 123.60 |
| 1 | Y | 398 | ASP | CB-CG-OD2 | 5.05 | 122.84 | 118.30 |
| 1 | O | 48 | ASP | CB-CG-OD2 | 5.05 | 122.84 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | Y | 193 | ASN | N-CA-CB | 5.02 | 119.64 | 110.60 |
| 1 | Y | 432 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | Y | 38 | ILE | CB-CA-C | -5.02 | 101.57 | 111.60 |
| 1 | O | 438 | VAL | CA-CB-CG2 | -5.01 | 103.38 | 110.90 |

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 | O | 3910 | 0 | 3841 | 747 | 0 |
| 1 | Y | 3910 | 0 | 3841 | 743 | 0 |
| 2 | O | 1 | 0 | 0 | 0 | 0 |
| 2 | Y | 1 | 0 | 0 | 0 | 0 |
| 3 | O | 31 | 0 | 14 | 4 | 0 |
| 3 | Y | 31 | 0 | 14 | 5 | 0 |
| 4 | O | 6 | 0 | 8 | 7 | 0 |
| 4 | Y | 6 | 0 | 8 | 2 | 0 |
| All | All | 7896 | 0 | 7726 | 1482 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 95.

All (1482) 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:Y:458:ASP:HA | 1:Y:461:GLN:HG3 | 1.25 | 1.13 |
| 1:O:48:ASP:HB3 | 1:O:51:GLU:HB3 | 1.16 | 1.13 |
| 1:O:415:ASN:ND2 | 1:O:418:LEU:H | 1.48 | 1.11 |
| 1:Y:31:SER:HB2 | 1:Y:63:VAL:HG22 | 1.28 | 1.08 |
| 1:O:83:ARG:HB2 | 4:O:600:GOL:H12 | 1.11 | 1.08 |
| 1:Y:459:GLU:HB2 | 1:Y:460:LEU:HD12 | 1.25 | 1.07 |
| 1:Y:84:GLU:HB2 | 1:Y:103:TRP:HB3 | 1.36 | 1.06 |
| 1:Y:31:SER:HB3 | 1:Y:59:THR:HA | 1.39 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:117:ARG:HH11 | 1:O:117:ARG:HB2 | 1.16 | 1.04 |
| 1:O:435:VAL:HG21 | 1:O:441:LEU:HD11 | 1.41 | 1.02 |
| 1:O:313:ILE:HD11 | 1:O:381:LEU:HD23 | 1.42 | 1.01 |
| 1:O:211:ARG:HG3 | 1:O:211:ARG:HH11 | 1.22 | 1.00 |
| 1:O:47:HIS:HB3 | 1:O:52:ILE:HD11 | 1.41 | 0.99 |
| 1:O:138:GLY:HA2 | 1:O:191:LEU:HD21 | 1.42 | 0.98 |
| 1:O:272:LEU:HD11 | 1:O:303:GLU:HG3 | 1.41 | 0.98 |
| 1:Y:246:GLN:HG3 | 1:Y:262:LYS:HZ1 | 1.28 | 0.97 |
| 1:Y:460:LEU:H | 1:Y:460:LEU:HD12 | 1.29 | 0.97 |
| 1:O:144:ILE:HD12 | 1:O:144:ILE:H | 1.28 | 0.96 |
| 1:O:460:LEU:HD12 | 1:O:460:LEU:H | 1.31 | 0.96 |
| 1:Y:117:ARG:HB2 | 1:Y:117:ARG:HH11 | 1.31 | 0.96 |
| 1:Y:229:ILE:HG21 | 1:Y:237:ILE:HG12 | 1.47 | 0.96 |
| 1:Y:27:ILE:HD12 | 1:Y:27:ILE:H | 1.31 | 0.96 |
| 1:Y:226:GLN:HB2 | 1:Y:236:ARG:HD3 | 1.50 | 0.93 |
| 1:O:137:SER:O | 1:O:138:GLY:C | 2.02 | 0.93 |
| 1:Y:152:ARG:HB3 | 1:Y:156:ARG:HH22 | 1.34 | 0.93 |
| 1:Y:413:VAL:HG12 | 1:Y:419:MET:HE3 | 1.51 | 0.92 |
| 1:O:468:ARG:HH11 | 1:O:468:ARG:HG3 | 1.32 | 0.92 |
| 1:O:415:ASN:HD21 | 1:O:417:PHE:HB3 | 1.33 | 0.92 |
| 1:Y:117:ARG:HB2 | 1:Y:117:ARG:NH1 | 1.84 | 0.91 |
| 1:Y:468:ARG:HD2 | 1:Y:469:GLU:N | 1.85 | 0.91 |
| 1:O:84:GLU:HB2 | 1:O:103:TRP:HB3 | 1.50 | 0.91 |
| 1:O:415:ASN:HD22 | 1:O:418:LEU:H | 1.01 | 0.91 |
| 1:O:27:ILE:H | 1:O:27:ILE:HD12 | 1.35 | 0.91 |
| 1:Y:91:LYS:HB2 | 1:Y:161:LEU:HD12 | 1.53 | 0.91 |
| 1:O:271:MET:HG2 | 1:O:395:MET:HE2 | 1.54 | 0.90 |
| 1:O:115:LEU:HD12 | 1:O:115:LEU:H | 1.38 | 0.89 |
| 1:Y:91:LYS:O | 1:Y:92:GLU:C | 2.05 | 0.89 |
| 1:O:413:VAL:HA | 1:O:419:MET:CE | 2.03 | 0.89 |
| 1:Y:459:GLU:HB2 | 1:Y:460:LEU:CD1 | 2.03 | 0.88 |
| 1:O:463:LYS:HA | 1:O:463:LYS:HE2 | 1.56 | 0.88 |
| 1:O:164:THR:H | 1:O:167:THR:HB | 1.39 | 0.87 |
| 1:Y:279:ALA:HB2 | 1:Y:300:TYR:CD2 | 2.09 | 0.87 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:CG2 | 2.04 | 0.87 |
| 1:Y:196:THR:H | 1:Y:197:LEU:HD22 | 1.39 | 0.87 |
| 1:Y:257:LYS:H | 1:Y:260:MET:HG3 | 1.40 | 0.87 |
| 1:O:3:LYS:HG3 | 1:O:73:GLN:HA | 1.57 | 0.87 |
| 1:O:203:MET:HA | 1:O:206:VAL:HG12 | 1.57 | 0.87 |
| 1:Y:211:ARG:HH11 | 1:Y:211:ARG:HG3 | 1.40 | 0.87 |
| 1:O:35:PHE:HB2 | 1:O:51:GLU:HG3 | 1.56 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:193:ASN:HB3 | 1:Y:196:THR:CG2 | 2.05 | 0.86 |
| 1:Y:31:SER:CB | 1:Y:63:VAL:HG22 | 2.05 | 0.86 |
| 1:O:63:VAL:HA | 1:O:66:LYS:HG2 | 1.55 | 0.85 |
| 1:O:91:LYS:HB2 | 1:O:161:LEU:HD12 | 1.57 | 0.85 |
| 1:Y:463:LYS:HE2 | 1:Y:463:LYS:HA | 1.56 | 0.85 |
| 1:Y:468:ARG:HD2 | 1:Y:469:GLU:H | 1.37 | 0.85 |
| 1:O:184:THR:HB | 1:O:247:GLN:HG2 | 1.59 | 0.85 |
| 1:Y:183:TYR:CE1 | 1:Y:217:VAL:HG12 | 2.12 | 0.85 |
| 1:O:90:GLU:HB3 | 1:O:93:THR:HG23 | 1.58 | 0.84 |
| 1:O:17:ARG:HH22 | 1:O:437:GLU:HG3 | 1.40 | 0.84 |
| 1:O:199:TRP:CZ2 | 1:O:214:LEU:HB3 | 2.13 | 0.83 |
| 1:Y:193:ASN:HB3 | 1:Y:196:THR:HB | 1.58 | 0.83 |
| 1:Y:84:GLU:HB2 | 1:Y:103:TRP:CB | 2.07 | 0.83 |
| 1:Y:240:SER:HB2 | 1:Y:450:ALA:CB | 2.08 | 0.83 |
| 1:Y:81:ASN:HD22 | 1:Y:81:ASN:N | 1.77 | 0.83 |
| 1:Y:328:ASP:HB3 | 1:Y:332:PHE:HE2 | 1.43 | 0.82 |
| 1:O:102:VAL:HG12 | 1:O:103:TRP:CD1 | 2.13 | 0.82 |
| 1:O:80:THR:HG21 | 1:O:245:ASP:HA | 1.61 | 0.82 |
| 1:O:47:HIS:HB3 | 1:O:52:ILE:CD1 | 2.08 | 0.82 |
| 1:Y:458:ASP:HA | 1:Y:461:GLN:CG | 2.09 | 0.82 |
| 1:Y:47:HIS:HB3 | 1:Y:52:ILE:HD11 | 1.60 | 0.82 |
| 1:O:415:ASN:HD22 | 1:O:418:LEU:N | 1.78 | 0.82 |
| 1:O:459:GLU:HB2 | 1:O:460:LEU:HD12 | 1.62 | 0.82 |
| 1:O:114:HIS:HA | 1:O:117:ARG:NH1 | 1.95 | 0.81 |
| 1:Y:433:PRO:HA | 1:Y:466:ILE:HA | 1.61 | 0.81 |
| 1:O:55:THR:HA | 1:O:58:TRP:CD1 | 2.16 | 0.81 |
| 1:O:91:LYS:O | 1:O:92:GLU:C | 2.12 | 0.81 |
| 1:O:313:ILE:HD11 | 1:O:381:LEU:CD2 | 2.11 | 0.81 |
| 1:O:48:ASP:CB | 1:O:51:GLU:HB3 | 2.08 | 0.80 |
| 1:O:91:LYS:NZ | 1:O:91:LYS:HB3 | 1.94 | 0.80 |
| 1:Y:189:THR:HB | 1:Y:191:LEU:HG | 1.63 | 0.80 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:HB | 1.62 | 0.80 |
| 1:O:373:ALA:O | 1:O:377:ILE:HG13 | 1.82 | 0.80 |
| 1:Y:195:HIS:ND1 | 1:Y:195:HIS:N | 2.29 | 0.80 |
| 1:Y:251:PHE:CE2 | 1:Y:446:LEU:HD12 | 2.17 | 0.80 |
| 1:Y:457:LEU:HA | 1:Y:460:LEU:HD13 | 1.61 | 0.80 |
| 1:O:253:GLN:HE21 | 1:O:262:LYS:CB | 1.96 | 0.79 |
| 1:O:138:GLY:HA2 | 1:O:191:LEU:CD2 | 2.12 | 0.79 |
| 1:O:199:TRP:CE2 | 1:O:214:LEU:HB3 | 2.18 | 0.79 |
| 1:Y:106:ARG:HD2 | 1:Y:349:THR:O | 1.82 | 0.79 |
| 1:O:188:ARG:HH21 | 1:O:289:THR:HG21 | 1.48 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:48:ASP:HB3 | 1:O:51:GLU:CB | 2.07 | 0.79 |
| 1:O:272:LEU:CD1 | 1:O:303:GLU:HG3 | 2.13 | 0.78 |
| 1:O:463:LYS:HA | 1:O:463:LYS:CE | 2.13 | 0.78 |
| 1:Y:458:ASP:CA | 1:Y:461:GLN:HG3 | 2.12 | 0.78 |
| 1:Y:413:VAL:HA | 1:Y:419:MET:CE | 2.13 | 0.78 |
| 1:Y:3:LYS:HA | 1:Y:73:GLN:HA | 1.64 | 0.78 |
| 1:O:438:VAL:HA | 1:O:441:LEU:HD12 | 1.65 | 0.78 |
| 1:Y:230:GLY:HA2 | 1:Y:235:THR:CB | 2.13 | 0.78 |
| 1:O:40:PRO:HG2 | 1:O:44:TRP:CB | 2.14 | 0.78 |
| 1:Y:415:ASN:HD21 | 1:Y:417:PHE:HB3 | 1.47 | 0.77 |
| 1:O:19:VAL:HG12 | 1:O:21:MET:HE2 | 1.66 | 0.77 |
| 1:O:146:ASP:HB3 | 1:O:152:ARG:HH12 | 1.49 | 0.77 |
| 1:Y:492:ARG:HG2 | 1:Y:492:ARG:HH11 | 1.47 | 0.77 |
| 1:O:253:GLN:HE21 | 1:O:262:LYS:HB2 | 1.49 | 0.77 |
| 1:Y:413:VAL:HG12 | 1:Y:419:MET:CE | 2.15 | 0.77 |
| 1:O:17:ARG:HH22 | 1:O:437:GLU:CG | 1.98 | 0.76 |
| 1:O:435:VAL:CG2 | 1:O:441:LEU:HD11 | 2.14 | 0.76 |
| 1:O:33:ARG:HH21 | 1:O:58:TRP:HB3 | 1.50 | 0.76 |
| 1:O:360:ALA:O | 1:O:361:ARG:HD3 | 1.84 | 0.76 |
| 1:O:155:ALA:HB1 | 1:O:210:PRO:HG2 | 1.66 | 0.76 |
| 1:Y:286:LEU:C | 1:Y:287:LEU:HD23 | 2.05 | 0.76 |
| 1:O:152:ARG:O | 1:O:155:ALA:HB3 | 1.85 | 0.76 |
| 1:Y:127:ASN:HB3 | 1:Y:193:ASN:ND2 | 2.00 | 0.76 |
| 1:Y:162:PHE:HB3 | 1:Y:213:MET:HG3 | 1.67 | 0.76 |
| 1:Y:373:ALA:O | 1:Y:377:ILE:HG13 | 1.84 | 0.76 |
| 1:O:413:VAL:HA | 1:O:419:MET:HE2 | 1.67 | 0.76 |
| 1:Y:360:ALA:O | 1:Y:361:ARG:HD3 | 1.85 | 0.76 |
| 1:Y:457:LEU:HD22 | 1:Y:460:LEU:HD13 | 1.66 | 0.76 |
| 1:Y:58:TRP:O | 1:Y:59:THR:C | 2.24 | 0.76 |
| 1:O:173:MET:HB3 | 1:O:227:THR:HG21 | 1.67 | 0.76 |
| 1:O:123:TYR:CZ | 1:O:202:LYS:HG3 | 2.20 | 0.76 |
| 1:O:164:THR:H | 1:O:167:THR:CB | 1.98 | 0.76 |
| 1:Y:141:VAL:O | 1:Y:145:LEU:HD22 | 1.86 | 0.75 |
| 1:Y:267:THR:OG1 | 3:Y:601:ACP:H3B2 | 1.86 | 0.75 |
| 1:O:195:HIS:N | 1:O:195:HIS:ND1 | 2.29 | 0.75 |
| 1:O:31:SER:OG | 1:O:62:GLU:HB2 | 1.85 | 0.75 |
| 1:Y:255:CYS:HB3 | 1:Y:260:MET:HB2 | 1.68 | 0.75 |
| 1:Y:269:CYS:HB2 | 1:Y:306:VAL:HB | 1.68 | 0.75 |
| 1:O:221:SER:CB | 1:O:296:GLY:HA3 | 2.16 | 0.75 |
| 1:Y:152:ARG:O | 1:Y:155:ALA:HB3 | 1.87 | 0.75 |
| 1:O:241:GLY:O | 1:O:242:ILE:HG13 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:447:ALA:O | 1:Y:450:ALA:HB3 | 1.86 | 0.75 |
| 1:O:141:VAL:O | 1:O:145:LEU:HD22 | 1.85 | 0.75 |
| 1:Y:193:ASN:HB3 | 1:Y:196:THR:CB | 2.17 | 0.75 |
| 1:O:153:GLU:C | 1:O:157:ARG:HD3 | 2.08 | 0.74 |
| 1:O:156:ARG:HB2 | 1:O:156:ARG:CZ | 2.16 | 0.74 |
| 1:Y:441:LEU:HD22 | 1:Y:445:TYR:CE1 | 2.22 | 0.74 |
| 1:O:184:THR:CG2 | 1:O:247:GLN:HG2 | 2.18 | 0.74 |
| 1:Y:8:ALA:O | 1:Y:9:LEU:HD13 | 1.87 | 0.74 |
| 1:O:137:SER:HA | 1:O:140:LYS:HD2 | 1.67 | 0.74 |
| 1:Y:410:GLY:O | 1:Y:413:VAL:HG22 | 1.87 | 0.74 |
| 1:Y:449:LEU:O | 1:Y:449:LEU:HD12 | 1.87 | 0.74 |
| 1:Y:85:THR:HA | 1:Y:101:ILE:O | 1.87 | 0.74 |
| 1:O:276:GLY:HA2 | 1:O:299:ASN:ND2 | 2.03 | 0.74 |
| 1:Y:168:TRP:O | 1:Y:172:LYS:HG2 | 1.88 | 0.74 |
| 1:Y:454:TRP:CD1 | 1:Y:460:LEU:HD11 | 2.22 | 0.74 |
| 1:O:332:PHE:O | 1:O:335:LYS:HB2 | 1.87 | 0.74 |
| 1:O:3:LYS:HG3 | 1:O:73:GLN:CA | 2.17 | 0.74 |
| 1:Y:183:TYR:CD1 | 1:Y:217:VAL:HG12 | 2.22 | 0.74 |
| 1:O:170:ILE:O | 1:O:171:TRP:C | 2.25 | 0.73 |
| 1:Y:120:LEU:HD12 | 1:Y:120:LEU:H | 1.54 | 0.73 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:CB | 2.18 | 0.73 |
| 1:O:41:LYS:HG3 | 1:O:42:PRO:HD2 | 1.70 | 0.73 |
| 1:O:80:THR:CG2 | 1:O:245:ASP:HA | 2.19 | 0.73 |
| 1:O:221:SER:HB3 | 1:O:296:GLY:HA3 | 1.70 | 0.73 |
| 1:O:184:THR:CB | 1:O:247:GLN:HG2 | 2.19 | 0.73 |
| 1:O:253:GLN:HG3 | 1:O:407:ARG:HD2 | 1.71 | 0.73 |
| 1:Y:44:TRP:CE2 | 1:Y:107:ARG:HB2 | 2.23 | 0.73 |
| 1:O:164:THR:O | 1:O:165:VAL:C | 2.26 | 0.72 |
| 1:O:226:GLN:CB | 1:O:236:ARG:HD3 | 2.18 | 0.72 |
| 1:O:261:ALA:HB2 | 1:O:273:MET:HG2 | 1.71 | 0.72 |
| 1:Y:415:ASN:ND2 | 1:Y:418:LEU:H | 1.86 | 0.72 |
| 1:Y:9:LEU:HD23 | 1:Y:77:ILE:HG23 | 1.71 | 0.72 |
| 1:Y:196:THR:N | 1:Y:197:LEU:HD22 | 2.03 | 0.72 |
| 1:O:200:ASP:OD1 | 1:O:202:LYS:HB2 | 1.88 | 0.72 |
| 1:O:358:PRO:HG2 | 1:O:359:TYR:CE2 | 2.24 | 0.72 |
| 1:O:245:ASP:O | 1:O:248:ALA:HB3 | 1.90 | 0.72 |
| 1:O:413:VAL:HA | 1:O:419:MET:HE3 | 1.70 | 0.72 |
| 1:O:83:ARG:HB2 | 4:O:600:GOL:C1 | 2.06 | 0.72 |
| 1:O:84:GLU:HB2 | 1:O:103:TRP:CB | 2.20 | 0.72 |
| 1:Y:17:ARG:HD3 | 1:Y:32:GLN:HE21 | 1.54 | 0.72 |
| 1:O:256:VAL:HG13 | 1:O:294:PRO:HG3 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:91:LYS:HG2 | 1:Y:92:GLU:N | 2.03 | 0.71 |
| 1:O:254:LEU:HD11 | 1:O:445:TYR:HE2 | 1.55 | 0.71 |
| 1:Y:84:GLU:CB | 1:Y:103:TRP:HB3 | 2.19 | 0.71 |
| 1:Y:142:LYS:O | 1:Y:143:TRP:C | 2.28 | 0.71 |
| 1:Y:279:ALA:HB2 | 1:Y:300:TYR:CG | 2.25 | 0.71 |
| 1:O:253:GLN:CG | 1:O:407:ARG:HD2 | 2.20 | 0.71 |
| 1:Y:88:VAL:CG2 | 1:Y:162:PHE:HB2 | 2.20 | 0.71 |
| 1:Y:262:LYS:HZ3 | 1:Y:264:THR:HB | 1.56 | 0.71 |
| 1:Y:463:LYS:CE | 1:Y:463:LYS:HA | 2.16 | 0.71 |
| 1:Y:137:SER:O | 1:Y:138:GLY:C | 2.28 | 0.71 |
| 1:O:9:LEU:HD12 | 1:O:56:GLN:NE2 | 2.05 | 0.71 |
| 1:O:90:GLU:OE2 | 1:O:93:THR:HG21 | 1.91 | 0.71 |
| 1:O:91:LYS:HB2 | 1:O:161:LEU:CD1 | 2.21 | 0.71 |
| 1:Y:27:ILE:CD1 | 1:Y:27:ILE:H | 2.03 | 0.70 |
| 1:Y:328:ASP:HB3 | 1:Y:332:PHE:CE2 | 2.25 | 0.70 |
| 1:Y:39:TYR:OH | 1:O:369:ARG:HD2 | 1.91 | 0.70 |
| 1:O:203:MET:HA | 1:O:206:VAL:CG1 | 2.20 | 0.70 |
| 1:O:403:LEU:N | 1:O:403:LEU:HD12 | 2.06 | 0.70 |
| 1:O:486:TRP:O | 1:O:490:VAL:HG23 | 1.90 | 0.70 |
| 1:Y:31:SER:HB3 | 1:Y:59:THR:CA | 2.20 | 0.70 |
| 1:Y:403:LEU:HD12 | 1:Y:403:LEU:N | 2.05 | 0.70 |
| 1:Y:348:PHE:CE1 | 1:Y:362:GLY:HA3 | 2.27 | 0.70 |
| 1:Y:413:VAL:CG1 | 1:Y:419:MET:HE3 | 2.22 | 0.70 |
| 1:Y:467:GLU:HG2 | 1:Y:468:ARG:N | 2.06 | 0.70 |
| 1:Y:422:GLN:O | 1:Y:426:LEU:HD22 | 1.92 | 0.70 |
| 1:O:117:ARG:HH11 | 1:O:117:ARG:CB | 1.98 | 0.70 |
| 1:O:33:ARG:NH2 | 1:O:58:TRP:HB3 | 2.07 | 0.70 |
| 1:Y:230:GLY:HA2 | 1:Y:235:THR:HB | 1.73 | 0.70 |
| 1:Y:413:VAL:HA | 1:Y:419:MET:HE2 | 1.71 | 0.70 |
| 1:Y:11:GLN:O | 1:Y:81:ASN:HA | 1.92 | 0.70 |
| 1:O:388:THR:O | 1:O:391:VAL:HG13 | 1.92 | 0.70 |
| 1:Y:88:VAL:HG22 | 1:Y:162:PHE:HB2 | 1.74 | 0.70 |
| 1:O:74:ILE:HD11 | 1:O:237:ILE:HG21 | 1.74 | 0.69 |
| 1:O:40:PRO:HG3 | 1:O:46:GLU:OE2 | 1.91 | 0.69 |
| 1:Y:154:ARG:HA | 1:Y:157:ARG:HG2 | 1.72 | 0.69 |
| 1:O:385:ALA:HB1 | 1:O:422:GLN:NE2 | 2.06 | 0.69 |
| 1:Y:262:LYS:HZ3 | 1:Y:264:THR:CB | 2.05 | 0.69 |
| 1:O:492:ARG:HH11 | 1:O:492:ARG:HG2 | 1.56 | 0.69 |
| 1:O:77:ILE:HB | 1:O:238:PRO:O | 1.92 | 0.69 |
| 1:O:451:VAL:HG12 | 1:O:453:PHE:HB2 | 1.74 | 0.69 |
| 1:Y:40:PRO:HG3 | 1:Y:46:GLU:CD | 2.12 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:154:ARG:O | 1:Y:155:ALA:C | 2.28 | 0.69 |
| 1:Y:246:GLN:HG3 | 1:Y:262:LYS:NZ | 2.04 | 0.69 |
| 1:Y:143:TRP:O | 1:Y:147:HIS:HB2 | 1.93 | 0.69 |
| 1:O:117:ARG:NH1 | 1:O:117:ARG:HB2 | 2.00 | 0.69 |
| 1:O:322:LEU:N | 1:O:322:LEU:HD23 | 2.07 | 0.69 |
| 1:Y:26:ASN:O | 1:Y:28:ILE:HD13 | 1.92 | 0.69 |
| 1:Y:246:GLN:HG2 | 1:Y:270:PHE:CB | 2.23 | 0.69 |
| 1:Y:123:TYR:CZ | 1:Y:202:LYS:HG3 | 2.27 | 0.69 |
| 1:O:70:SER:H | 1:O:73:GLN:HE21 | 1.41 | 0.69 |
| 1:Y:207:LEU:HB3 | 1:Y:209:ILE:HD12 | 1.73 | 0.69 |
| 1:O:439:THR:HG22 | 1:O:440:ALA:N | 2.07 | 0.68 |
| 1:Y:222:GLU:HG2 | 1:Y:224:TYR:CE1 | 2.28 | 0.68 |
| 1:Y:35:PHE:HB2 | 1:Y:51:GLU:HG2 | 1.75 | 0.68 |
| 1:O:444:ALA:O | 1:O:445:TYR:C | 2.32 | 0.68 |
| 1:Y:115:LEU:H | 1:Y:115:LEU:HD12 | 1.57 | 0.68 |
| 1:Y:257:LYS:C | 1:Y:274:ASN:HD22 | 1.97 | 0.68 |
| 1:Y:317:ARG:O | 1:Y:321:LYS:HA | 1.93 | 0.68 |
| 1:Y:170:ILE:HG22 | 1:Y:171:TRP:N | 2.07 | 0.68 |
| 1:O:317:ARG:HG2 | 1:O:318:ASP:N | 2.08 | 0.68 |
| 1:Y:203:MET:HA | 1:Y:206:VAL:HG12 | 1.75 | 0.68 |
| 1:Y:337:GLN:HA | 1:Y:337:GLN:NE2 | 2.09 | 0.68 |
| 1:O:193:ASN:CB | 1:O:196:THR:HB | 2.24 | 0.68 |
| 1:Y:271:MET:HG2 | 1:Y:395:MET:CE | 2.23 | 0.68 |
| 1:Y:124:ILE:HG12 | 1:Y:203:MET:HE3 | 1.76 | 0.68 |
| 1:O:271:MET:C | 1:O:272:LEU:HD12 | 2.13 | 0.68 |
| 1:Y:156:ARG:HB2 | 1:Y:156:ARG:CZ | 2.24 | 0.68 |
| 1:O:182:ASP:HB3 | 1:O:242:ILE:CG2 | 2.24 | 0.68 |
| 1:Y:151:SER:O | 1:Y:152:ARG:C | 2.30 | 0.68 |
| 1:Y:169:LEU:O | 1:Y:172:LYS:HB2 | 1.94 | 0.68 |
| 1:O:31:SER:HB2 | 1:O:63:VAL:CG2 | 2.25 | 0.67 |
| 1:O:20:VAL:HG23 | 1:O:63:VAL:HG11 | 1.77 | 0.67 |
| 1:Y:124:ILE:HG12 | 1:Y:203:MET:CE | 2.24 | 0.67 |
| 1:O:44:TRP:CE2 | 1:O:107:ARG:HB2 | 2.30 | 0.67 |
| 1:O:227:THR:OG1 | 1:O:239:ILE:HD11 | 1.94 | 0.67 |
| 1:O:47:HIS:O | 1:O:49:PRO:HD3 | 1.93 | 0.67 |
| 1:Y:193:ASN:CB | 1:Y:196:THR:HB | 2.24 | 0.67 |
| 1:Y:286:LEU:HD11 | 1:Y:394:ALA:CB | 2.25 | 0.67 |
| 1:O:226:GLN:HB2 | 1:O:236:ARG:HD3 | 1.76 | 0.67 |
| 1:Y:20:VAL:HG12 | 1:Y:21:MET:N | 2.09 | 0.67 |
| 1:Y:61:VAL:HG12 | 1:Y:62:GLU:N | 2.08 | 0.67 |
| 1:O:63:VAL:O | 1:O:64:LEU:C | 2.32 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:363:ALA:C | 1:Y:364:ILE:HD13 | 2.15 | 0.67 |
| 1:Y:82:GLN:O | 1:Y:165:VAL:HG21 | 1.94 | 0.67 |
| 1:Y:322:LEU:HD23 | 1:Y:322:LEU:N | 2.09 | 0.67 |
| 1:Y:392:LEU:HD23 | 1:Y:393:GLU:N | 2.10 | 0.67 |
| 1:O:113:GLU:O | 1:O:116:LYS:HB2 | 1.95 | 0.67 |
| 1:Y:20:VAL:O | 1:Y:28:ILE:N | 2.28 | 0.67 |
| 1:O:229:ILE:HG21 | 1:O:237:ILE:HG12 | 1.78 | 0.66 |
| 1:Y:276:GLY:O | 1:Y:300:TYR:N | 2.29 | 0.66 |
| 1:O:19:VAL:HG12 | 1:O:21:MET:CE | 2.25 | 0.66 |
| 1:O:278:LYS:HE3 | 1:O:280:VAL:HG23 | 1.77 | 0.66 |
| 1:O:20:VAL:O | 1:O:28:ILE:N | 2.29 | 0.66 |
| 1:Y:197:LEU:N | 1:Y:197:LEU:HD22 | 2.10 | 0.66 |
| 1:Y:47:HIS:O | 1:Y:99:ASN:HB3 | 1.96 | 0.66 |
| 1:O:207:LEU:HB3 | 1:O:209:ILE:CD1 | 2.26 | 0.66 |
| 1:O:90:GLU:OE1 | 1:O:95:LYS:HG2 | 1.94 | 0.66 |
| 1:Y:345:VAL:O | 1:Y:362:GLY:HA2 | 1.96 | 0.66 |
| 1:O:164:THR:O | 1:O:167:THR:N | 2.29 | 0.66 |
| 1:O:40:PRO:HG2 | 1:O:44:TRP:HB3 | 1.77 | 0.66 |
| 1:O:181:THR:HG23 | 1:O:182:ASP:O | 1.95 | 0.66 |
| 1:O:3:LYS:HA | 1:O:73:GLN:HA | 1.77 | 0.66 |
| 1:O:91:LYS:O | 1:O:94:GLY:N | 2.29 | 0.66 |
| 1:Y:138:GLY:O | 1:Y:141:VAL:HG23 | 1.95 | 0.66 |
| 1:Y:22:ASP:OD2 | 1:Y:26:ASN:HB2 | 1.96 | 0.66 |
| 1:O:197:LEU:N | 1:O:197:LEU:HD22 | 2.10 | 0.66 |
| 1:O:118:ASP:N | 1:O:118:ASP:OD1 | 2.29 | 0.66 |
| 1:O:468:ARG:HG3 | 1:O:468:ARG:NH1 | 2.00 | 0.66 |
| 1:Y:153:GLU:O | 1:Y:156:ARG:N | 2.29 | 0.66 |
| 1:O:271:MET:HG2 | 1:O:395:MET:CE | 2.26 | 0.65 |
| 1:Y:128:THR:HG21 | 1:Y:190:MET:HA | 1.79 | 0.65 |
| 1:Y:166:ASP:OD2 | 1:Y:242:ILE:HG21 | 1.95 | 0.65 |
| 1:O:125:ARG:NH1 | 1:O:282:SER:O | 2.29 | 0.65 |
| 1:O:144:ILE:CD1 | 1:O:144:ILE:H | 2.06 | 0.65 |
| 1:O:26:ASN:O | 1:O:28:ILE:HD13 | 1.97 | 0.65 |
| 1:O:478:GLU:OE1 | 1:O:478:GLU:HA | 1.96 | 0.65 |
| 1:Y:205:GLU:O | 1:Y:208:ASP:N | 2.30 | 0.65 |
| 1:Y:179:HIS:CD2 | 1:Y:215:PRO:HA | 2.30 | 0.65 |
| 1:O:84:GLU:CB | 1:O:103:TRP:HB3 | 2.26 | 0.65 |
| 1:Y:85:THR:HG23 | 1:Y:102:VAL:HA | 1.78 | 0.65 |
| 1:Y:19:VAL:HG22 | 1:Y:30:VAL:HG22 | 1.79 | 0.65 |
| 1:O:183:TYR:CD1 | 1:O:217:VAL:HG12 | 2.31 | 0.65 |
| 1:O:410:GLY:O | 1:O:413:VAL:HG13 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:78:GLY:C | 1:O:79:ILE:HG12 | 2.16 | 0.65 |
| 1:O:114:HIS:HA | 1:O:117:ARG:CZ | 2.26 | 0.65 |
| 1:O:352:GLY:O | 1:O:355:TYR:N | 2.29 | 0.65 |
| 1:O:81:ASN:N | 1:O:81:ASN:HD22 | 1.95 | 0.65 |
| 1:Y:91:LYS:O | 1:Y:94:GLY:N | 2.30 | 0.65 |
| 1:O:152:ARG:HB3 | 1:O:156:ARG:HH22 | 1.61 | 0.65 |
| 1:Y:58:TRP:O | 1:Y:61:VAL:N | 2.30 | 0.65 |
| 1:O:205:GLU:O | 1:O:208:ASP:N | 2.29 | 0.65 |
| 1:O:219:ARG:NH2 | 1:O:295:THR:OG1 | 2.29 | 0.65 |
| 1:O:489:ALA:O | 1:O:492:ARG:N | 2.29 | 0.65 |
| 1:O:65:ALA:O | 1:O:67:ALA:N | 2.30 | 0.65 |
| 1:O:137:SER:O | 1:O:140:LYS:N | 2.30 | 0.65 |
| 1:O:179:HIS:CD2 | 1:O:215:PRO:HA | 2.32 | 0.65 |
| 1:O:84:GLU:OE1 | 1:O:84:GLU:N | 2.29 | 0.65 |
| 1:O:88:VAL:HG22 | 1:O:162:PHE:HB2 | 1.78 | 0.65 |
| 1:O:40:PRO:HG2 | 1:O:44:TRP:HB2 | 1.77 | 0.65 |
| 1:Y:212:GLU:O | 1:Y:214:LEU:N | 2.29 | 0.65 |
| 1:Y:58:TRP:O | 1:Y:60:LEU:N | 2.30 | 0.65 |
| 1:O:144:ILE:O | 1:O:147:HIS:N | 2.30 | 0.65 |
| 1:O:420:GLN:NE2 | 1:O:424:ASP:OD1 | 2.29 | 0.65 |
| 1:O:451:VAL:CG1 | 1:O:453:PHE:HB2 | 2.26 | 0.65 |
| 1:Y:4:LYS:N | 1:Y:73:GLN:O | 2.30 | 0.65 |
| 1:O:220:SER:HB3 | 1:O:242:ILE:O | 1.97 | 0.64 |
| 1:Y:237:ILE:HG22 | 1:Y:238:PRO:N | 2.12 | 0.64 |
| 1:O:146:ASP:HB3 | 1:O:152:ARG:NH1 | 2.11 | 0.64 |
| 1:Y:137:SER:OG | 1:Y:189:THR:HA | 1.97 | 0.64 |
| 1:Y:420:GLN:NE2 | 1:Y:424:ASP:OD1 | 2.30 | 0.64 |
| 1:O:120:LEU:O | 1:O:124:ILE:HG13 | 1.97 | 0.64 |
| 1:O:171:TRP:CE2 | 1:O:176:GLY:HA2 | 2.32 | 0.64 |
| 1:Y:63:VAL:HA | 1:Y:66:LYS:HD3 | 1.78 | 0.64 |
| 1:Y:205:GLU:HG2 | 1:Y:206:VAL:N | 2.12 | 0.64 |
| 1:Y:314:GLN:O | 1:Y:318:ASP:N | 2.29 | 0.64 |
| 1:Y:153:GLU:O | 1:Y:154:ARG:C | 2.32 | 0.64 |
| 1:Y:364:ILE:HD13 | 1:Y:364:ILE:N | 2.13 | 0.64 |
| 1:O:127:ASN:HD22 | 1:O:193:ASN:HD21 | 1.46 | 0.64 |
| 1:O:216:GLU:HG2 | 1:O:218:ARG:HH11 | 1.62 | 0.64 |
| 1:O:230:GLY:HA2 | 1:O:235:THR:CB | 2.27 | 0.64 |
| 1:O:31:SER:HB3 | 1:O:59:THR:HA | 1.79 | 0.64 |
| 1:O:46:GLU:O | 1:O:47:HIS:ND1 | 2.30 | 0.64 |
| 1:O:183:TYR:CE1 | 1:O:217:VAL:HG12 | 2.33 | 0.64 |
| 1:O:33:ARG:HE | 1:O:58:TRP:CB | 2.11 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:87:ILE:HD13 | 1:O:168:TRP:HB2 | 1.79 | 0.64 |
| 1:Y:109:ALA:O | 1:Y:112:CYS:HB2 | 1.98 | 0.64 |
| 1:Y:3:LYS:HG3 | 1:Y:72:ASP:O | 1.98 | 0.64 |
| 1:Y:396:GLN:HA | 1:Y:399:SER:OG | 1.98 | 0.64 |
| 1:O:272:LEU:HD11 | 1:O:303:GLU:CG | 2.22 | 0.63 |
| 1:Y:130:LEU:HD23 | 1:Y:130:LEU:N | 2.07 | 0.63 |
| 1:Y:157:ARG:HG3 | 1:Y:159:GLU:OE1 | 1.98 | 0.63 |
| 1:O:143:TRP:O | 1:O:147:HIS:HB2 | 1.98 | 0.63 |
| 1:O:353:ALA:HB2 | 1:O:356:TRP:CZ2 | 2.34 | 0.63 |
| 1:Y:359:TYR:HB3 | 1:Y:497:GLU:HB3 | 1.80 | 0.63 |
| 1:O:286:LEU:HD11 | 1:O:394:ALA:CB | 2.29 | 0.63 |
| 1:O:386:TYR:HB3 | 1:O:486:TRP:CE2 | 2.33 | 0.63 |
| 1:Y:413:VAL:HA | 1:Y:419:MET:HE3 | 1.81 | 0.63 |
| 1:Y:496:TRP:O | 1:O:488:LYS:HE2 | 1.98 | 0.63 |
| 1:O:181:THR:HG23 | 1:O:182:ASP:N | 2.13 | 0.63 |
| 1:O:20:VAL:HG12 | 1:O:21:MET:N | 2.14 | 0.63 |
| 1:Y:153:GLU:C | 1:Y:157:ARG:HD3 | 2.18 | 0.63 |
| 1:Y:18:ALA:CB | 1:Y:63:VAL:HG21 | 2.29 | 0.63 |
| 1:Y:229:ILE:CG2 | 1:Y:237:ILE:HG12 | 2.23 | 0.63 |
| 1:Y:9:LEU:HD23 | 1:Y:77:ILE:CG2 | 2.29 | 0.63 |
| 1:Y:40:PRO:HG3 | 1:Y:46:GLU:OE2 | 1.99 | 0.63 |
| 1:Y:62:GLU:O | 1:Y:63:VAL:C | 2.32 | 0.63 |
| 1:O:111:ILE:CD1 | 1:O:142:LYS:HG2 | 2.29 | 0.63 |
| 1:O:80:THR:HG21 | 1:O:248:ALA:CB | 2.27 | 0.63 |
| 1:O:458:ASP:O | 1:O:461:GLN:HB2 | 1.98 | 0.63 |
| 1:O:11:GLN:O | 1:O:81:ASN:HA | 1.98 | 0.63 |
| 1:O:88:VAL:HG13 | 1:O:161:LEU:O | 1.99 | 0.63 |
| 1:Y:182:ASP:HA | 1:Y:218:ARG:O | 1.99 | 0.63 |
| 1:Y:29:SER:OG | 1:Y:63:VAL:HG12 | 1.99 | 0.63 |
| 1:O:267:THR:OG1 | 3:O:601:ACP:H3B1 | 1.98 | 0.62 |
| 1:O:459:GLU:HB2 | 1:O:460:LEU:CD1 | 2.28 | 0.62 |
| 1:Y:257:LYS:O | 1:Y:260:MET:HG2 | 1.98 | 0.62 |
| 1:Y:140:LYS:O | 1:Y:144:ILE:HD12 | 1.99 | 0.62 |
| 1:O:179:HIS:O | 1:O:216:GLU:N | 2.29 | 0.62 |
| 1:O:67:ALA:HB3 | 1:O:69:ILE:CD1 | 2.29 | 0.62 |
| 1:Y:179:HIS:CE1 | 1:Y:215:PRO:HB3 | 2.34 | 0.62 |
| 1:Y:186:ALA:O | 1:Y:187:SER:C | 2.38 | 0.62 |
| 1:Y:14:THR:N | 3:Y:601:ACP:O2G | 2.30 | 0.62 |
| 1:O:166:ASP:OD1 | 1:O:167:THR:N | 2.31 | 0.62 |
| 1:O:208:ASP:O | 1:O:209:ILE:HG13 | 1.99 | 0.62 |
| 1:O:438:VAL:HA | 1:O:441:LEU:CD1 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:447:ALA:O | 1:O:450:ALA:HB3 | 2.00 | 0.62 |
| 1:Y:478:GLU:OE1 | 1:Y:478:GLU:HA | 1.97 | 0.62 |
| 1:O:455:GLN:HG3 | 1:O:455:GLN:O | 1.99 | 0.62 |
| 1:O:91:LYS:HB3 | 1:O:91:LYS:HZ3 | 1.65 | 0.62 |
| 1:Y:120:LEU:HD12 | 1:Y:120:LEU:N | 2.13 | 0.62 |
| 1:Y:53:TRP:CH2 | 1:Y:172:LYS:HB3 | 2.34 | 0.62 |
| 1:Y:211:ARG:CG | 1:Y:211:ARG:HH11 | 2.12 | 0.62 |
| 1:Y:337:GLN:HA | 1:Y:337:GLN:HE21 | 1.64 | 0.62 |
| 1:Y:272:LEU:HG | 1:Y:303:GLU:HB2 | 1.81 | 0.62 |
| 1:O:117:ARG:O | 1:O:119:GLY:N | 2.30 | 0.62 |
| 1:O:164:THR:O | 1:O:166:ASP:N | 2.32 | 0.62 |
| 1:O:350:GLY:HA2 | 1:O:360:ALA:O | 2.00 | 0.62 |
| 1:O:483:TYR:O | 1:O:487:LYS:HG3 | 2.00 | 0.62 |
| 1:Y:87:ILE:HG22 | 1:Y:88:VAL:H | 1.65 | 0.62 |
| 1:O:140:LYS:O | 1:O:143:TRP:N | 2.33 | 0.62 |
| 1:Y:488:LYS:HD2 | 1:O:496:TRP:CH2 | 2.34 | 0.62 |
| 1:Y:16:SER:HB3 | 1:Y:56:GLN:HA | 1.82 | 0.61 |
| 1:Y:344:VAL:HG22 | 1:Y:364:ILE:HD12 | 1.81 | 0.61 |
| 1:O:105:CYS:SG | 1:O:107:ARG:HB3 | 2.40 | 0.61 |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:CA | 2.12 | 0.61 |
| 1:Y:141:VAL:O | 1:Y:144:ILE:HB | 1.99 | 0.61 |
| 1:Y:310:GLY:O | 1:Y:313:ILE:N | 2.33 | 0.61 |
| 1:O:475:GLU:O | 1:O:478:GLU:HB2 | 2.00 | 0.61 |
| 1:Y:257:LYS:N | 1:Y:260:MET:HG3 | 2.14 | 0.61 |
| 1:Y:286:LEU:HD11 | 1:Y:394:ALA:HB1 | 1.81 | 0.61 |
| 1:O:390:ASP:HA | 1:O:483:TYR:OH | 2.00 | 0.61 |
| 1:Y:330:GLU:O | 1:Y:334:THR:HG23 | 2.00 | 0.61 |
| 1:O:226:GLN:HB3 | 1:O:236:ARG:HD3 | 1.81 | 0.61 |
| 1:Y:127:ASN:HD22 | 1:Y:193:ASN:HD21 | 1.47 | 0.61 |
| 1:Y:287:LEU:N | 1:Y:287:LEU:HD23 | 2.15 | 0.61 |
| 1:Y:38:ILE:O | 1:Y:40:PRO:HD3 | 2.00 | 0.61 |
| 1:Y:81:ASN:N | 1:Y:81:ASN:ND2 | 2.42 | 0.61 |
| 1:O:279:ALA:HB2 | 1:O:300:TYR:CD2 | 2.36 | 0.61 |
| 1:Y:114:HIS:O | 1:Y:115:LEU:C | 2.39 | 0.61 |
| 1:O:110:GLU:O | 1:O:113:GLU:HB2 | 2.00 | 0.61 |
| 1:Y:138:GLY:HA2 | 1:Y:191:LEU:CD2 | 2.31 | 0.61 |
| 1:O:202:LYS:O | 1:O:206:VAL:HB | 2.00 | 0.61 |
| 1:Y:442:GLY:O | 1:Y:445:TYR:N | 2.33 | 0.61 |
| 1:O:91:LYS:CB | 1:O:161:LEU:HD12 | 2.29 | 0.61 |
| 1:O:196:THR:HG22 | 1:O:198:ASP:N | 2.16 | 0.61 |
| 1:O:387:GLN:O | 1:O:390:ASP:HB2 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:142:LYS:O | 1:Y:145:LEU:N | 2.34 | 0.61 |
| 1:Y:123:TYR:CD2 | 1:Y:203:MET:HE2 | 2.35 | 0.61 |
| 1:O:164:THR:N | 1:O:167:THR:HB | 2.13 | 0.60 |
| 1:O:213:MET:HG2 | 1:O:214:LEU:HD12 | 1.83 | 0.60 |
| 1:O:63:VAL:CA | 1:O:66:LYS:HG2 | 2.30 | 0.60 |
| 1:Y:152:ARG:CB | 1:Y:156:ARG:HH22 | 2.12 | 0.60 |
| 1:O:216:GLU:HG2 | 1:O:218:ARG:NH1 | 2.17 | 0.60 |
| 1:O:29:SER:OG | 1:O:30:VAL:N | 2.29 | 0.60 |
| 1:Y:123:TYR:OH | 1:Y:202:LYS:HG3 | 2.01 | 0.60 |
| 1:Y:201:ASP:O | 1:Y:202:LYS:C | 2.38 | 0.60 |
| 1:Y:222:GLU:HG3 | 1:Y:223:VAL:N | 2.15 | 0.60 |
| 1:O:262:LYS:HD2 | 1:O:262:LYS:O | 2.01 | 0.60 |
| 1:O:405:ALA:HB1 | 1:O:431:GLU:OE2 | 2.01 | 0.60 |
| 1:Y:118:ASP:HB2 | 1:Y:120:LEU:HD11 | 1.81 | 0.60 |
| 1:Y:179:HIS:CG | 1:Y:215:PRO:HB3 | 2.37 | 0.60 |
| 1:Y:262:LYS:NZ | 1:Y:264:THR:HB | 2.15 | 0.60 |
| 1:Y:283:GLU:OE1 | 1:Y:283:GLU:HA | 2.00 | 0.60 |
| 1:Y:387:GLN:O | 1:Y:391:VAL:HG12 | 2.01 | 0.60 |
| 1:O:142:LYS:HE3 | 1:O:146:ASP:CG | 2.22 | 0.60 |
| 1:Y:477:THR:O | 1:Y:478:GLU:C | 2.39 | 0.60 |
| 1:Y:179:HIS:ND1 | 1:Y:215:PRO:HB3 | 2.16 | 0.60 |
| 1:Y:295:THR:N | 1:Y:297:GLU:OE1 | 2.32 | 0.60 |
| 1:O:111:ILE:HD13 | 1:O:142:LYS:HG2 | 1.82 | 0.60 |
| 1:O:123:TYR:CD2 | 1:O:203:MET:HE2 | 2.36 | 0.60 |
| 1:O:211:ARG:NH1 | 1:O:211:ARG:HG3 | 1.98 | 0.60 |
| 1:O:227:THR:N | 1:O:237:ILE:O | 2.33 | 0.60 |
| 1:O:279:ALA:HB2 | 1:O:300:TYR:CE2 | 2.37 | 0.60 |
| 1:O:85:THR:HA | 1:O:101:ILE:O | 2.01 | 0.60 |
| 1:O:297:GLU:N | 1:O:297:GLU:OE1 | 2.28 | 0.60 |
| 1:Y:257:LYS:O | 1:Y:258:GLU:C | 2.39 | 0.60 |
| 1:O:203:MET:CA | 1:O:206:VAL:HG12 | 2.30 | 0.60 |
| 1:O:90:GLU:N | 1:O:95:LYS:O | 2.29 | 0.60 |
| 1:Y:87:ILE:HD12 | 1:Y:163:GLY:O | 2.02 | 0.60 |
| 1:O:278:LYS:CE | 1:O:280:VAL:HG23 | 2.31 | 0.60 |
| 1:O:90:GLU:HB3 | 1:O:93:THR:CG2 | 2.31 | 0.60 |
| 1:Y:275:THR:OG1 | 1:Y:300:TYR:HB2 | 2.01 | 0.60 |
| 1:Y:388:THR:O | 1:Y:391:VAL:HG13 | 2.01 | 0.60 |
| 1:Y:35:PHE:CB | 1:Y:51:GLU:HG2 | 2.32 | 0.60 |
| 1:Y:81:ASN:HD22 | 1:Y:81:ASN:H | 1.47 | 0.60 |
| 1:O:180:VAL:HG23 | 1:O:216:GLU:O | 2.02 | 0.59 |
| 1:O:84:GLU:HG2 | 1:O:135:TYR:CD1 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:255:CYS:CB | 1:Y:260:MET:HB2 | 2.31 | 0.59 |
| 1:O:130:LEU:O | 1:O:131:VAL:HG23 | 2.02 | 0.59 |
| 1:Y:253:GLN:HE21 | 1:Y:262:LYS:HB2 | 1.67 | 0.59 |
| 1:O:286:LEU:O | 1:O:287:LEU:HD23 | 2.02 | 0.59 |
| 1:O:454:TRP:HD1 | 1:O:459:GLU:CD | 2.06 | 0.59 |
| 1:Y:123:TYR:CE2 | 1:Y:203:MET:HE2 | 2.37 | 0.59 |
| 1:Y:21:MET:CE | 1:Y:444:ALA:HB2 | 2.32 | 0.59 |
| 1:Y:44:TRP:CZ2 | 1:Y:107:ARG:HB2 | 2.37 | 0.59 |
| 1:Y:183:TYR:HE1 | 1:Y:217:VAL:HG12 | 1.62 | 0.59 |
| 1:Y:46:GLU:O | 1:Y:47:HIS:ND1 | 2.32 | 0.59 |
| 1:O:224:TYR:CZ | 1:O:242:ILE:HD12 | 2.37 | 0.59 |
| 1:O:497:GLU:HA | 1:O:497:GLU:OE1 | 2.01 | 0.59 |
| 1:Y:203:MET:O | 1:Y:206:VAL:HG12 | 2.03 | 0.59 |
| 1:Y:261:ALA:HB2 | 1:Y:273:MET:CG | 2.33 | 0.59 |
| 1:Y:20:VAL:HB | 1:Y:28:ILE:HB | 1.84 | 0.59 |
| 1:Y:30:VAL:C | 1:Y:63:VAL:HG13 | 2.22 | 0.59 |
| 1:Y:423:SER:CB | 1:Y:430:VAL:HG23 | 2.32 | 0.59 |
| 1:Y:62:GLU:O | 1:Y:66:LYS:HG2 | 2.02 | 0.59 |
| 1:O:254:LEU:CD1 | 1:O:445:TYR:HE2 | 2.15 | 0.59 |
| 1:O:78:GLY:O | 1:O:79:ILE:HG12 | 2.03 | 0.59 |
| 1:O:89:TRP:HB2 | 1:O:95:LYS:O | 2.02 | 0.59 |
| 1:Y:390:ASP:HA | 1:Y:483:TYR:OH | 2.02 | 0.59 |
| 1:O:246:GLN:NE2 | 1:O:246:GLN:N | 2.50 | 0.59 |
| 1:O:265:TYR:HE1 | 1:O:408:VAL:CG1 | 2.16 | 0.59 |
| 1:O:83:ARG:CB | 4:O:600:GOL:H12 | 2.07 | 0.59 |
| 1:Y:144:ILE:HD12 | 1:Y:144:ILE:H | 1.67 | 0.59 |
| 1:Y:70:SER:H | 1:Y:73:GLN:HE21 | 1.51 | 0.59 |
| 1:O:173:MET:HB3 | 1:O:227:THR:CG2 | 2.32 | 0.59 |
| 1:O:205:GLU:HG2 | 1:O:206:VAL:N | 2.17 | 0.59 |
| 1:O:229:ILE:CG2 | 1:O:237:ILE:HG12 | 2.33 | 0.59 |
| 1:O:27:ILE:H | 1:O:27:ILE:CD1 | 2.01 | 0.59 |
| 1:O:59:THR:O | 1:O:63:VAL:HG23 | 2.03 | 0.59 |
| 1:Y:188:ARG:HH21 | 1:Y:289:THR:HG21 | 1.67 | 0.59 |
| 1:Y:22:ASP:OD1 | 1:Y:24:ASP:N | 2.35 | 0.59 |
| 1:Y:242:ILE:HG22 | 1:Y:243:ALA:H | 1.67 | 0.59 |
| 1:Y:415:ASN:O | 1:Y:419:MET:HG2 | 2.03 | 0.59 |
| 1:O:394:ALA:O | 1:O:395:MET:C | 2.41 | 0.59 |
| 1:Y:148:VAL:HG12 | 1:Y:151:SER:OG | 2.03 | 0.59 |
| 1:Y:48:ASP:O | 1:Y:52:ILE:HD13 | 2.03 | 0.59 |
| 1:O:186:ALA:O | 1:O:187:SER:C | 2.40 | 0.59 |
| 1:O:5:TYR:O | 1:O:75:ALA:N | 2.29 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:247:GLN:N | 1:O:247:GLN:OE1 | 2.36 | 0.58 |
| 1:O:17:ARG:NH2 | 1:O:437:GLU:HG3 | 2.15 | 0.58 |
| 1:Y:240:SER:HB2 | 1:Y:450:ALA:HB3 | 1.85 | 0.58 |
| 1:Y:432:ARG:HD2 | 1:Y:436:ARG:NH2 | 2.17 | 0.58 |
| 1:O:415:ASN:ND2 | 1:O:418:LEU:N | 2.34 | 0.58 |
| 1:Y:317:ARG:HG2 | 1:Y:318:ASP:N | 2.17 | 0.58 |
| 1:O:87:ILE:HD13 | 1:O:168:TRP:CB | 2.33 | 0.58 |
| 1:O:415:ASN:O | 1:O:419:MET:HG2 | 2.02 | 0.58 |
| 1:O:438:VAL:O | 1:O:441:LEU:HB2 | 2.02 | 0.58 |
| 1:O:47:HIS:CB | 1:O:52:ILE:HD11 | 2.25 | 0.58 |
| 1:Y:280:VAL:HG12 | 1:Y:281:LYS:N | 2.19 | 0.58 |
| 1:Y:91:LYS:NZ | 1:Y:91:LYS:HB3 | 2.16 | 0.58 |
| 1:O:345:VAL:O | 1:O:362:GLY:HA2 | 2.03 | 0.58 |
| 1:O:422:GLN:O | 1:O:425:ILE:HG22 | 2.03 | 0.58 |
| 1:O:47:HIS:O | 1:O:99:ASN:HB3 | 2.03 | 0.58 |
| 1:Y:21:MET:HE3 | 1:Y:444:ALA:HB2 | 1.84 | 0.58 |
| 1:Y:48:ASP:C | 1:Y:52:ILE:HD13 | 2.23 | 0.58 |
| 1:Y:372:ASN:O | 1:Y:375:HIS:N | 2.36 | 0.58 |
| 1:O:81:ASN:N | 1:O:81:ASN:ND2 | 2.51 | 0.58 |
| 1:Y:204:LEU:HD22 | 1:Y:209:ILE:O | 2.04 | 0.58 |
| 1:Y:220:SER:O | 1:Y:241:GLY:HA2 | 2.03 | 0.58 |
| 1:Y:458:ASP:O | 1:Y:461:GLN:HB2 | 2.03 | 0.58 |
| 1:Y:118:ASP:OD1 | 1:Y:118:ASP:N | 2.35 | 0.58 |
| 1:O:237:ILE:N | 1:O:237:ILE:HD13 | 2.19 | 0.58 |
| 1:O:50:MET:O | 1:O:53:TRP:HB3 | 2.04 | 0.58 |
| 1:Y:396:GLN:HA | 1:Y:399:SER:HG | 1.69 | 0.58 |
| 1:Y:86:THR:HG23 | 1:Y:162:PHE:HE2 | 1.68 | 0.58 |
| 1:O:115:LEU:CD1 | 1:O:115:LEU:H | 2.14 | 0.58 |
| 1:O:179:HIS:CE1 | 1:O:215:PRO:HB3 | 2.39 | 0.58 |
| 1:O:203:MET:O | 1:O:207:LEU:N | 2.30 | 0.58 |
| 1:Y:104:GLN:CG | 1:Y:349:THR:HG21 | 2.33 | 0.58 |
| 1:Y:293:GLY:N | 1:Y:297:GLU:O | 2.37 | 0.58 |
| 1:Y:445:TYR:O | 1:Y:446:LEU:C | 2.42 | 0.58 |
| 1:Y:432:ARG:O | 1:Y:466:ILE:HG12 | 2.04 | 0.58 |
| 1:Y:31:SER:OG | 1:Y:63:VAL:N | 2.36 | 0.58 |
| 1:Y:70:SER:O | 1:Y:73:GLN:HG3 | 2.04 | 0.58 |
| 1:Y:193:ASN:HB3 | 1:Y:196:THR:HG21 | 1.83 | 0.57 |
| 1:O:142:LYS:O | 1:O:143:TRP:C | 2.41 | 0.57 |
| 1:O:193:ASN:CG | 1:O:196:THR:HB | 2.24 | 0.57 |
| 1:O:314:GLN:O | 1:O:318:ASP:N | 2.37 | 0.57 |
| 1:Y:103:TRP:HA | 1:Y:140:LYS:HE3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:240:SER:HB2 | 1:Y:450:ALA:HB1 | 1.82 | 0.57 |
| 1:Y:128:THR:HB | 1:Y:130:LEU:HB2 | 1.86 | 0.57 |
| 1:O:463:LYS:HZ3 | 1:O:465:VAL:HG23 | 1.69 | 0.57 |
| 1:Y:144:ILE:O | 1:Y:145:LEU:C | 2.42 | 0.57 |
| 1:O:184:THR:HG22 | 1:O:291:ALA:HA | 1.85 | 0.57 |
| 1:O:78:GLY:HA2 | 1:O:447:ALA:HB2 | 1.85 | 0.57 |
| 1:O:83:ARG:HE | 4:O:600:GOL:C2 | 2.16 | 0.57 |
| 1:Y:492:ARG:CG | 1:Y:492:ARG:HH11 | 2.15 | 0.57 |
| 1:O:219:ARG:HG3 | 1:O:296:GLY:O | 2.04 | 0.57 |
| 1:Y:104:GLN:HG3 | 1:Y:349:THR:HG21 | 1.87 | 0.57 |
| 1:Y:172:LYS:O | 1:Y:175:GLN:N | 2.38 | 0.57 |
| 1:Y:20:VAL:C | 1:Y:21:MET:HG3 | 2.24 | 0.57 |
| 1:O:182:ASP:CG | 1:O:242:ILE:HG22 | 2.23 | 0.57 |
| 1:O:382:GLU:O | 1:O:383:SER:C | 2.40 | 0.57 |
| 1:O:423:SER:HB2 | 1:O:430:VAL:HG23 | 1.87 | 0.57 |
| 1:Y:71:SER:HB2 | 1:Y:235:THR:CG2 | 2.35 | 0.57 |
| 1:Y:154:ARG:HB2 | 1:Y:159:GLU:HB3 | 1.86 | 0.57 |
| 1:O:185:ASN:O | 1:O:188:ARG:HB2 | 2.05 | 0.57 |
| 1:O:445:TYR:O | 1:O:448:GLY:N | 2.37 | 0.57 |
| 1:O:89:TRP:HB2 | 1:O:95:LYS:C | 2.24 | 0.57 |
| 1:Y:88:VAL:HG22 | 1:Y:162:PHE:HA | 1.87 | 0.57 |
| 1:O:230:GLY:HA2 | 1:O:235:THR:OG1 | 2.05 | 0.56 |
| 1:O:17:ARG:HG2 | 1:O:32:GLN:HG2 | 1.86 | 0.56 |
| 1:O:253:GLN:HE21 | 1:O:262:LYS:HB3 | 1.68 | 0.56 |
| 1:O:442:GLY:O | 1:O:444:ALA:N | 2.38 | 0.56 |
| 1:O:468:ARG:HD2 | 1:O:469:GLU:N | 2.20 | 0.56 |
| 1:Y:110:GLU:O | 1:Y:113:GLU:N | 2.38 | 0.56 |
| 1:Y:156:ARG:C | 1:Y:158:GLY:H | 2.09 | 0.56 |
| 1:Y:53:TRP:CZ2 | 1:Y:172:LYS:HB3 | 2.39 | 0.56 |
| 1:Y:194:ILE:HG13 | 1:Y:195:HIS:CE1 | 2.40 | 0.56 |
| 1:Y:453:PHE:HD2 | 1:Y:454:TRP:CE3 | 2.23 | 0.56 |
| 1:O:85:THR:OG1 | 1:O:103:TRP:HD1 | 1.89 | 0.56 |
| 1:O:196:THR:N | 1:O:197:LEU:HD22 | 2.21 | 0.56 |
| 1:Y:496:TRP:CH2 | 1:O:488:LYS:HD2 | 2.40 | 0.56 |
| 1:Y:137:SER:HA | 1:Y:140:LYS:HD2 | 1.87 | 0.56 |
| 1:Y:192:PHE:CZ | 1:Y:197:LEU:HA | 2.41 | 0.56 |
| 1:Y:246:GLN:HG2 | 1:Y:270:PHE:HB2 | 1.85 | 0.56 |
| 1:O:203:MET:O | 1:O:206:VAL:HG12 | 2.05 | 0.56 |
| 1:O:256:VAL:HG13 | 1:O:294:PRO:CG | 2.35 | 0.56 |
| 1:Y:110:GLU:O | 1:Y:113:GLU:HB2 | 2.06 | 0.56 |
| 1:Y:181:THR:HG23 | 1:Y:182:ASP:N | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:154:ARG:O | 1:O:159:GLU:HB2 | 2.05 | 0.56 |
| 1:O:83:ARG:HE | 4:O:600:GOL:C1 | 2.19 | 0.56 |
| 1:Y:184:THR:HA | 1:Y:290:ILE:HG22 | 1.88 | 0.56 |
| 1:O:170:ILE:HG22 | 1:O:171:TRP:N | 2.21 | 0.56 |
| 1:O:183:TYR:CB | 1:O:290:ILE:HG21 | 2.36 | 0.56 |
| 1:O:221:SER:HB3 | 1:O:295:THR:O | 2.06 | 0.56 |
| 1:O:83:ARG:HE | 4:O:600:GOL:H12 | 1.70 | 0.56 |
| 1:Y:207:LEU:HB3 | 1:Y:209:ILE:CD1 | 2.36 | 0.56 |
| 1:Y:357:ASP:O | 1:Y:359:TYR:N | 2.39 | 0.56 |
| 1:Y:78:GLY:HA2 | 1:Y:447:ALA:HB2 | 1.88 | 0.56 |
| 1:O:130:LEU:HD13 | 1:O:136:PHE:CD1 | 2.41 | 0.56 |
| 1:O:41:LYS:HG3 | 1:O:42:PRO:CD | 2.35 | 0.56 |
| 1:O:442:GLY:O | 1:O:443:ALA:C | 2.42 | 0.56 |
| 1:O:251:PHE:CE2 | 1:O:446:LEU:HD13 | 2.41 | 0.56 |
| 1:O:484:ALA:O | 1:O:487:LYS:N | 2.36 | 0.56 |
| 1:Y:105:CYS:SG | 1:Y:107:ARG:HB3 | 2.46 | 0.56 |
| 1:Y:71:SER:HB2 | 1:Y:235:THR:HG21 | 1.87 | 0.56 |
| 1:O:20:VAL:O | 1:O:28:ILE:HB | 2.05 | 0.56 |
| 1:Y:262:LYS:O | 1:Y:262:LYS:HD2 | 2.06 | 0.56 |
| 1:Y:154:ARG:HG3 | 1:Y:160:LEU:CD1 | 2.36 | 0.55 |
| 1:Y:21:MET:HE3 | 1:Y:444:ALA:CB | 2.37 | 0.55 |
| 1:Y:246:GLN:HG2 | 1:Y:270:PHE:HB3 | 1.87 | 0.55 |
| 1:O:258:GLU:N | 1:O:274:ASN:HD22 | 2.04 | 0.55 |
| 1:Y:441:LEU:HD22 | 1:Y:445:TYR:HE1 | 1.67 | 0.55 |
| 1:O:448:GLY:O | 1:O:453:PHE:N | 2.35 | 0.55 |
| 1:O:44:TRP:HA | 1:O:105:CYS:SG | 2.46 | 0.55 |
| 1:Y:340:ASN:HB2 | 1:Y:375:HIS:CD2 | 2.42 | 0.55 |
| 1:O:115:LEU:HD12 | 1:O:115:LEU:N | 2.11 | 0.55 |
| 1:O:389:ARG:HA | 1:O:426:LEU:HD11 | 1.88 | 0.55 |
| 1:O:425:ILE:HG22 | 1:O:426:LEU:HD22 | 1.88 | 0.55 |
| 1:O:430:VAL:O | 1:O:469:GLU:HA | 2.06 | 0.55 |
| 1:O:6:ILE:O | 1:O:20:VAL:HG13 | 2.06 | 0.55 |
| 1:Y:111:ILE:HG22 | 1:Y:115:LEU:HD13 | 1.88 | 0.55 |
| 1:Y:21:MET:HA | 1:Y:26:ASN:O | 2.06 | 0.55 |
| 1:Y:498:GLU:OE1 | 1:Y:498:GLU:HA | 2.06 | 0.55 |
| 1:Y:53:TRP:HA | 1:Y:53:TRP:CE3 | 2.41 | 0.55 |
| 1:O:405:ALA:HA | 1:O:429:ARG:O | 2.07 | 0.55 |
| 1:O:97:ILE:O | 1:O:98:TYR:HB2 | 2.07 | 0.55 |
| 1:Y:113:GLU:O | 1:Y:116:LYS:HB2 | 2.06 | 0.55 |
| 1:Y:181:THR:O | 1:Y:218:ARG:N | 2.30 | 0.55 |
| 1:Y:271:MET:C | 1:Y:272:LEU:HD12 | 2.26 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:351:LEU:HB2 | 1:Y:357:ASP:H | 1.72 | 0.55 |
| 1:Y:40:PRO:HG2 | 1:Y:44:TRP:HB3 | 1.87 | 0.55 |
| 1:O:254:LEU:HD11 | 1:O:445:TYR:CE2 | 2.40 | 0.55 |
| 1:Y:227:THR:N | 1:Y:237:ILE:O | 2.28 | 0.55 |
| 1:Y:265:TYR:HE1 | 1:Y:408:VAL:CG1 | 2.19 | 0.55 |
| 1:Y:425:ILE:HD12 | 1:Y:479:ARG:HG2 | 1.89 | 0.55 |
| 1:O:137:SER:O | 1:O:139:THR:N | 2.39 | 0.55 |
| 1:O:286:LEU:HD11 | 1:O:394:ALA:HB3 | 1.89 | 0.55 |
| 1:Y:286:LEU:HD11 | 1:Y:395:MET:N | 2.22 | 0.55 |
| 1:Y:392:LEU:O | 1:Y:395:MET:HB3 | 2.07 | 0.55 |
| 1:O:430:VAL:O | 1:O:470:PHE:N | 2.29 | 0.55 |
| 1:Y:279:ALA:HB2 | 1:Y:300:TYR:CE2 | 2.40 | 0.55 |
| 1:Y:445:TYR:O | 1:Y:448:GLY:N | 2.39 | 0.55 |
| 1:O:80:THR:HG22 | 1:O:245:ASP:N | 2.22 | 0.55 |
| 1:Y:164:THR:O | 1:Y:165:VAL:C | 2.45 | 0.55 |
| 1:Y:404:HIS:O | 1:Y:429:ARG:HD2 | 2.07 | 0.55 |
| 1:Y:91:LYS:HZ3 | 1:Y:91:LYS:HB3 | 1.71 | 0.55 |
| 1:O:275:THR:HG1 | 1:O:300:TYR:HB2 | 1.72 | 0.54 |
| 1:O:463:LYS:NZ | 1:O:465:VAL:HG23 | 2.21 | 0.54 |
| 1:Y:18:ALA:HB3 | 1:Y:63:VAL:HG21 | 1.87 | 0.54 |
| 1:Y:368:THR:HG23 | 1:Y:369:ARG:N | 2.20 | 0.54 |
| 1:Y:415:ASN:HD22 | 1:Y:418:LEU:H | 1.52 | 0.54 |
| 1:O:170:ILE:HA | 1:O:173:MET:HG3 | 1.89 | 0.54 |
| 1:O:193:ASN:O | 1:O:197:LEU:N | 2.40 | 0.54 |
| 1:Y:87:ILE:HD13 | 1:Y:168:TRP:HB2 | 1.88 | 0.54 |
| 1:Y:189:THR:HB | 1:Y:191:LEU:CG | 2.35 | 0.54 |
| 1:Y:344:VAL:CG2 | 1:Y:364:ILE:HG23 | 2.37 | 0.54 |
| 1:Y:85:THR:OG1 | 1:Y:103:TRP:HD1 | 1.90 | 0.54 |
| 1:O:258:GLU:HA | 1:O:274:ASN:O | 2.07 | 0.54 |
| 1:Y:228:ASN:HD21 | 1:Y:235:THR:N | 2.05 | 0.54 |
| 1:Y:424:ASP:OD1 | 1:Y:473:GLY:N | 2.29 | 0.54 |
| 1:Y:63:VAL:HA | 1:Y:66:LYS:CD | 2.38 | 0.54 |
| 1:Y:11:GLN:HE22 | 1:Y:82:GLN:HE21 | 1.55 | 0.54 |
| 1:O:150:GLY:HA3 | 1:O:154:ARG:HD2 | 1.89 | 0.54 |
| 1:O:265:TYR:HE1 | 1:O:408:VAL:HG12 | 1.72 | 0.54 |
| 1:Y:141:VAL:C | 1:Y:145:LEU:HD22 | 2.27 | 0.54 |
| 1:Y:460:LEU:H | 1:Y:460:LEU:CD1 | 1.98 | 0.54 |
| 1:O:162:PHE:HB3 | 1:O:213:MET:HG3 | 1.90 | 0.54 |
| 1:O:35:PHE:HB2 | 1:O:51:GLU:CG | 2.33 | 0.54 |
| 1:Y:41:LYS:O | 1:Y:44:TRP:HB2 | 2.08 | 0.54 |
| 1:O:249:ALA:HB2 | 1:O:439:THR:OG1 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:218:ARG:HG3 | 1:Y:218:ARG:NH1 | 2.23 | 0.54 |
| 1:Y:53:TRP:HA | 1:Y:53:TRP:HE3 | 1.72 | 0.54 |
| 1:O:101:ILE:HD13 | 1:O:107:ARG:CZ | 2.37 | 0.54 |
| 1:O:240:SER:HB2 | 1:O:450:ALA:HB3 | 1.89 | 0.54 |
| 1:Y:138:GLY:HA2 | 1:Y:191:LEU:HD21 | 1.88 | 0.54 |
| 1:Y:413:VAL:CB | 1:Y:419:MET:HE3 | 2.38 | 0.54 |
| 1:O:142:LYS:HE3 | 1:O:146:ASP:OD2 | 2.07 | 0.54 |
| 1:O:20:VAL:HB | 1:O:28:ILE:HB | 1.89 | 0.54 |
| 1:Y:38:ILE:O | 1:Y:45:VAL:HA | 2.08 | 0.54 |
| 1:O:139:THR:OG1 | 1:O:140:LYS:N | 2.41 | 0.54 |
| 1:O:88:VAL:HA | 1:O:161:LEU:O | 2.08 | 0.54 |
| 1:Y:29:SER:OG | 1:Y:30:VAL:N | 2.42 | 0.54 |
| 1:Y:286:LEU:HD21 | 1:Y:394:ALA:CB | 2.37 | 0.54 |
| 1:Y:445:TYR:O | 1:Y:447:ALA:N | 2.41 | 0.54 |
| 1:O:41:LYS:CG | 1:O:42:PRO:HD2 | 2.37 | 0.53 |
| 1:Y:203:MET:O | 1:Y:207:LEU:HB2 | 2.08 | 0.53 |
| 1:Y:86:THR:HG23 | 1:Y:162:PHE:CE2 | 2.43 | 0.53 |
| 1:Y:170:ILE:O | 1:Y:171:TRP:C | 2.45 | 0.53 |
| 1:Y:227:THR:O | 1:Y:236:ARG:HA | 2.08 | 0.53 |
| 1:Y:80:THR:HG22 | 1:Y:243:ALA:O | 2.08 | 0.53 |
| 1:Y:28:ILE:HD13 | 1:Y:28:ILE:N | 2.21 | 0.53 |
| 1:Y:332:PHE:O | 1:Y:335:LYS:HB2 | 2.09 | 0.53 |
| 1:Y:416:ASN:O | 1:Y:417:PHE:C | 2.46 | 0.53 |
| 1:Y:446:LEU:O | 1:Y:450:ALA:HB2 | 2.08 | 0.53 |
| 1:O:272:LEU:N | 1:O:272:LEU:HD12 | 2.23 | 0.53 |
| 1:O:280:VAL:HG13 | 1:O:281:LYS:N | 2.23 | 0.53 |
| 1:Y:325:ASP:O | 1:Y:326:ALA:C | 2.44 | 0.53 |
| 1:Y:498:GLU:OE2 | 1:O:488:LYS:HE3 | 2.08 | 0.53 |
| 1:Y:18:ALA:HB3 | 1:Y:63:VAL:CG2 | 2.38 | 0.53 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:HG21 | 1.89 | 0.53 |
| 1:Y:246:GLN:CG | 1:Y:270:PHE:HB2 | 2.38 | 0.53 |
| 1:Y:422:GLN:HE21 | 1:Y:426:LEU:HD22 | 1.74 | 0.53 |
| 1:Y:137:SER:O | 1:Y:140:LYS:N | 2.42 | 0.53 |
| 1:O:219:ARG:HG2 | 1:O:221:SER:H | 1.74 | 0.53 |
| 1:O:363:ALA:HB3 | 1:O:365:PHE:CE1 | 2.43 | 0.53 |
| 1:Y:17:ARG:HH22 | 1:Y:437:GLU:HG3 | 1.72 | 0.53 |
| 1:O:207:LEU:HB3 | 1:O:209:ILE:HD11 | 1.89 | 0.53 |
| 1:O:220:SER:HB2 | 1:O:292:CYS:SG | 2.48 | 0.53 |
| 1:O:293:GLY:O | 1:O:295:THR:N | 2.42 | 0.53 |
| 1:O:401:ILE:HG22 | 1:O:402:ARG:N | 2.23 | 0.53 |
| 1:Y:127:ASN:ND2 | 1:Y:193:ASN:HD21 | 2.06 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:152:ARG:HB3 | 1:Y:156:ARG:NH2 | 2.14 | 0.53 |
| 1:Y:201:ASP:HA | 1:Y:204:LEU:HB2 | 1.91 | 0.53 |
| 1:Y:372:ASN:OD1 | 1:Y:374:ASN:HB2 | 2.09 | 0.53 |
| 1:Y:405:ALA:HB1 | 1:Y:431:GLU:OE2 | 2.07 | 0.53 |
| 1:Y:451:VAL:O | 1:Y:451:VAL:HG13 | 2.07 | 0.53 |
| 1:O:198:ASP:C | 1:O:199:TRP:O | 2.43 | 0.53 |
| 1:O:63:VAL:HA | 1:O:66:LYS:CG | 2.33 | 0.53 |
| 1:Y:111:ILE:CG2 | 1:Y:115:LEU:HD13 | 2.39 | 0.53 |
| 1:O:460:LEU:CD1 | 1:O:460:LEU:H | 1.96 | 0.53 |
| 1:Y:416:ASN:OD1 | 1:Y:432:ARG:NH1 | 2.30 | 0.53 |
| 1:Y:441:LEU:O | 1:Y:444:ALA:HB3 | 2.09 | 0.53 |
| 1:O:434:GLU:OE1 | 1:O:465:VAL:HB | 2.08 | 0.53 |
| 1:O:490:VAL:O | 1:O:494:MET:HG2 | 2.09 | 0.53 |
| 1:O:183:TYR:HB3 | 1:O:290:ILE:HG21 | 1.91 | 0.52 |
| 1:Y:67:ALA:HB3 | 1:Y:69:ILE:CD1 | 2.38 | 0.52 |
| 1:O:156:ARG:C | 1:O:158:GLY:H | 2.13 | 0.52 |
| 1:O:244:GLY:O | 1:O:245:ASP:C | 2.44 | 0.52 |
| 1:O:253:GLN:NE2 | 1:O:262:LYS:HB2 | 2.21 | 0.52 |
| 1:O:263:ASN:HB2 | 1:O:406:LEU:HD11 | 1.91 | 0.52 |
| 1:Y:271:MET:HG2 | 1:Y:395:MET:HE2 | 1.90 | 0.52 |
| 1:Y:423:SER:HB2 | 1:Y:428:THR:O | 2.10 | 0.52 |
| 1:Y:420:GLN:HE21 | 1:Y:424:ASP:CG | 2.12 | 0.52 |
| 1:O:123:TYR:HD2 | 1:O:203:MET:CE | 2.22 | 0.52 |
| 1:O:140:LYS:O | 1:O:141:VAL:C | 2.48 | 0.52 |
| 1:O:142:LYS:O | 1:O:145:LEU:N | 2.43 | 0.52 |
| 1:Y:113:GLU:HA | 1:Y:113:GLU:OE1 | 2.08 | 0.52 |
| 1:O:422:GLN:O | 1:O:426:LEU:HD22 | 2.10 | 0.52 |
| 1:Y:146:ASP:HB3 | 1:Y:152:ARG:HH12 | 1.74 | 0.52 |
| 1:O:228:ASN:HD21 | 1:O:235:THR:N | 2.07 | 0.52 |
| 1:O:453:PHE:HD2 | 1:O:454:TRP:CZ3 | 2.28 | 0.52 |
| 1:Y:22:ASP:O | 1:Y:25:ALA:N | 2.31 | 0.52 |
| 1:Y:295:THR:HG23 | 1:Y:297:GLU:OE1 | 2.09 | 0.52 |
| 1:Y:308:MET:HB2 | 1:Y:346:PRO:HB2 | 1.91 | 0.52 |
| 1:Y:483:TYR:O | 1:Y:486:TRP:HB3 | 2.09 | 0.52 |
| 1:O:142:LYS:HG3 | 1:O:143:TRP:N | 2.24 | 0.52 |
| 1:O:60:LEU:HD12 | 1:O:60:LEU:C | 2.30 | 0.52 |
| 1:Y:164:THR:O | 1:Y:167:THR:N | 2.42 | 0.52 |
| 1:Y:205:GLU:O | 1:Y:206:VAL:C | 2.43 | 0.52 |
| 1:Y:50:MET:O | 1:Y:53:TRP:HB3 | 2.09 | 0.52 |
| 1:O:154:ARG:HA | 1:O:159:GLU:OE1 | 2.10 | 0.52 |
| 1:O:65:ALA:O | 1:O:68:ASP:N | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:9:LEU:HB2 | 1:O:79:ILE:HD13 | 1.91 | 0.52 |
| 1:Y:154:ARG:HA | 1:Y:157:ARG:CG | 2.40 | 0.52 |
| 1:O:172:LYS:N | 1:O:172:LYS:HD2 | 2.25 | 0.52 |
| 1:O:415:ASN:HB3 | 1:O:418:LEU:HB2 | 1.92 | 0.52 |
| 1:Y:151:SER:O | 1:Y:153:GLU:N | 2.43 | 0.52 |
| 1:Y:78:GLY:C | 1:Y:79:ILE:HG12 | 2.29 | 0.52 |
| 1:O:67:ALA:HB3 | 1:O:69:ILE:HD12 | 1.91 | 0.52 |
| 1:Y:91:LYS:O | 1:Y:93:THR:N | 2.43 | 0.52 |
| 1:Y:102:VAL:O | 1:Y:103:TRP:C | 2.47 | 0.51 |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CD1 | 2.45 | 0.51 |
| 1:Y:87:ILE:HG22 | 1:Y:88:VAL:N | 2.25 | 0.51 |
| 1:O:116:LYS:HG2 | 1:O:132:ILE:HG21 | 1.92 | 0.51 |
| 1:O:330:GLU:O | 1:O:334:THR:HG23 | 2.09 | 0.51 |
| 1:O:14:THR:N | 3:O:601:ACP:O3G | 2.43 | 0.51 |
| 1:Y:144:ILE:HG22 | 1:Y:145:LEU:N | 2.24 | 0.51 |
| 1:Y:272:LEU:HD11 | 1:Y:303:GLU:HG3 | 1.92 | 0.51 |
| 1:Y:12:GLY:HA3 | 3:Y:601:ACP:O3G | 2.11 | 0.51 |
| 1:O:188:ARG:NH2 | 1:O:289:THR:HG21 | 2.21 | 0.51 |
| 1:O:298:VAL:HG12 | 1:O:299:ASN:N | 2.25 | 0.51 |
| 1:O:80:THR:CG2 | 1:O:248:ALA:HB2 | 2.41 | 0.51 |
| 1:Y:16:SER:HB3 | 1:Y:56:GLN:OE1 | 2.10 | 0.51 |
| 1:O:261:ALA:HB2 | 1:O:273:MET:CG | 2.39 | 0.51 |
| 1:O:271:MET:O | 1:O:272:LEU:HD12 | 2.11 | 0.51 |
| 1:O:38:ILE:O | 1:O:40:PRO:HD3 | 2.11 | 0.51 |
| 1:Y:423:SER:HB2 | 1:Y:430:VAL:HG23 | 1.91 | 0.51 |
| 1:O:409:ASP:C | 1:O:413:VAL:HG11 | 2.30 | 0.51 |
| 1:Y:130:LEU:HD12 | 1:Y:190:MET:HB2 | 1.91 | 0.51 |
| 1:Y:235:THR:O | 1:Y:237:ILE:HD13 | 2.11 | 0.51 |
| 1:O:193:ASN:OD1 | 1:O:196:THR:HB | 2.10 | 0.51 |
| 1:O:455:GLN:O | 1:O:456:ASN:HB2 | 2.09 | 0.51 |
| 1:O:144:ILE:O | 1:O:145:LEU:C | 2.49 | 0.51 |
| 1:O:218:ARG:HH11 | 1:O:218:ARG:CG | 2.24 | 0.51 |
| 1:O:278:LYS:HG2 | 1:O:278:LYS:O | 2.09 | 0.51 |
| 1:O:438:VAL:HG12 | 1:O:439:THR:N | 2.24 | 0.51 |
| 1:O:482:ARG:CG | 1:O:482:ARG:HH11 | 2.24 | 0.51 |
| 1:Y:172:LYS:O | 1:Y:173:MET:C | 2.49 | 0.51 |
| 1:Y:33:ARG:NE | 1:Y:58:TRP:CE3 | 2.79 | 0.51 |
| 1:O:154:ARG:O | 1:O:159:GLU:N | 2.30 | 0.51 |
| 1:Y:432:ARG:HB3 | 1:Y:468:ARG:HB3 | 1.93 | 0.51 |
| 1:Y:89:TRP:HB2 | 1:Y:95:LYS:O | 2.10 | 0.51 |
| 1:Y:89:TRP:HD1 | 1:Y:90:GLU:O | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:38:ILE:O | 1:O:45:VAL:HA | 2.10 | 0.51 |
| 1:O:77:ILE:HG22 | 1:O:239:ILE:HG23 | 1.93 | 0.51 |
| 1:Y:115:LEU:N | 1:Y:115:LEU:HD12 | 2.24 | 0.51 |
| 1:Y:179:HIS:CE1 | 1:Y:215:PRO:HG3 | 2.46 | 0.51 |
| 1:Y:89:TRP:HB2 | 1:Y:95:LYS:C | 2.32 | 0.51 |
| 1:O:41:LYS:CB | 1:O:42:PRO:HD2 | 2.41 | 0.51 |
| 1:O:56:GLN:O | 1:O:59:THR:HB | 2.11 | 0.51 |
| 1:Y:352:GLY:O | 1:Y:353:ALA:C | 2.44 | 0.51 |
| 1:Y:422:GLN:NE2 | 1:Y:426:LEU:HD22 | 2.25 | 0.51 |
| 1:O:359:TYR:CZ | 1:O:499:HIS:CE1 | 2.99 | 0.50 |
| 1:O:445:TYR:O | 1:O:446:LEU:C | 2.48 | 0.50 |
| 1:Y:124:ILE:CG1 | 1:Y:203:MET:HE3 | 2.40 | 0.50 |
| 1:Y:222:GLU:O | 1:Y:240:SER:HA | 2.11 | 0.50 |
| 1:O:114:HIS:CD2 | 1:O:117:ARG:NH2 | 2.79 | 0.50 |
| 1:O:137:SER:O | 1:O:138:GLY:O | 2.29 | 0.50 |
| 1:O:142:LYS:O | 1:O:146:ASP:OD1 | 2.29 | 0.50 |
| 1:O:185:ASN:ND2 | 1:O:244:GLY:N | 2.59 | 0.50 |
| 1:O:283:GLU:HA | 1:O:283:GLU:OE1 | 2.10 | 0.50 |
| 1:O:453:PHE:HD2 | 1:O:454:TRP:CE3 | 2.29 | 0.50 |
| 1:Y:108:THR:HG1 | 1:Y:139:THR:HG1 | 1.57 | 0.50 |
| 1:Y:237:ILE:N | 1:Y:237:ILE:HD13 | 2.26 | 0.50 |
| 1:Y:456:ASN:O | 1:Y:459:GLU:OE2 | 2.29 | 0.50 |
| 1:Y:491:LYS:O | 1:Y:493:ALA:N | 2.44 | 0.50 |
| 1:Y:91:LYS:HB2 | 1:Y:161:LEU:CD1 | 2.34 | 0.50 |
| 1:O:163:GLY:HA3 | 1:O:167:THR:HB | 1.94 | 0.50 |
| 1:O:182:ASP:OD1 | 1:O:185:ASN:HB2 | 2.12 | 0.50 |
| 1:O:428:THR:HG23 | 1:O:429:ARG:N | 2.26 | 0.50 |
| 1:Y:242:ILE:HG22 | 1:Y:243:ALA:N | 2.25 | 0.50 |
| 1:O:184:THR:HA | 1:O:290:ILE:HG22 | 1.94 | 0.50 |
| 1:Y:170:ILE:HA | 1:Y:173:MET:HG3 | 1.93 | 0.50 |
| 1:Y:253:GLN:HE21 | 1:Y:262:LYS:CB | 2.23 | 0.50 |
| 1:Y:267:THR:CB | 3:Y:601:ACP:H3B2 | 2.42 | 0.50 |
| 1:Y:453:PHE:CD2 | 1:Y:454:TRP:CZ3 | 2.99 | 0.50 |
| 1:Y:5:TYR:O | 1:Y:75:ALA:N | 2.33 | 0.50 |
| 1:O:103:TRP:N | 1:O:103:TRP:CD1 | 2.80 | 0.50 |
| 1:O:95:LYS:HG3 | 1:O:96:PRO:N | 2.25 | 0.50 |
| 1:Y:12:GLY:O | 1:Y:35:PHE:HZ | 1.95 | 0.50 |
| 1:Y:211:ARG:NH1 | 1:Y:211:ARG:HG3 | 2.15 | 0.50 |
| 1:Y:257:LYS:CA | 1:Y:274:ASN:HD22 | 2.24 | 0.50 |
| 1:Y:63:VAL:O | 1:Y:64:LEU:O | 2.29 | 0.50 |
| 1:O:101:ILE:HD13 | 1:O:107:ARG:NE | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:163:GLY:CA | 1:O:167:THR:HB | 2.42 | 0.50 |
| 1:O:263:ASN:ND2 | 1:O:265:TYR:CE1 | 2.80 | 0.50 |
| 1:O:44:TRP:CE3 | 1:O:107:ARG:NH2 | 2.80 | 0.50 |
| 1:O:37:GLN:NE2 | 1:O:47:HIS:CE1 | 2.80 | 0.50 |
| 1:O:153:GLU:O | 1:O:157:ARG:HD3 | 2.12 | 0.50 |
| 1:O:310:GLY:HA3 | 3:O:601:ACP:O3' | 2.10 | 0.50 |
| 1:Y:114:HIS:O | 1:Y:117:ARG:N | 2.44 | 0.50 |
| 1:Y:3:LYS:HG3 | 1:Y:73:GLN:CA | 2.41 | 0.50 |
| 1:Y:444:ALA:O | 1:Y:445:TYR:O | 2.30 | 0.50 |
| 1:Y:3:LYS:HG3 | 1:Y:73:GLN:HA | 1.93 | 0.50 |
| 1:O:123:TYR:CE2 | 1:O:203:MET:HE2 | 2.47 | 0.50 |
| 1:O:144:ILE:HD12 | 1:O:144:ILE:N | 2.10 | 0.50 |
| 1:O:278:LYS:HD2 | 1:O:280:VAL:HG23 | 1.93 | 0.50 |
| 1:O:348:PHE:CD1 | 1:O:348:PHE:N | 2.79 | 0.50 |
| 1:O:386:TYR:HB3 | 1:O:486:TRP:CD2 | 2.45 | 0.50 |
| 1:Y:257:LYS:H | 1:Y:260:MET:CG | 2.19 | 0.50 |
| 1:Y:343:TYR:CD2 | 1:Y:486:TRP:HA | 2.47 | 0.50 |
| 1:Y:74:ILE:HD11 | 1:Y:237:ILE:HG21 | 1.94 | 0.50 |
| 1:O:148:VAL:HG12 | 1:O:151:SER:HB3 | 1.92 | 0.50 |
| 1:O:198:ASP:O | 1:O:199:TRP:O | 2.30 | 0.50 |
| 1:O:44:TRP:N | 1:O:44:TRP:CD1 | 2.79 | 0.50 |
| 1:Y:188:ARG:NH2 | 1:Y:289:THR:HG21 | 2.26 | 0.50 |
| 1:Y:87:ILE:O | 1:Y:88:VAL:HG23 | 2.11 | 0.50 |
| 1:Y:90:GLU:N | 1:Y:95:LYS:O | 2.36 | 0.50 |
| 1:O:11:GLN:NE2 | 1:O:82:GLN:HG2 | 2.27 | 0.49 |
| 1:O:138:GLY:O | 1:O:141:VAL:HG23 | 2.12 | 0.49 |
| 1:O:166:ASP:O | 1:O:167:THR:C | 2.51 | 0.49 |
| 1:O:200:ASP:O | 1:O:201:ASP:C | 2.50 | 0.49 |
| 1:O:237:ILE:CG2 | 1:O:238:PRO:HD2 | 2.42 | 0.49 |
| 1:O:457:LEU:HD22 | 1:O:460:LEU:HD13 | 1.93 | 0.49 |
| 1:Y:114:HIS:N | 1:Y:114:HIS:CD2 | 2.78 | 0.49 |
| 1:Y:203:MET:CA | 1:Y:206:VAL:HG12 | 2.42 | 0.49 |
| 1:Y:253:GLN:HG3 | 1:Y:407:ARG:HD2 | 1.94 | 0.49 |
| 1:Y:44:TRP:CD1 | 1:Y:44:TRP:N | 2.78 | 0.49 |
| 1:O:202:LYS:HA | 1:O:205:GLU:OE2 | 2.12 | 0.49 |
| 1:O:275:THR:OG1 | 1:O:300:TYR:HB2 | 2.12 | 0.49 |
| 1:O:326:ALA:O | 1:O:327:TYR:C | 2.49 | 0.49 |
| 1:Y:88:VAL:HG22 | 1:Y:162:PHE:CB | 2.43 | 0.49 |
| 1:Y:298:VAL:O | 1:Y:299:ASN:OD1 | 2.30 | 0.49 |
| 1:Y:344:VAL:HG22 | 1:Y:364:ILE:HG23 | 1.94 | 0.49 |
| 1:Y:77:ILE:N | 1:Y:238:PRO:O | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:153:GLU:HA | 1:O:156:ARG:NH1 | 2.27 | 0.49 |
| 1:O:325:ASP:O | 1:O:328:ASP:HB2 | 2.12 | 0.49 |
| 1:O:488:LYS:O | 1:O:492:ARG:HD3 | 2.12 | 0.49 |
| 1:Y:445:TYR:CD2 | 1:Y:457:LEU:HD11 | 2.48 | 0.49 |
| 1:Y:70:SER:N | 1:Y:73:GLN:HE21 | 2.08 | 0.49 |
| 1:O:22:ASP:OD2 | 1:O:26:ASN:HB2 | 2.11 | 0.49 |
| 1:O:83:ARG:HE | 4:O:600:GOL:H2 | 1.78 | 0.49 |
| 1:Y:229:ILE:HG23 | 1:Y:237:ILE:CD1 | 2.43 | 0.49 |
| 1:Y:271:MET:O | 1:Y:272:LEU:HD12 | 2.12 | 0.49 |
| 1:Y:455:GLN:O | 1:Y:456:ASN:OD1 | 2.30 | 0.49 |
| 1:O:155:ALA:CB | 1:O:210:PRO:HG2 | 2.38 | 0.49 |
| 1:O:199:TRP:CG | 1:O:214:LEU:HD23 | 2.47 | 0.49 |
| 1:O:375:HIS:O | 1:O:376:ILE:C | 2.50 | 0.49 |
| 1:Y:173:MET:C | 1:Y:175:GLN:H | 2.15 | 0.49 |
| 1:Y:454:TRP:HD1 | 1:Y:459:GLU:CD | 2.15 | 0.49 |
| 1:O:420:GLN:HE21 | 1:O:424:ASP:CG | 2.16 | 0.49 |
| 1:Y:256:VAL:CG1 | 1:Y:294:PRO:HG3 | 2.42 | 0.49 |
| 1:Y:441:LEU:CD2 | 1:Y:445:TYR:HE1 | 2.26 | 0.49 |
| 1:Y:220:SER:O | 1:Y:446:LEU:HD23 | 2.12 | 0.49 |
| 1:O:21:MET:HB3 | 1:O:26:ASN:O | 2.13 | 0.49 |
| 1:O:272:LEU:HG | 1:O:303:GLU:HB2 | 1.94 | 0.49 |
| 1:O:271:MET:CG | 1:O:395:MET:HE2 | 2.37 | 0.49 |
| 1:O:422:GLN:NE2 | 1:O:426:LEU:HD21 | 2.28 | 0.49 |
| 1:O:54:ALA:O | 1:O:55:THR:C | 2.49 | 0.49 |
| 1:O:7:VAL:HG12 | 1:O:9:LEU:HD22 | 1.95 | 0.49 |
| 1:Y:205:GLU:C | 1:Y:208:ASP:H | 2.16 | 0.49 |
| 1:Y:324:ASN:ND2 | 1:Y:324:ASN:N | 2.61 | 0.49 |
| 1:Y:31:SER:CB | 1:Y:59:THR:HA | 2.28 | 0.49 |
| 1:Y:86:THR:HG22 | 1:Y:87:ILE:N | 2.27 | 0.49 |
| 1:O:108:THR:HG21 | 1:O:140:LYS:HA | 1.95 | 0.49 |
| 1:O:264:THR:HA | 1:O:409:ASP:O | 2.13 | 0.49 |
| 1:O:91:LYS:O | 1:O:92:GLU:O | 2.30 | 0.49 |
| 1:O:39:TYR:HA | 1:O:44:TRP:O | 2.12 | 0.49 |
| 1:O:451:VAL:O | 1:O:452:GLY:C | 2.46 | 0.49 |
| 1:Y:123:TYR:HD2 | 1:Y:203:MET:CE | 2.26 | 0.49 |
| 1:Y:261:ALA:HB2 | 1:Y:273:MET:HG3 | 1.94 | 0.49 |
| 1:Y:7:VAL:O | 1:Y:77:ILE:HA | 2.13 | 0.49 |
| 1:O:48:ASP:O | 1:O:51:GLU:N | 2.46 | 0.49 |
| 1:Y:133:ASP:OD1 | 1:Y:135:TYR:HB2 | 2.12 | 0.49 |
| 1:Y:408:VAL:O | 1:Y:409:ASP:HB3 | 2.13 | 0.49 |
| 1:O:196:THR:HG22 | 1:O:198:ASP:H | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:219:ARG:HG2 | 1:O:220:SER:N | 2.28 | 0.48 |
| 1:O:451:VAL:HG13 | 1:O:451:VAL:O | 2.11 | 0.48 |
| 1:O:91:LYS:HG2 | 1:O:92:GLU:N | 2.26 | 0.48 |
| 1:Y:218:ARG:HH11 | 1:Y:218:ARG:CG | 2.25 | 0.48 |
| 1:Y:261:ALA:HB2 | 1:Y:273:MET:HG2 | 1.95 | 0.48 |
| 1:Y:69:ILE:HG22 | 1:Y:70:SER:N | 2.28 | 0.48 |
| 1:O:141:VAL:C | 1:O:145:LEU:HD22 | 2.34 | 0.48 |
| 1:Y:166:ASP:OD2 | 1:Y:185:ASN:OD1 | 2.31 | 0.48 |
| 1:Y:391:VAL:O | 1:Y:394:ALA:HB3 | 2.12 | 0.48 |
| 1:O:199:TRP:CD2 | 1:O:214:LEU:HD23 | 2.48 | 0.48 |
| 1:O:389:ARG:O | 1:O:392:LEU:N | 2.46 | 0.48 |
| 1:Y:185:ASN:O | 1:Y:188:ARG:HB2 | 2.13 | 0.48 |
| 1:O:113:GLU:O | 1:O:117:ARG:HD3 | 2.13 | 0.48 |
| 1:O:481:TYR:O | 1:O:484:ALA:HB3 | 2.13 | 0.48 |
| 1:Y:146:ASP:OD1 | 1:Y:146:ASP:N | 2.39 | 0.48 |
| 1:Y:348:PHE:CD1 | 1:Y:348:PHE:N | 2.78 | 0.48 |
| 1:Y:9:LEU:CD2 | 1:Y:77:ILE:HG23 | 2.41 | 0.48 |
| 1:O:201:ASP:O | 1:O:202:LYS:C | 2.52 | 0.48 |
| 1:O:221:SER:HB2 | 1:O:296:GLY:HA3 | 1.92 | 0.48 |
| 1:O:387:GLN:O | 1:O:388:THR:C | 2.51 | 0.48 |
| 1:O:93:THR:OG1 | 1:O:95:LYS:HB3 | 2.12 | 0.48 |
| 1:Y:142:LYS:HG3 | 1:Y:143:TRP:N | 2.27 | 0.48 |
| 1:Y:54:ALA:O | 1:Y:57:SER:HB2 | 2.13 | 0.48 |
| 1:O:124:ILE:HG12 | 1:O:203:MET:CE | 2.43 | 0.48 |
| 1:O:40:PRO:HD2 | 1:O:44:TRP:O | 2.14 | 0.48 |
| 1:O:132:ILE:O | 1:O:133:ASP:HB2 | 2.11 | 0.48 |
| 1:O:150:GLY:HA3 | 1:O:154:ARG:CD | 2.43 | 0.48 |
| 1:O:263:ASN:ND2 | 1:O:265:TYR:CZ | 2.80 | 0.48 |
| 1:Y:17:ARG:HD3 | 1:Y:32:GLN:NE2 | 2.26 | 0.48 |
| 1:Y:17:ARG:HG2 | 1:Y:32:GLN:HG2 | 1.95 | 0.48 |
| 1:Y:271:MET:HE1 | 1:Y:392:LEU:HB2 | 1.96 | 0.48 |
| 1:O:61:VAL:O | 1:O:62:GLU:C | 2.51 | 0.48 |
| 1:Y:128:THR:C | 1:Y:130:LEU:H | 2.17 | 0.48 |
| 1:Y:22:ASP:O | 1:Y:23:HIS:C | 2.51 | 0.48 |
| 1:O:276:GLY:HA2 | 1:O:299:ASN:HD22 | 1.77 | 0.48 |
| 1:O:462:GLU:C | 1:O:464:ALA:H | 2.15 | 0.48 |
| 1:O:90:GLU:HB2 | 1:O:93:THR:OG1 | 2.14 | 0.48 |
| 1:Y:222:GLU:HG3 | 1:Y:223:VAL:H | 1.79 | 0.48 |
| 1:O:278:LYS:HG3 | 1:O:279:ALA:N | 2.27 | 0.48 |
| 1:Y:227:THR:O | 1:Y:237:ILE:N | 2.34 | 0.48 |
| 1:Y:50:MET:O | 1:Y:51:GLU:C | 2.51 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:140:LYS:O | 1:O:144:ILE:HD12 | 2.14 | 0.47 |
| 1:O:154:ARG:CA | 1:O:159:GLU:HB2 | 2.44 | 0.47 |
| 1:O:129:GLY:HA3 | 1:O:288:THR:HB | 1.94 | 0.47 |
| 1:Y:115:LEU:H | 1:Y:115:LEU:CD1 | 2.26 | 0.47 |
| 1:Y:20:VAL:HG12 | 1:Y:21:MET:H | 1.77 | 0.47 |
| 1:Y:289:THR:O | 1:Y:301:ALA:N | 2.43 | 0.47 |
| 1:Y:479:ARG:HH11 | 1:Y:479:ARG:CG | 2.27 | 0.47 |
| 1:O:118:ASP:HB2 | 1:O:120:LEU:HD11 | 1.95 | 0.47 |
| 1:O:9:LEU:HD13 | 1:O:9:LEU:HA | 1.43 | 0.47 |
| 1:Y:207:LEU:O | 1:Y:208:ASP:HB3 | 2.13 | 0.47 |
| 1:Y:247:GLN:NE2 | 1:Y:290:ILE:O | 2.47 | 0.47 |
| 1:Y:357:ASP:OD2 | 1:Y:494:MET:HB3 | 2.14 | 0.47 |
| 1:Y:50:MET:O | 1:Y:53:TRP:N | 2.47 | 0.47 |
| 1:O:273:MET:HB2 | 1:O:395:MET:CE | 2.44 | 0.47 |
| 1:O:451:VAL:HG12 | 1:O:453:PHE:CB | 2.44 | 0.47 |
| 1:O:458:ASP:HA | 1:O:461:GLN:HB2 | 1.95 | 0.47 |
| 1:Y:140:LYS:O | 1:Y:143:TRP:HB3 | 2.13 | 0.47 |
| 1:Y:179:HIS:O | 1:Y:216:GLU:N | 2.42 | 0.47 |
| 1:Y:193:ASN:CG | 1:Y:196:THR:HB | 2.33 | 0.47 |
| 1:Y:367:LEU:HD11 | 1:O:364:ILE:HD13 | 1.96 | 0.47 |
| 1:Y:468:ARG:HG2 | 1:Y:468:ARG:HH11 | 1.78 | 0.47 |
| 1:Y:80:THR:HG21 | 1:Y:248:ALA:HB2 | 1.95 | 0.47 |
| 1:Y:350:GLY:HA2 | 1:Y:360:ALA:O | 2.14 | 0.47 |
| 1:O:20:VAL:C | 1:O:21:MET:HG3 | 2.34 | 0.47 |
| 1:O:22:ASP:O | 1:O:25:ALA:N | 2.43 | 0.47 |
| 1:O:247:GLN:O | 1:O:250:LEU:HB3 | 2.15 | 0.47 |
| 1:O:24:ASP:HB3 | 1:O:26:ASN:HD21 | 1.80 | 0.47 |
| 1:O:80:THR:HG21 | 1:O:248:ALA:HB2 | 1.96 | 0.47 |
| 1:O:278:LYS:CD | 1:O:280:VAL:HG23 | 2.44 | 0.47 |
| 1:O:31:SER:HB2 | 1:O:63:VAL:HG23 | 1.96 | 0.47 |
| 1:Y:329:SER:HB2 | 1:Y:381:LEU:HD11 | 1.95 | 0.47 |
| 1:Y:9:LEU:HD13 | 1:Y:9:LEU:HA | 1.67 | 0.47 |
| 1:O:103:TRP:HB2 | 1:O:135:TYR:CE1 | 2.50 | 0.47 |
| 1:O:130:LEU:HD12 | 1:O:190:MET:HB2 | 1.97 | 0.47 |
| 1:O:24:ASP:O | 1:O:25:ALA:HB3 | 2.15 | 0.47 |
| 1:O:257:LYS:O | 1:O:258:GLU:O | 2.32 | 0.47 |
| 1:O:382:GLU:O | 1:O:384:ILE:N | 2.48 | 0.47 |
| 1:O:77:ILE:CG2 | 1:O:79:ILE:HD11 | 2.44 | 0.47 |
| 1:Y:117:ARG:CZ | 1:Y:117:ARG:HB2 | 2.42 | 0.47 |
| 1:Y:154:ARG:HG3 | 1:Y:160:LEU:HD11 | 1.96 | 0.47 |
| 1:Y:342:VAL:HA | 1:Y:365:PHE:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:415:ASN:ND2 | 1:Y:417:PHE:HB3 | 2.25 | 0.47 |
| 1:Y:418:LEU:HA | 1:Y:418:LEU:HD23 | 1.73 | 0.47 |
| 1:Y:438:VAL:HA | 1:Y:441:LEU:HD12 | 1.96 | 0.47 |
| 1:O:127:ASN:HB3 | 1:O:193:ASN:ND2 | 2.30 | 0.47 |
| 1:Y:310:GLY:O | 1:Y:313:ILE:HB | 2.15 | 0.47 |
| 1:Y:356:TRP:O | 1:Y:358:PRO:HD3 | 2.15 | 0.47 |
| 1:Y:343:TYR:CE2 | 1:Y:486:TRP:CA | 2.98 | 0.47 |
| 1:Y:69:ILE:H | 1:Y:69:ILE:HD12 | 1.80 | 0.47 |
| 1:O:158:GLY:H | 1:O:212:GLU:HG2 | 1.78 | 0.47 |
| 1:O:404:HIS:O | 1:O:429:ARG:HD2 | 2.15 | 0.47 |
| 1:Y:121:GLU:O | 1:Y:122:ASP:C | 2.53 | 0.47 |
| 1:Y:169:LEU:O | 1:Y:173:MET:HG2 | 2.14 | 0.47 |
| 1:Y:201:ASP:O | 1:Y:204:LEU:N | 2.48 | 0.47 |
| 1:Y:428:THR:HG23 | 1:Y:429:ARG:N | 2.30 | 0.47 |
| 1:O:482:ARG:NH1 | 1:O:482:ARG:HG3 | 2.30 | 0.47 |
| 1:O:95:LYS:HG3 | 1:O:96:PRO:O | 2.14 | 0.47 |
| 1:Y:24:ASP:O | 1:Y:25:ALA:HB3 | 2.14 | 0.47 |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:HA2 | 1.79 | 0.47 |
| 1:O:468:ARG:HH11 | 1:O:468:ARG:CG | 2.15 | 0.47 |
| 1:O:494:MET:O | 1:O:495:ALA:HB3 | 2.15 | 0.47 |
| 1:O:148:VAL:CG1 | 1:O:151:SER:HB3 | 2.45 | 0.46 |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:N | 2.13 | 0.46 |
| 1:O:351:LEU:HA | 1:O:351:LEU:HD12 | 1.74 | 0.46 |
| 1:Y:403:LEU:CD1 | 1:Y:403:LEU:N | 2.78 | 0.46 |
| 1:O:39:TYR:O | 1:O:40:PRO:C | 2.53 | 0.46 |
| 1:O:74:ILE:HD12 | 1:O:76:ALA:N | 2.30 | 0.46 |
| 1:Y:180:VAL:CG2 | 1:Y:181:THR:N | 2.78 | 0.46 |
| 1:Y:219:ARG:O | 1:Y:224:TYR:OH | 2.27 | 0.46 |
| 1:Y:253:GLN:O | 1:Y:254:LEU:HB2 | 2.15 | 0.46 |
| 1:Y:392:LEU:HD23 | 1:Y:393:GLU:HG2 | 1.96 | 0.46 |
| 1:O:117:ARG:HD3 | 1:O:117:ARG:H | 1.81 | 0.46 |
| 1:O:439:THR:O | 1:O:442:GLY:N | 2.48 | 0.46 |
| 1:O:484:ALA:O | 1:O:485:GLY:C | 2.53 | 0.46 |
| 1:Y:152:ARG:C | 1:Y:155:ALA:HB3 | 2.36 | 0.46 |
| 1:O:184:THR:O | 1:O:187:SER:HB3 | 2.16 | 0.46 |
| 1:Y:18:ALA:HB1 | 1:Y:63:VAL:HG21 | 1.97 | 0.46 |
| 1:Y:351:LEU:HB3 | 1:Y:355:TYR:HB2 | 1.97 | 0.46 |
| 1:Y:343:TYR:CE2 | 1:Y:486:TRP:HA | 2.51 | 0.46 |
| 1:O:158:GLY:N | 1:O:212:GLU:HG2 | 2.30 | 0.46 |
| 1:O:284:ASN:OD1 | 1:O:398:ASP:OD1 | 2.34 | 0.46 |
| 1:Y:104:GLN:HG2 | 1:Y:349:THR:HG21 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:203:MET:HA | 1:Y:206:VAL:CG1 | 2.42 | 0.46 |
| 1:Y:237:ILE:N | 1:Y:237:ILE:CD1 | 2.78 | 0.46 |
| 1:Y:256:VAL:HG12 | 1:Y:294:PRO:HG3 | 1.98 | 0.46 |
| 1:Y:438:VAL:O | 1:Y:441:LEU:HB2 | 2.16 | 0.46 |
| 1:Y:457:LEU:HA | 1:Y:460:LEU:CD1 | 2.39 | 0.46 |
| 1:Y:5:TYR:O | 1:Y:74:ILE:HA | 2.15 | 0.46 |
| 1:O:145:LEU:N | 1:O:145:LEU:HD13 | 2.26 | 0.46 |
| 1:O:224:TYR:CE2 | 1:O:242:ILE:HD12 | 2.51 | 0.46 |
| 1:O:245:ASP:OD1 | 1:O:246:GLN:NE2 | 2.48 | 0.46 |
| 1:O:435:VAL:CG2 | 1:O:436:ARG:N | 2.79 | 0.46 |
| 1:Y:170:ILE:N | 1:Y:170:ILE:CD1 | 2.79 | 0.46 |
| 1:Y:422:GLN:NE2 | 1:Y:426:LEU:CD2 | 2.78 | 0.46 |
| 1:Y:453:PHE:HD2 | 1:Y:454:TRP:CZ3 | 2.34 | 0.46 |
| 1:Y:468:ARG:CG | 1:Y:468:ARG:HH11 | 2.27 | 0.46 |
| 1:O:154:ARG:HA | 1:O:159:GLU:HB2 | 1.97 | 0.46 |
| 1:O:163:GLY:HA2 | 1:O:167:THR:HG21 | 1.98 | 0.46 |
| 1:O:172:LYS:O | 1:O:175:GLN:N | 2.40 | 0.46 |
| 1:O:269:CYS:HB2 | 1:O:306:VAL:HB | 1.96 | 0.46 |
| 1:O:316:LEU:HD23 | 1:O:316:LEU:HA | 1.26 | 0.46 |
| 1:O:347:ALA:O | 1:O:361:ARG:HA | 2.16 | 0.46 |
| 1:O:476:THR:O | 1:O:477:THR:C | 2.51 | 0.46 |
| 1:O:5:TYR:N | 1:O:73:GLN:O | 2.44 | 0.46 |
| 1:O:77:ILE:CG2 | 1:O:239:ILE:HG23 | 2.45 | 0.46 |
| 1:O:78:GLY:HA3 | 1:O:443:ALA:O | 2.15 | 0.46 |
| 1:O:85:THR:HG23 | 1:O:102:VAL:HA | 1.97 | 0.46 |
| 1:Y:114:HIS:O | 1:Y:116:LYS:N | 2.48 | 0.46 |
| 1:Y:435:VAL:HG21 | 1:Y:441:LEU:HD11 | 1.97 | 0.46 |
| 1:Y:88:VAL:HG22 | 1:Y:162:PHE:CA | 2.46 | 0.46 |
| 1:O:142:LYS:CG | 1:O:143:TRP:N | 2.79 | 0.46 |
| 1:O:52:ILE:O | 1:O:55:THR:OG1 | 2.34 | 0.46 |
| 1:O:70:SER:O | 1:O:73:GLN:HG3 | 2.16 | 0.46 |
| 1:Y:181:THR:CG2 | 1:Y:182:ASP:N | 2.79 | 0.46 |
| 1:Y:124:ILE:HG12 | 1:Y:203:MET:HE1 | 1.98 | 0.46 |
| 1:Y:262:LYS:C | 1:Y:262:LYS:HD2 | 2.36 | 0.46 |
| 1:O:113:GLU:HA | 1:O:113:GLU:OE1 | 2.14 | 0.46 |
| 1:O:317:ARG:O | 1:O:321:LYS:HA | 2.15 | 0.46 |
| 1:O:33:ARG:HE | 1:O:58:TRP:HB3 | 1.80 | 0.46 |
| 1:O:5:TYR:O | 1:O:74:ILE:HA | 2.16 | 0.46 |
| 1:O:11:GLN:NE2 | 1:O:82:GLN:HE21 | 2.14 | 0.46 |
| 1:Y:22:ASP:OD1 | 1:Y:25:ALA:N | 2.49 | 0.46 |
| 1:Y:104:GLN:NE2 | 1:Y:308:MET:CE | 2.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:389:ARG:O | 1:Y:390:ASP:C | 2.52 | 0.46 |
| 1:Y:47:HIS:O | 1:Y:49:PRO:HD3 | 2.16 | 0.46 |
| 1:Y:64:LEU:HB2 | 1:Y:65:ALA:H | 1.54 | 0.46 |
| 1:O:145:LEU:HB3 | 1:O:152:ARG:CZ | 2.46 | 0.46 |
| 1:O:88:VAL:CG2 | 1:O:162:PHE:HB2 | 2.46 | 0.46 |
| 1:Y:120:LEU:O | 1:Y:124:ILE:HG13 | 2.16 | 0.46 |
| 1:Y:244:GLY:O | 1:Y:245:ASP:C | 2.52 | 0.46 |
| 1:Y:254:LEU:O | 1:Y:256:VAL:N | 2.48 | 0.46 |
| 1:Y:50:MET:O | 1:Y:52:ILE:N | 2.49 | 0.46 |
| 1:O:161:LEU:CD2 | 1:O:179:HIS:CE1 | 2.99 | 0.45 |
| 1:O:179:HIS:CD2 | 1:O:215:PRO:CA | 2.99 | 0.45 |
| 1:O:196:THR:C | 1:O:197:LEU:HD22 | 2.37 | 0.45 |
| 1:O:467:GLU:OE2 | 1:O:468:ARG:HB2 | 2.15 | 0.45 |
| 1:Y:124:ILE:CD1 | 1:Y:203:MET:HE3 | 2.46 | 0.45 |
| 1:Y:222:GLU:HG2 | 1:Y:224:TYR:CD1 | 2.52 | 0.45 |
| 1:Y:441:LEU:HD23 | 1:Y:441:LEU:HA | 1.67 | 0.45 |
| 1:Y:482:ARG:HG3 | 1:Y:482:ARG:NH1 | 2.30 | 0.45 |
| 1:Y:57:SER:O | 1:Y:60:LEU:HD23 | 2.16 | 0.45 |
| 1:O:179:HIS:CG | 1:O:215:PRO:HB3 | 2.52 | 0.45 |
| 1:O:199:TRP:HB3 | 1:O:204:LEU:HD11 | 1.98 | 0.45 |
| 1:O:428:THR:CG2 | 1:O:429:ARG:N | 2.79 | 0.45 |
| 1:O:251:PHE:CE2 | 1:O:446:LEU:CD1 | 2.98 | 0.45 |
| 1:O:78:GLY:HA2 | 1:O:241:GLY:HA3 | 1.97 | 0.45 |
| 1:Y:101:ILE:HD13 | 1:Y:107:ARG:NE | 2.31 | 0.45 |
| 1:Y:193:ASN:OD1 | 1:Y:196:THR:HB | 2.16 | 0.45 |
| 1:Y:284:ASN:OD1 | 1:Y:398:ASP:OD1 | 2.34 | 0.45 |
| 1:Y:394:ALA:O | 1:Y:395:MET:C | 2.52 | 0.45 |
| 1:O:117:ARG:HD3 | 1:O:117:ARG:N | 2.31 | 0.45 |
| 1:O:191:LEU:HD23 | 1:O:207:LEU:CD1 | 2.46 | 0.45 |
| 1:O:230:GLY:HA2 | 1:O:235:THR:HB | 1.98 | 0.45 |
| 1:O:285:GLY:O | 1:O:356:TRP:NE1 | 2.39 | 0.45 |
| 1:O:309:ALA:O | 1:O:312:SER:OG | 2.30 | 0.45 |
| 1:O:310:GLY:O | 1:O:313:ILE:N | 2.49 | 0.45 |
| 1:O:401:ILE:CG2 | 1:O:402:ARG:N | 2.79 | 0.45 |
| 1:O:60:LEU:HD12 | 1:O:60:LEU:O | 2.16 | 0.45 |
| 1:O:145:LEU:HD12 | 1:O:145:LEU:HA | 1.54 | 0.45 |
| 1:O:214:LEU:CD1 | 1:O:214:LEU:N | 2.79 | 0.45 |
| 1:O:251:PHE:O | 1:O:254:LEU:HD12 | 2.16 | 0.45 |
| 1:O:298:VAL:O | 1:O:299:ASN:OD1 | 2.35 | 0.45 |
| 1:Y:183:TYR:O | 1:Y:184:THR:C | 2.55 | 0.45 |
| 1:Y:80:THR:HG21 | 1:Y:248:ALA:CB | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:264:THR:CG2 | 1:Y:265:TYR:N | 2.79 | 0.45 |
| 1:Y:423:SER:HB3 | 1:Y:430:VAL:HG23 | 1.98 | 0.45 |
| 1:Y:461:GLN:HE21 | 1:Y:461:GLN:HB3 | 1.56 | 0.45 |
| 1:O:218:ARG:NH1 | 1:O:218:ARG:CG | 2.79 | 0.45 |
| 1:O:438:VAL:CA | 1:O:441:LEU:HD12 | 2.41 | 0.45 |
| 1:Y:161:LEU:CD2 | 1:Y:179:HIS:NE2 | 2.80 | 0.45 |
| 1:Y:206:VAL:CG1 | 1:Y:207:LEU:N | 2.79 | 0.45 |
| 1:Y:425:ILE:HA | 1:Y:425:ILE:HD12 | 1.53 | 0.45 |
| 1:O:153:GLU:O | 1:O:156:ARG:N | 2.49 | 0.45 |
| 1:O:86:THR:CG2 | 1:O:162:PHE:CE2 | 2.99 | 0.45 |
| 1:O:183:TYR:CD2 | 1:O:298:VAL:CG2 | 2.99 | 0.45 |
| 1:O:419:MET:O | 1:O:420:GLN:C | 2.52 | 0.45 |
| 1:O:13:THR:HB | 3:O:601:ACP:O3G | 2.16 | 0.45 |
| 1:O:8:ALA:O | 1:O:9:LEU:HD13 | 2.16 | 0.45 |
| 1:Y:179:HIS:CE1 | 1:Y:215:PRO:CB | 3.00 | 0.45 |
| 1:Y:256:VAL:N | 1:Y:260:MET:HG3 | 2.31 | 0.45 |
| 1:Y:328:ASP:O | 1:Y:329:SER:C | 2.53 | 0.45 |
| 1:Y:428:THR:CG2 | 1:Y:429:ARG:N | 2.80 | 0.45 |
| 1:Y:53:TRP:CA | 1:Y:53:TRP:CE3 | 3.00 | 0.45 |
| 1:O:105:CYS:SG | 1:O:107:ARG:NH1 | 2.89 | 0.45 |
| 1:O:184:THR:OG1 | 1:O:243:ALA:HA | 2.17 | 0.45 |
| 1:O:406:LEU:CD2 | 1:O:407:ARG:N | 2.79 | 0.45 |
| 1:O:33:ARG:NE | 1:O:58:TRP:HB3 | 2.32 | 0.45 |
| 1:Y:212:GLU:C | 1:Y:214:LEU:H | 2.19 | 0.45 |
| 1:Y:3:LYS:HA | 1:Y:73:GLN:CA | 2.40 | 0.45 |
| 1:Y:466:ILE:O | 1:Y:466:ILE:HD13 | 2.17 | 0.45 |
| 1:O:180:VAL:CG2 | 1:O:181:THR:N | 2.80 | 0.45 |
| 1:O:71:SER:OG | 1:O:230:GLY:O | 2.30 | 0.45 |
| 1:O:182:ASP:OD1 | 1:O:242:ILE:HG22 | 2.17 | 0.45 |
| 1:O:257:LYS:CA | 1:O:274:ASN:HD22 | 2.30 | 0.45 |
| 1:O:352:GLY:O | 1:O:353:ALA:C | 2.51 | 0.45 |
| 1:Y:130:LEU:HB3 | 1:Y:131:VAL:H | 1.41 | 0.45 |
| 1:Y:435:VAL:CG2 | 1:Y:436:ARG:N | 2.79 | 0.45 |
| 1:O:290:ILE:CG2 | 1:O:291:ALA:N | 2.80 | 0.45 |
| 1:O:33:ARG:CZ | 1:O:58:TRP:HB3 | 2.47 | 0.45 |
| 1:Y:230:GLY:CA | 1:Y:235:THR:HB | 2.44 | 0.45 |
| 1:Y:426:LEU:HD12 | 1:Y:426:LEU:HA | 1.71 | 0.45 |
| 1:O:11:GLN:HE22 | 1:O:82:GLN:HG2 | 1.82 | 0.45 |
| 1:O:265:TYR:CE1 | 1:O:408:VAL:CG1 | 2.99 | 0.45 |
| 1:O:467:GLU:HG2 | 1:O:467:GLU:O | 2.09 | 0.45 |
| 1:Y:142:LYS:O | 1:Y:145:LEU:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:312:SER:O | 1:Y:315:TRP:HB3 | 2.17 | 0.45 |
| 1:Y:79:ILE:HD11 | 1:Y:239:ILE:HG23 | 1.98 | 0.45 |
| 1:O:237:ILE:N | 1:O:237:ILE:CD1 | 2.80 | 0.44 |
| 1:O:422:GLN:NE2 | 1:O:426:LEU:CD2 | 2.79 | 0.44 |
| 1:O:463:LYS:NZ | 1:O:465:VAL:CG2 | 2.80 | 0.44 |
| 1:Y:102:VAL:O | 1:Y:104:GLN:N | 2.50 | 0.44 |
| 1:Y:149:GLU:OE1 | 1:Y:149:GLU:HA | 2.17 | 0.44 |
| 1:Y:182:ASP:CG | 1:Y:242:ILE:HB | 2.37 | 0.44 |
| 1:Y:271:MET:HG2 | 1:Y:271:MET:O | 2.13 | 0.44 |
| 1:Y:309:ALA:O | 1:Y:312:SER:OG | 2.32 | 0.44 |
| 1:Y:478:GLU:O | 1:Y:481:TYR:N | 2.50 | 0.44 |
| 1:Y:488:LYS:O | 1:Y:492:ARG:HD3 | 2.17 | 0.44 |
| 1:O:146:ASP:N | 1:O:146:ASP:OD1 | 2.38 | 0.44 |
| 1:O:389:ARG:O | 1:O:390:ASP:C | 2.56 | 0.44 |
| 1:O:3:LYS:HG3 | 1:O:72:ASP:O | 2.17 | 0.44 |
| 1:O:65:ALA:C | 1:O:67:ALA:H | 2.21 | 0.44 |
| 1:Y:111:ILE:O | 1:Y:112:CYS:C | 2.50 | 0.44 |
| 1:Y:214:LEU:CD1 | 1:Y:214:LEU:N | 2.79 | 0.44 |
| 1:Y:495:ALA:O | 1:O:492:ARG:NH2 | 2.50 | 0.44 |
| 1:Y:59:THR:O | 1:Y:60:LEU:C | 2.56 | 0.44 |
| 1:O:186:ALA:HB2 | 1:O:217:VAL:HG13 | 2.00 | 0.44 |
| 1:O:357:ASP:OD1 | 1:O:358:PRO:HD2 | 2.17 | 0.44 |
| 1:O:37:GLN:HB3 | 1:O:39:TYR:CZ | 2.52 | 0.44 |
| 1:O:37:GLN:HE22 | 1:O:47:HIS:CE1 | 2.34 | 0.44 |
| 1:O:53:TRP:O | 1:O:54:ALA:C | 2.56 | 0.44 |
| 1:O:80:THR:C | 1:O:81:ASN:HD22 | 2.20 | 0.44 |
| 1:Y:142:LYS:O | 1:Y:146:ASP:OD1 | 2.35 | 0.44 |
| 1:Y:148:VAL:CG1 | 1:Y:149:GLU:N | 2.80 | 0.44 |
| 1:Y:222:GLU:CG | 1:Y:223:VAL:N | 2.80 | 0.44 |
| 1:Y:70:SER:H | 1:Y:73:GLN:HG3 | 1.82 | 0.44 |
| 1:O:41:LYS:CG | 1:O:42:PRO:N | 2.81 | 0.44 |
| 1:O:83:ARG:NH1 | 1:O:246:GLN:HB2 | 2.33 | 0.44 |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CE1 | 2.52 | 0.44 |
| 1:Y:31:SER:HB2 | 1:Y:63:VAL:CG2 | 2.20 | 0.44 |
| 1:Y:3:LYS:HG3 | 1:Y:72:ASP:C | 2.37 | 0.44 |
| 1:Y:56:GLN:O | 1:Y:56:GLN:HG3 | 2.18 | 0.44 |
| 1:O:302:LEU:HD23 | 1:O:302:LEU:HA | 1.62 | 0.44 |
| 1:O:415:ASN:ND2 | 1:O:417:PHE:HB3 | 2.15 | 0.44 |
| 1:Y:228:ASN:HD22 | 1:Y:230:GLY:N | 2.16 | 0.44 |
| 1:O:298:VAL:CG1 | 1:O:299:ASN:N | 2.81 | 0.44 |
| 1:Y:154:ARG:CA | 1:Y:159:GLU:HB2 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:255:CYS:HA | 1:Y:260:MET:CB | 2.47 | 0.44 |
| 1:Y:265:TYR:N | 1:Y:409:ASP:O | 2.51 | 0.44 |
| 1:Y:41:LYS:HB2 | 1:Y:42:PRO:HD2 | 2.00 | 0.44 |
| 1:Y:434:GLU:HB2 | 1:Y:465:VAL:O | 2.17 | 0.44 |
| 1:Y:43:GLY:C | 1:Y:44:TRP:HD1 | 2.20 | 0.44 |
| 1:O:130:LEU:HD13 | 1:O:136:PHE:CG | 2.52 | 0.44 |
| 1:O:21:MET:HA | 1:O:26:ASN:O | 2.18 | 0.44 |
| 1:O:439:THR:CG2 | 1:O:440:ALA:N | 2.79 | 0.44 |
| 1:Y:200:ASP:OD1 | 1:Y:202:LYS:HB2 | 2.18 | 0.44 |
| 1:Y:257:LYS:CA | 1:Y:274:ASN:ND2 | 2.81 | 0.44 |
| 1:Y:272:LEU:CD1 | 1:Y:272:LEU:N | 2.80 | 0.44 |
| 1:Y:253:GLN:CG | 1:Y:407:ARG:HD2 | 2.47 | 0.44 |
| 1:O:183:TYR:O | 1:O:187:SER:N | 2.37 | 0.44 |
| 1:Y:218:ARG:CG | 1:Y:218:ARG:NH1 | 2.79 | 0.44 |
| 1:Y:279:ALA:CB | 1:Y:300:TYR:CG | 2.99 | 0.44 |
| 1:Y:74:ILE:HD12 | 1:Y:75:ALA:N | 2.32 | 0.44 |
| 1:Y:97:ILE:HG13 | 1:Y:97:ILE:H | 1.66 | 0.44 |
| 1:O:148:VAL:CG1 | 1:O:149:GLU:N | 2.80 | 0.44 |
| 1:O:185:ASN:ND2 | 1:O:244:GLY:CA | 2.79 | 0.44 |
| 1:O:354:PRO:HD2 | 1:O:355:TYR:CE2 | 2.53 | 0.44 |
| 1:O:442:GLY:O | 1:O:445:TYR:N | 2.51 | 0.44 |
| 1:O:474:ILE:HA | 1:O:474:ILE:HD12 | 1.79 | 0.44 |
| 1:O:5:TYR:CE2 | 1:O:28:ILE:HG13 | 2.53 | 0.44 |
| 1:Y:111:ILE:O | 1:Y:115:LEU:HD13 | 2.18 | 0.44 |
| 1:Y:172:LYS:HA | 1:Y:172:LYS:HD2 | 1.48 | 0.44 |
| 1:O:169:LEU:HA | 1:O:169:LEU:HD13 | 1.39 | 0.43 |
| 1:O:453:PHE:CD2 | 1:O:454:TRP:CZ3 | 3.05 | 0.43 |
| 1:O:482:ARG:CG | 1:O:482:ARG:NH1 | 2.79 | 0.43 |
| 1:O:74:ILE:HD12 | 1:O:74:ILE:C | 2.38 | 0.43 |
| 1:Y:348:PHE:HD1 | 1:Y:348:PHE:N | 2.14 | 0.43 |
| 1:Y:445:TYR:HD2 | 1:Y:457:LEU:HD11 | 1.81 | 0.43 |
| 1:Y:270:PHE:CZ | 4:Y:600:GOL:H11 | 2.53 | 0.43 |
| 1:Y:74:ILE:C | 1:Y:74:ILE:HD12 | 2.38 | 0.43 |
| 1:O:192:PHE:CZ | 1:O:197:LEU:HA | 2.53 | 0.43 |
| 1:O:246:GLN:HE21 | 1:O:246:GLN:H | 1.65 | 0.43 |
| 1:O:257:LYS:O | 1:O:258:GLU:C | 2.56 | 0.43 |
| 1:O:394:ALA:O | 1:O:397:ALA:N | 2.51 | 0.43 |
| 1:Y:88:VAL:HA | 1:Y:161:LEU:O | 2.17 | 0.43 |
| 1:Y:476:THR:O | 1:Y:477:THR:C | 2.56 | 0.43 |
| 1:Y:16:SER:CB | 1:Y:56:GLN:HA | 2.48 | 0.43 |
| 1:Y:64:LEU:O | 1:Y:65:ALA:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:114:HIS:O | 1:O:117:ARG:N | 2.51 | 0.43 |
| 1:O:109:ALA:HA | 1:O:134:PRO:HG3 | 2.01 | 0.43 |
| 1:O:123:TYR:OH | 1:O:200:ASP:OD2 | 2.31 | 0.43 |
| 1:O:84:GLU:HG2 | 1:O:135:TYR:O | 2.19 | 0.43 |
| 1:Y:161:LEU:HD22 | 1:Y:179:HIS:CE1 | 2.52 | 0.43 |
| 1:Y:286:LEU:O | 1:Y:287:LEU:HD23 | 2.17 | 0.43 |
| 1:Y:91:LYS:CB | 1:Y:91:LYS:NZ | 2.79 | 0.43 |
| 1:O:141:VAL:O | 1:O:142:LYS:C | 2.57 | 0.43 |
| 1:O:219:ARG:HD3 | 1:O:221:SER:O | 2.18 | 0.43 |
| 1:O:28:ILE:HD13 | 1:O:28:ILE:N | 2.32 | 0.43 |
| 1:Y:110:GLU:O | 1:Y:111:ILE:C | 2.55 | 0.43 |
| 1:Y:436:ARG:C | 1:Y:438:VAL:H | 2.20 | 0.43 |
| 1:Y:482:ARG:CG | 1:Y:482:ARG:HH11 | 2.30 | 0.43 |
| 1:Y:484:ALA:O | 1:Y:485:GLY:C | 2.54 | 0.43 |
| 1:O:363:ALA:HB3 | 1:O:365:PHE:HE1 | 1.81 | 0.43 |
| 1:O:385:ALA:CB | 1:O:422:GLN:NE2 | 2.79 | 0.43 |
| 1:O:443:ALA:O | 1:O:444:ALA:O | 2.35 | 0.43 |
| 1:Y:199:TRP:CE2 | 1:Y:214:LEU:HD23 | 2.53 | 0.43 |
| 1:Y:302:LEU:HD23 | 1:Y:302:LEU:HA | 1.33 | 0.43 |
| 1:Y:41:LYS:CB | 1:Y:42:PRO:HD2 | 2.48 | 0.43 |
| 1:Y:468:ARG:CG | 1:Y:468:ARG:NH1 | 2.80 | 0.43 |
| 1:Y:489:ALA:O | 1:Y:490:VAL:C | 2.57 | 0.43 |
| 1:Y:83:ARG:HB2 | 1:Y:83:ARG:HE | 1.64 | 0.43 |
| 1:O:182:ASP:HB3 | 1:O:242:ILE:HG21 | 1.99 | 0.43 |
| 1:O:33:ARG:NE | 1:O:58:TRP:CB | 2.80 | 0.43 |
| 1:O:84:GLU:OE1 | 1:O:103:TRP:HB3 | 2.19 | 0.43 |
| 1:Y:151:SER:O | 1:Y:155:ALA:N | 2.46 | 0.43 |
| 1:Y:439:THR:O | 1:Y:440:ALA:C | 2.56 | 0.43 |
| 1:Y:8:ALA:C | 1:Y:9:LEU:HD22 | 2.39 | 0.43 |
| 1:O:204:LEU:HA | 1:O:204:LEU:HD23 | 1.48 | 0.43 |
| 1:O:251:PHE:CD1 | 1:O:256:VAL:HG21 | 2.54 | 0.43 |
| 1:Y:13:THR:N | 3:Y:601:ACP:O2G | 2.52 | 0.43 |
| 1:Y:343:TYR:HE2 | 1:Y:486:TRP:HB2 | 1.83 | 0.43 |
| 1:O:171:TRP:NE1 | 1:O:176:GLY:HA2 | 2.33 | 0.43 |
| 1:O:409:ASP:CA | 1:O:413:VAL:HG11 | 2.49 | 0.43 |
| 1:O:457:LEU:HA | 1:O:457:LEU:HD22 | 1.39 | 0.43 |
| 1:O:460:LEU:O | 1:O:462:GLU:N | 2.52 | 0.43 |
| 1:Y:475:GLU:O | 1:Y:478:GLU:HB2 | 2.19 | 0.43 |
| 1:Y:74:ILE:HD12 | 1:Y:76:ALA:N | 2.33 | 0.43 |
| 1:O:257:LYS:C | 1:O:274:ASN:HD22 | 2.21 | 0.43 |
| 1:O:460:LEU:C | 1:O:462:GLU:H | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:179:HIS:CD2 | 1:Y:215:PRO:CA | 2.99 | 0.43 |
| 1:Y:286:LEU:HD21 | 1:Y:394:ALA:HB3 | 2.01 | 0.43 |
| 1:Y:293:GLY:O | 1:Y:295:THR:N | 2.52 | 0.43 |
| 1:Y:433:PRO:O | 1:Y:436:ARG:NH1 | 2.52 | 0.43 |
| 1:Y:154:ARG:HA | 1:Y:159:GLU:HB2 | 2.01 | 0.43 |
| 1:Y:179:HIS:CE1 | 1:Y:215:PRO:CG | 3.02 | 0.43 |
| 1:Y:193:ASN:O | 1:Y:197:LEU:N | 2.52 | 0.43 |
| 1:Y:199:TRP:HZ2 | 1:Y:215:PRO:O | 2.01 | 0.43 |
| 1:Y:251:PHE:C | 1:Y:254:LEU:H | 2.21 | 0.43 |
| 1:Y:35:PHE:HB2 | 1:Y:51:GLU:CG | 2.47 | 0.43 |
| 1:Y:40:PRO:HD2 | 1:Y:44:TRP:C | 2.38 | 0.43 |
| 1:Y:38:ILE:HG22 | 1:Y:40:PRO:HD3 | 2.01 | 0.43 |
| 1:Y:482:ARG:O | 1:Y:483:TYR:C | 2.53 | 0.43 |
| 1:O:144:ILE:O | 1:O:147:HIS:HB2 | 2.19 | 0.42 |
| 1:O:228:ASN:HB2 | 1:O:236:ARG:CZ | 2.49 | 0.42 |
| 1:O:276:GLY:O | 1:O:300:TYR:N | 2.52 | 0.42 |
| 1:O:477:THR:O | 1:O:478:GLU:C | 2.57 | 0.42 |
| 1:Y:153:GLU:H | 1:Y:153:GLU:HG2 | 1.68 | 0.42 |
| 1:Y:203:MET:C | 1:Y:206:VAL:HG12 | 2.40 | 0.42 |
| 1:Y:325:ASP:O | 1:Y:328:ASP:N | 2.51 | 0.42 |
| 1:Y:251:PHE:CD2 | 1:Y:446:LEU:HD12 | 2.54 | 0.42 |
| 1:Y:45:VAL:O | 1:Y:102:VAL:HG23 | 2.19 | 0.42 |
| 1:Y:467:GLU:OE2 | 1:Y:468:ARG:HB2 | 2.18 | 0.42 |
| 1:Y:478:GLU:O | 1:Y:481:TYR:HB3 | 2.19 | 0.42 |
| 1:O:124:ILE:HG12 | 1:O:203:MET:HE1 | 2.00 | 0.42 |
| 1:O:154:ARG:H | 1:O:154:ARG:HG2 | 1.34 | 0.42 |
| 1:O:86:THR:HG23 | 1:O:162:PHE:CE2 | 2.54 | 0.42 |
| 1:O:415:ASN:ND2 | 1:O:418:LEU:HB2 | 2.33 | 0.42 |
| 1:Y:130:LEU:CD1 | 1:Y:136:PHE:CD1 | 3.01 | 0.42 |
| 1:Y:174:THR:O | 1:Y:175:GLN:C | 2.55 | 0.42 |
| 1:Y:401:ILE:HG22 | 1:Y:402:ARG:N | 2.34 | 0.42 |
| 1:O:251:PHE:CE1 | 1:O:256:VAL:HG21 | 2.55 | 0.42 |
| 1:O:183:TYR:CD2 | 1:O:298:VAL:HG22 | 2.55 | 0.42 |
| 1:Y:91:LYS:HZ2 | 1:Y:161:LEU:CD1 | 2.33 | 0.42 |
| 1:Y:229:ILE:HG23 | 1:Y:237:ILE:HD13 | 2.01 | 0.42 |
| 1:Y:421:PHE:O | 1:Y:422:GLN:C | 2.57 | 0.42 |
| 1:O:152:ARG:C | 1:O:155:ALA:HB3 | 2.39 | 0.42 |
| 1:O:262:LYS:HA | 1:O:407:ARG:O | 2.19 | 0.42 |
| 1:O:487:LYS:O | 1:O:491:LYS:HG3 | 2.20 | 0.42 |
| 1:O:7:VAL:HG12 | 1:O:9:LEU:CD2 | 2.49 | 0.42 |
| 1:Y:372:ASN:OD1 | 1:Y:374:ASN:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:415:ASN:C | 1:Y:415:ASN:HD22 | 2.23 | 0.42 |
| 1:Y:479:ARG:HG3 | 1:Y:479:ARG:HH11 | 1.83 | 0.42 |
| 1:O:286:LEU:HD11 | 1:O:395:MET:N | 2.35 | 0.42 |
| 1:Y:204:LEU:O | 1:Y:209:ILE:N | 2.39 | 0.42 |
| 1:Y:79:ILE:HD11 | 1:Y:239:ILE:CG2 | 2.49 | 0.42 |
| 1:Y:242:ILE:O | 1:Y:243:ALA:HB2 | 2.19 | 0.42 |
| 1:O:102:VAL:HG23 | 1:O:102:VAL:H | 1.50 | 0.42 |
| 1:O:308:MET:HB2 | 1:O:346:PRO:HB2 | 2.00 | 0.42 |
| 1:O:265:TYR:CE1 | 1:O:408:VAL:HG11 | 2.55 | 0.42 |
| 1:Y:273:MET:HB2 | 1:Y:395:MET:CE | 2.50 | 0.42 |
| 1:Y:28:ILE:HA | 1:Y:28:ILE:HD12 | 1.79 | 0.42 |
| 1:O:120:LEU:O | 1:O:121:GLU:C | 2.57 | 0.42 |
| 1:O:246:GLN:NE2 | 1:O:246:GLN:H | 2.16 | 0.42 |
| 1:O:40:PRO:HD2 | 1:O:44:TRP:C | 2.40 | 0.42 |
| 1:O:486:TRP:CD1 | 1:O:487:LYS:HG2 | 2.54 | 0.42 |
| 1:O:70:SER:O | 1:O:72:ASP:N | 2.53 | 0.42 |
| 1:O:84:GLU:HG2 | 1:O:135:TYR:CE1 | 2.55 | 0.42 |
| 1:Y:154:ARG:O | 1:Y:155:ALA:O | 2.38 | 0.42 |
| 1:Y:169:LEU:HA | 1:Y:169:LEU:HD12 | 1.57 | 0.42 |
| 1:Y:280:VAL:HG12 | 1:Y:281:LYS:H | 1.83 | 0.42 |
| 1:Y:368:THR:CG2 | 1:Y:369:ARG:N | 2.82 | 0.42 |
| 1:O:101:ILE:HD13 | 1:O:107:ARG:CD | 2.50 | 0.42 |
| 1:O:432:ARG:HA | 1:O:433:PRO:HD2 | 1.84 | 0.42 |
| 1:O:445:TYR:O | 1:O:447:ALA:N | 2.53 | 0.42 |
| 1:O:457:LEU:HA | 1:O:460:LEU:HD13 | 2.00 | 0.42 |
| 1:O:466:ILE:HD13 | 1:O:466:ILE:C | 2.39 | 0.42 |
| 1:O:87:ILE:HD11 | 1:O:165:VAL:N | 2.34 | 0.42 |
| 1:Y:214:LEU:HD12 | 1:Y:214:LEU:N | 2.33 | 0.42 |
| 1:Y:347:ALA:O | 1:Y:362:GLY:N | 2.52 | 0.42 |
| 1:Y:67:ALA:CB | 1:Y:69:ILE:CD1 | 2.98 | 0.42 |
| 1:O:117:ARG:C | 1:O:119:GLY:H | 2.18 | 0.42 |
| 1:O:13:THR:O | 1:O:13:THR:HG22 | 2.19 | 0.42 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:HG22 | 1.95 | 0.42 |
| 1:O:338:ASN:OD1 | 1:O:340:ASN:N | 2.43 | 0.42 |
| 1:O:50:MET:O | 1:O:53:TRP:N | 2.53 | 0.42 |
| 1:Y:155:ALA:HB1 | 1:Y:210:PRO:HG2 | 2.01 | 0.42 |
| 1:Y:81:ASN:H | 1:Y:81:ASN:ND2 | 2.12 | 0.42 |
| 1:Y:95:LYS:HA | 1:Y:96:PRO:HD3 | 1.92 | 0.42 |
| 1:O:109:ALA:O | 1:O:112:CYS:HB2 | 2.20 | 0.42 |
| 1:O:114:HIS:CD2 | 1:O:117:ARG:HH22 | 2.38 | 0.42 |
| 1:O:422:GLN:HG3 | 1:O:426:LEU:HD23 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:309:ALA:HA | 1:Y:384:ILE:HD13 | 2.02 | 0.42 |
| 1:Y:320:MET:O | 1:Y:321:LYS:HB2 | 2.20 | 0.42 |
| 1:Y:70:SER:O | 1:Y:71:SER:C | 2.59 | 0.42 |
| 1:O:246:GLN:NE2 | 1:O:246:GLN:CA | 2.80 | 0.41 |
| 1:O:378:ARG:O | 1:O:379:ALA:C | 2.57 | 0.41 |
| 1:Y:154:ARG:HG2 | 1:Y:154:ARG:H | 1.41 | 0.41 |
| 1:Y:20:VAL:CG1 | 1:Y:21:MET:N | 2.80 | 0.41 |
| 1:Y:355:TYR:O | 1:Y:356:TRP:HB2 | 2.20 | 0.41 |
| 1:Y:364:ILE:CD1 | 1:Y:364:ILE:N | 2.83 | 0.41 |
| 1:O:154:ARG:HA | 1:O:157:ARG:HG2 | 2.02 | 0.41 |
| 1:O:272:LEU:N | 1:O:272:LEU:CD1 | 2.82 | 0.41 |
| 1:O:374:ASN:O | 1:O:375:HIS:C | 2.58 | 0.41 |
| 1:O:487:LYS:O | 1:O:488:LYS:C | 2.58 | 0.41 |
| 1:O:3:LYS:HD2 | 1:O:72:ASP:O | 2.20 | 0.41 |
| 1:Y:453:PHE:CE2 | 1:Y:454:TRP:CZ3 | 3.08 | 0.41 |
| 1:Y:482:ARG:NH1 | 1:Y:482:ARG:CG | 2.80 | 0.41 |
| 1:O:207:LEU:HB3 | 1:O:209:ILE:HD12 | 1.99 | 0.41 |
| 1:O:82:GLN:OE1 | 1:O:102:VAL:HG13 | 2.21 | 0.41 |
| 1:Y:128:THR:HB | 1:Y:130:LEU:H | 1.85 | 0.41 |
| 1:Y:180:VAL:HA | 1:Y:216:GLU:O | 2.20 | 0.41 |
| 1:Y:237:ILE:CG2 | 1:Y:238:PRO:N | 2.80 | 0.41 |
| 1:Y:3:LYS:HZ2 | 1:Y:75:ALA:HA | 1.85 | 0.41 |
| 1:O:124:ILE:CD1 | 1:O:203:MET:CE | 2.98 | 0.41 |
| 1:O:311:ALA:O | 1:O:312:SER:C | 2.59 | 0.41 |
| 1:O:406:LEU:HD22 | 1:O:407:ARG:N | 2.35 | 0.41 |
| 1:Y:328:ASP:O | 1:Y:332:PHE:HD2 | 2.03 | 0.41 |
| 1:Y:492:ARG:NH1 | 1:Y:492:ARG:CG | 2.80 | 0.41 |
| 1:O:199:TRP:HZ2 | 1:O:215:PRO:O | 2.02 | 0.41 |
| 1:O:245:ASP:OD1 | 1:O:246:GLN:N | 2.54 | 0.41 |
| 1:O:251:PHE:CE2 | 1:O:446:LEU:HB2 | 2.55 | 0.41 |
| 1:O:489:ALA:O | 1:O:490:VAL:C | 2.59 | 0.41 |
| 1:O:86:THR:C | 1:O:87:ILE:HG13 | 2.40 | 0.41 |
| 1:Y:348:PHE:CD1 | 1:Y:362:GLY:HA3 | 2.55 | 0.41 |
| 1:Y:286:LEU:CD1 | 1:Y:394:ALA:HB1 | 2.47 | 0.41 |
| 1:O:44:TRP:CE3 | 1:O:107:ARG:CZ | 3.04 | 0.41 |
| 1:O:183:TYR:HA | 1:O:186:ALA:HB3 | 2.03 | 0.41 |
| 1:O:286:LEU:HD11 | 1:O:394:ALA:HB1 | 2.00 | 0.41 |
| 1:O:372:ASN:OD1 | 1:O:374:ASN:N | 2.54 | 0.41 |
| 1:O:389:ARG:HB2 | 1:O:426:LEU:HD13 | 2.03 | 0.41 |
| 1:Y:144:ILE:O | 1:Y:147:HIS:N | 2.53 | 0.41 |
| 1:Y:272:LEU:CD1 | 1:Y:303:GLU:HG3 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:376:ILE:HD12 | 1:Y:376:ILE:HA | 1.69 | 0.41 |
| 1:Y:449:LEU:HD13 | 1:Y:449:LEU:HA | 1.55 | 0.41 |
| 1:O:111:ILE:O | 1:O:112:CYS:C | 2.58 | 0.41 |
| 1:O:123:TYR:CE2 | 1:O:202:LYS:CB | 3.04 | 0.41 |
| 1:O:410:GLY:O | 1:O:413:VAL:HG22 | 2.20 | 0.41 |
| 1:O:343:TYR:CE1 | 1:O:486:TRP:HB2 | 2.55 | 0.41 |
| 1:Y:251:PHE:O | 1:Y:254:LEU:HD12 | 2.20 | 0.41 |
| 1:Y:250:LEU:CD1 | 1:Y:255:CYS:HB2 | 2.51 | 0.41 |
| 1:Y:466:ILE:HD13 | 1:Y:466:ILE:C | 2.41 | 0.41 |
| 1:Y:488:LYS:HD3 | 1:O:496:TRP:CZ3 | 2.56 | 0.41 |
| 1:O:296:GLY:N | 1:O:297:GLU:OE1 | 2.53 | 0.41 |
| 1:O:347:ALA:O | 1:O:348:PHE:C | 2.58 | 0.41 |
| 1:Y:142:LYS:HE3 | 1:Y:146:ASP:OD2 | 2.21 | 0.41 |
| 1:Y:77:ILE:O | 1:Y:239:ILE:HA | 2.21 | 0.41 |
| 1:Y:256:VAL:CG1 | 1:Y:294:PRO:CG | 2.99 | 0.41 |
| 1:O:133:ASP:OD1 | 1:O:135:TYR:N | 2.43 | 0.41 |
| 1:O:151:SER:HA | 1:O:160:LEU:CD1 | 2.51 | 0.41 |
| 1:O:20:VAL:HG23 | 1:O:63:VAL:CG1 | 2.50 | 0.41 |
| 1:O:213:MET:HG2 | 1:O:214:LEU:CD1 | 2.49 | 0.41 |
| 1:O:255:CYS:SG | 1:O:260:MET:HB3 | 2.61 | 0.41 |
| 1:O:270:PHE:CD1 | 1:O:270:PHE:N | 2.89 | 0.41 |
| 1:Y:154:ARG:CB | 1:Y:159:GLU:CB | 2.99 | 0.41 |
| 1:Y:154:ARG:HG3 | 1:Y:160:LEU:HD12 | 2.02 | 0.41 |
| 1:Y:183:TYR:N | 1:Y:183:TYR:CD1 | 2.79 | 0.41 |
| 1:Y:188:ARG:HH21 | 1:Y:289:THR:CG2 | 2.33 | 0.41 |
| 1:Y:127:ASN:CB | 1:Y:193:ASN:ND2 | 2.79 | 0.41 |
| 1:Y:434:GLU:N | 1:Y:465:VAL:O | 2.54 | 0.41 |
| 1:Y:83:ARG:N | 4:Y:600:GOL:O2 | 2.53 | 0.41 |
| 1:O:394:ALA:O | 1:O:398:ASP:N | 2.41 | 0.41 |
| 1:O:98:TYR:CD1 | 1:O:99:ASN:N | 2.89 | 0.41 |
| 1:Y:183:TYR:CD1 | 1:Y:217:VAL:CG1 | 3.00 | 0.41 |
| 1:Y:375:HIS:O | 1:Y:376:ILE:C | 2.57 | 0.41 |
| 1:Y:391:VAL:HG22 | 1:Y:392:LEU:N | 2.35 | 0.41 |
| 1:Y:401:ILE:CG2 | 1:Y:402:ARG:N | 2.84 | 0.41 |
| 1:Y:474:ILE:HD12 | 1:Y:474:ILE:HA | 1.73 | 0.41 |
| 1:Y:8:ALA:HB2 | 1:Y:21:MET:HE1 | 2.03 | 0.41 |
| 1:O:168:TRP:O | 1:O:172:LYS:HG2 | 2.20 | 0.41 |
| 1:O:254:LEU:O | 1:O:256:VAL:N | 2.54 | 0.41 |
| 1:O:348:PHE:CE1 | 1:O:362:GLY:HA3 | 2.56 | 0.41 |
| 1:O:372:ASN:O | 1:O:373:ALA:C | 2.59 | 0.41 |
| 1:O:405:ALA:HB1 | 1:O:431:GLU:CD | 2.42 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:9:LEU:CD1 | 1:O:18:ALA:CB | 2.99 | 0.41 |
| 1:Y:123:TYR:CD2 | 1:Y:203:MET:CE | 3.00 | 0.41 |
| 1:Y:142:LYS:O | 1:Y:144:ILE:N | 2.54 | 0.41 |
| 1:Y:152:ARG:CB | 1:Y:156:ARG:NH2 | 2.80 | 0.41 |
| 1:O:257:LYS:H | 1:O:260:MET:HG3 | 1.86 | 0.40 |
| 1:Y:91:LYS:HZ2 | 1:Y:161:LEU:HD11 | 1.86 | 0.40 |
| 1:Y:334:THR:H | 1:Y:334:THR:HG23 | 1.49 | 0.40 |
| 1:Y:413:VAL:CA | 1:Y:419:MET:HE3 | 2.49 | 0.40 |
| 1:O:222:GLU:HG3 | 1:O:223:VAL:N | 2.36 | 0.40 |
| 1:O:344:VAL:O | 1:O:346:PRO:HD3 | 2.20 | 0.40 |
| 1:Y:166:ASP:O | 1:Y:167:THR:C | 2.58 | 0.40 |
| 1:Y:277:GLU:O | 1:Y:300:TYR:HE2 | 2.04 | 0.40 |
| 1:O:115:LEU:O | 1:O:120:LEU:HD12 | 2.22 | 0.40 |
| 1:O:38:ILE:HG22 | 1:O:40:PRO:N | 2.36 | 0.40 |
| 1:Y:124:ILE:CD1 | 1:Y:203:MET:CE | 3.00 | 0.40 |
| 1:Y:295:THR:HG23 | 1:Y:297:GLU:CD | 2.42 | 0.40 |
| 1:Y:316:LEU:HA | 1:Y:316:LEU:HD23 | 1.27 | 0.40 |
| 1:Y:351:LEU:HD22 | 1:Y:360:ALA:CB | 2.52 | 0.40 |
| 1:Y:439:THR:O | 1:Y:442:GLY:N | 2.55 | 0.40 |
| 1:Y:48:ASP:O | 1:Y:52:ILE:N | 2.41 | 0.40 |
| 1:Y:54:ALA:O | 1:Y:57:SER:N | 2.49 | 0.40 |
| 1:O:181:THR:HG22 | 1:O:217:VAL:HG13 | 2.02 | 0.40 |
| 1:O:41:LYS:CB | 1:O:42:PRO:CD | 2.99 | 0.40 |
| 1:O:480:ASN:O | 1:O:481:TYR:C | 2.58 | 0.40 |
| 1:Y:381:LEU:HA | 1:Y:381:LEU:HD23 | 1.85 | 0.40 |
| 1:Y:422:GLN:HA | 1:Y:422:GLN:NE2 | 2.37 | 0.40 |
| 1:Y:453:PHE:CD2 | 1:Y:454:TRP:CE3 | 3.07 | 0.40 |
| 1:O:44:TRP:CD2 | 1:O:107:ARG:HB2 | 2.56 | 0.40 |
| 1:O:228:ASN:HB2 | 1:O:236:ARG:NH2 | 2.37 | 0.40 |
| 1:O:336:VAL:HG11 | 1:O:375:HIS:CD2 | 2.56 | 0.40 |
| 1:O:347:ALA:HB2 | 1:O:351:LEU:HD13 | 2.03 | 0.40 |
| 1:O:389:ARG:HB2 | 1:O:426:LEU:CD1 | 2.50 | 0.40 |
| 1:O:422:GLN:HG3 | 1:O:426:LEU:CD2 | 2.51 | 0.40 |
| 1:Y:121:GLU:O | 1:Y:124:ILE:N | 2.55 | 0.40 |
| 1:Y:162:PHE:O | 1:Y:215:PRO:HD3 | 2.21 | 0.40 |
| 1:Y:71:SER:OG | 1:Y:230:GLY:O | 2.29 | 0.40 |
| 1:Y:251:PHE:O | 1:Y:254:LEU:HA | 2.22 | 0.40 |
| 1:Y:324:ASN:ND2 | 1:Y:324:ASN:H | 2.19 | 0.40 |
| 1:Y:432:ARG:HG2 | 1:Y:436:ARG:NH1 | 2.37 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|----------|-------------|---|
| 1 | O | 490/501 (98%) | 341 (70%) | 102 (21%) | 47 (10%) | 1 | 3 |
| 1 | Y | 490/501 (98%) | 354 (72%) | 87 (18%) | 49 (10%) | 1 | 3 |
| All | All | 980/1002 (98%) | 695 (71%) | 189 (19%) | 96 (10%) | 1 | 3 |

All (96) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Y | 58 | TRP |
| 1 | Y | 59 | THR |
| 1 | Y | 64 | LEU |
| 1 | Y | 151 | SER |
| 1 | Y | 165 | VAL |
| 1 | Y | 212 | GLU |
| 1 | Y | 213 | MET |
| 1 | Y | 445 | TYR |
| 1 | Y | 446 | LEU |
| 1 | Y | 456 | ASN |
| 1 | O | 66 | LYS |
| 1 | O | 165 | VAL |
| 1 | O | 187 | SER |
| 1 | O | 199 | TRP |
| 1 | O | 258 | GLU |
| 1 | O | 443 | ALA |
| 1 | O | 445 | TYR |
| 1 | O | 446 | LEU |
| 1 | Y | 53 | TRP |
| 1 | Y | 65 | ALA |
| 1 | Y | 92 | GLU |
| 1 | Y | 172 | LYS |
| 1 | Y | 187 | SER |
| 1 | Y | 188 | ARG |
| 1 | Y | 196 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Y | 202 | LYS |
| 1 | Y | 358 | PRO |
| 1 | Y | 439 | THR |
| 1 | Y | 461 | GLN |
| 1 | Y | 477 | THR |
| 1 | O | 64 | LEU |
| 1 | O | 71 | SER |
| 1 | O | 99 | ASN |
| 1 | O | 118 | ASP |
| 1 | O | 119 | GLY |
| 1 | O | 138 | GLY |
| 1 | O | 141 | VAL |
| 1 | O | 172 | LYS |
| 1 | O | 188 | ARG |
| 1 | O | 276 | GLY |
| 1 | O | 294 | PRO |
| 1 | O | 444 | ALA |
| 1 | O | 456 | ASN |
| 1 | Y | 54 | ALA |
| 1 | Y | 61 | VAL |
| 1 | Y | 121 | GLU |
| 1 | Y | 130 | LEU |
| 1 | Y | 138 | GLY |
| 1 | Y | 143 | TRP |
| 1 | Y | 153 | GLU |
| 1 | Y | 199 | TRP |
| 1 | Y | 441 | LEU |
| 1 | Y | 459 | GLU |
| 1 | Y | 478 | GLU |
| 1 | Y | 492 | ARG |
| 1 | O | 143 | TRP |
| 1 | O | 201 | ASP |
| 1 | O | 212 | GLU |
| 1 | O | 213 | MET |
| 1 | O | 390 | ASP |
| 1 | O | 442 | GLY |
| 1 | O | 461 | GLN |
| 1 | Y | 71 | SER |
| 1 | Y | 99 | ASN |
| 1 | Y | 147 | HIS |
| 1 | Y | 175 | GLN |
| 1 | Y | 418 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 55 | THR |
| 1 | O | 140 | LYS |
| 1 | O | 151 | SER |
| 1 | O | 202 | LYS |
| 1 | Y | 110 | GLU |
| 1 | Y | 142 | LYS |
| 1 | Y | 145 | LEU |
| 1 | Y | 298 | VAL |
| 1 | O | 63 | VAL |
| 1 | O | 92 | GLU |
| 1 | O | 111 | ILE |
| 1 | O | 121 | GLU |
| 1 | O | 145 | LEU |
| 1 | O | 242 | ILE |
| 1 | O | 298 | VAL |
| 1 | O | 418 | LEU |
| 1 | O | 459 | GLU |
| 1 | O | 110 | GLU |
| 1 | O | 114 | HIS |
| 1 | O | 131 | VAL |
| 1 | O | 157 | ARG |
| 1 | Y | 27 | ILE |
| 1 | Y | 238 | PRO |
| 1 | Y | 346 | PRO |
| 1 | Y | 411 | GLY |
| 1 | O | 490 | VAL |
| 1 | Y | 170 | ILE |
| 1 | Y | 490 | VAL |
| 1 | O | 144 | ILE |

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 | O | 408/412 (99%) | 258 (63%) | 150 (37%) | 0 1 |
| 1 | Y | 408/412 (99%) | 259 (64%) | 149 (36%) | 0 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|---------------|-----------|-----------|-------------------|
| All | All | 816/824 (99%) | 517 (63%) | 299 (37%) | 0 1 |

All (299) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Y | 2 | GLU |
| 1 | Y | 3 | LYS |
| 1 | Y | 4 | LYS |
| 1 | Y | 11 | GLN |
| 1 | Y | 13 | THR |
| 1 | Y | 21 | MET |
| 1 | Y | 24 | ASP |
| 1 | Y | 28 | ILE |
| 1 | Y | 32 | GLN |
| 1 | Y | 33 | ARG |
| 1 | Y | 34 | GLU |
| 1 | Y | 41 | LYS |
| 1 | Y | 46 | GLU |
| 1 | Y | 53 | TRP |
| 1 | Y | 57 | SER |
| 1 | Y | 60 | LEU |
| 1 | Y | 62 | GLU |
| 1 | Y | 63 | VAL |
| 1 | Y | 64 | LEU |
| 1 | Y | 71 | SER |
| 1 | Y | 73 | GLN |
| 1 | Y | 74 | ILE |
| 1 | Y | 79 | ILE |
| 1 | Y | 80 | THR |
| 1 | Y | 81 | ASN |
| 1 | Y | 87 | ILE |
| 1 | Y | 91 | LYS |
| 1 | Y | 92 | GLU |
| 1 | Y | 93 | THR |
| 1 | Y | 95 | LYS |
| 1 | Y | 97 | ILE |
| 1 | Y | 106 | ARG |
| 1 | Y | 107 | ARG |
| 1 | Y | 116 | LYS |
| 1 | Y | 117 | ARG |
| 1 | Y | 118 | ASP |
| 1 | Y | 120 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Y | 124 | ILE |
| 1 | Y | 128 | THR |
| 1 | Y | 130 | LEU |
| 1 | Y | 137 | SER |
| 1 | Y | 139 | THR |
| 1 | Y | 141 | VAL |
| 1 | Y | 142 | LYS |
| 1 | Y | 145 | LEU |
| 1 | Y | 146 | ASP |
| 1 | Y | 148 | VAL |
| 1 | Y | 149 | GLU |
| 1 | Y | 151 | SER |
| 1 | Y | 154 | ARG |
| 1 | Y | 156 | ARG |
| 1 | Y | 157 | ARG |
| 1 | Y | 162 | PHE |
| 1 | Y | 164 | THR |
| 1 | Y | 165 | VAL |
| 1 | Y | 169 | LEU |
| 1 | Y | 170 | ILE |
| 1 | Y | 172 | LYS |
| 1 | Y | 173 | MET |
| 1 | Y | 175 | GLN |
| 1 | Y | 178 | VAL |
| 1 | Y | 180 | VAL |
| 1 | Y | 181 | THR |
| 1 | Y | 187 | SER |
| 1 | Y | 191 | LEU |
| 1 | Y | 195 | HIS |
| 1 | Y | 196 | THR |
| 1 | Y | 205 | GLU |
| 1 | Y | 211 | ARG |
| 1 | Y | 213 | MET |
| 1 | Y | 218 | ARG |
| 1 | Y | 222 | GLU |
| 1 | Y | 227 | THR |
| 1 | Y | 228 | ASN |
| 1 | Y | 229 | ILE |
| 1 | Y | 235 | THR |
| 1 | Y | 236 | ARG |
| 1 | Y | 237 | ILE |
| 1 | Y | 239 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Y | 240 | SER |
| 1 | Y | 242 | ILE |
| 1 | Y | 246 | GLN |
| 1 | Y | 253 | GLN |
| 1 | Y | 257 | LYS |
| 1 | Y | 260 | MET |
| 1 | Y | 262 | LYS |
| 1 | Y | 271 | MET |
| 1 | Y | 273 | MET |
| 1 | Y | 278 | LYS |
| 1 | Y | 281 | LYS |
| 1 | Y | 287 | LEU |
| 1 | Y | 290 | ILE |
| 1 | Y | 295 | THR |
| 1 | Y | 302 | LEU |
| 1 | Y | 312 | SER |
| 1 | Y | 314 | GLN |
| 1 | Y | 317 | ARG |
| 1 | Y | 324 | ASN |
| 1 | Y | 325 | ASP |
| 1 | Y | 335 | LYS |
| 1 | Y | 339 | THR |
| 1 | Y | 351 | LEU |
| 1 | Y | 364 | ILE |
| 1 | Y | 368 | THR |
| 1 | Y | 369 | ARG |
| 1 | Y | 376 | ILE |
| 1 | Y | 383 | SER |
| 1 | Y | 384 | ILE |
| 1 | Y | 389 | ARG |
| 1 | Y | 390 | ASP |
| 1 | Y | 391 | VAL |
| 1 | Y | 392 | LEU |
| 1 | Y | 402 | ARG |
| 1 | Y | 406 | LEU |
| 1 | Y | 407 | ARG |
| 1 | Y | 409 | ASP |
| 1 | Y | 415 | ASN |
| 1 | Y | 418 | LEU |
| 1 | Y | 423 | SER |
| 1 | Y | 425 | ILE |
| 1 | Y | 426 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Y | 428 | THR |
| 1 | Y | 429 | ARG |
| 1 | Y | 431 | GLU |
| 1 | Y | 434 | GLU |
| 1 | Y | 436 | ARG |
| 1 | Y | 437 | GLU |
| 1 | Y | 438 | VAL |
| 1 | Y | 445 | TYR |
| 1 | Y | 446 | LEU |
| 1 | Y | 449 | LEU |
| 1 | Y | 451 | VAL |
| 1 | Y | 454 | TRP |
| 1 | Y | 455 | GLN |
| 1 | Y | 457 | LEU |
| 1 | Y | 461 | GLN |
| 1 | Y | 462 | GLU |
| 1 | Y | 463 | LYS |
| 1 | Y | 466 | ILE |
| 1 | Y | 467 | GLU |
| 1 | Y | 468 | ARG |
| 1 | Y | 469 | GLU |
| 1 | Y | 474 | ILE |
| 1 | Y | 479 | ARG |
| 1 | Y | 482 | ARG |
| 1 | Y | 483 | TYR |
| 1 | Y | 488 | LYS |
| 1 | Y | 492 | ARG |
| 1 | Y | 494 | MET |
| 1 | O | 3 | LYS |
| 1 | O | 4 | LYS |
| 1 | O | 5 | TYR |
| 1 | O | 9 | LEU |
| 1 | O | 11 | GLN |
| 1 | O | 21 | MET |
| 1 | O | 24 | ASP |
| 1 | O | 27 | ILE |
| 1 | O | 28 | ILE |
| 1 | O | 29 | SER |
| 1 | O | 31 | SER |
| 1 | O | 32 | GLN |
| 1 | O | 33 | ARG |
| 1 | O | 34 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 41 | LYS |
| 1 | O | 51 | GLU |
| 1 | O | 52 | ILE |
| 1 | O | 57 | SER |
| 1 | O | 60 | LEU |
| 1 | O | 64 | LEU |
| 1 | O | 71 | SER |
| 1 | O | 72 | ASP |
| 1 | O | 73 | GLN |
| 1 | O | 74 | ILE |
| 1 | O | 80 | THR |
| 1 | O | 81 | ASN |
| 1 | O | 82 | GLN |
| 1 | O | 86 | THR |
| 1 | O | 87 | ILE |
| 1 | O | 91 | LYS |
| 1 | O | 92 | GLU |
| 1 | O | 93 | THR |
| 1 | O | 95 | LYS |
| 1 | O | 102 | VAL |
| 1 | O | 104 | GLN |
| 1 | O | 106 | ARG |
| 1 | O | 107 | ARG |
| 1 | O | 117 | ARG |
| 1 | O | 118 | ASP |
| 1 | O | 124 | ILE |
| 1 | O | 125 | ARG |
| 1 | O | 128 | THR |
| 1 | O | 131 | VAL |
| 1 | O | 135 | TYR |
| 1 | O | 136 | PHE |
| 1 | O | 137 | SER |
| 1 | O | 139 | THR |
| 1 | O | 141 | VAL |
| 1 | O | 142 | LYS |
| 1 | O | 145 | LEU |
| 1 | O | 147 | HIS |
| 1 | O | 149 | GLU |
| 1 | O | 153 | GLU |
| 1 | O | 154 | ARG |
| 1 | O | 156 | ARG |
| 1 | O | 157 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 161 | LEU |
| 1 | O | 162 | PHE |
| 1 | O | 164 | THR |
| 1 | O | 165 | VAL |
| 1 | O | 169 | LEU |
| 1 | O | 170 | ILE |
| 1 | O | 172 | LYS |
| 1 | O | 173 | MET |
| 1 | O | 178 | VAL |
| 1 | O | 181 | THR |
| 1 | O | 182 | ASP |
| 1 | O | 188 | ARG |
| 1 | O | 191 | LEU |
| 1 | O | 195 | HIS |
| 1 | O | 196 | THR |
| 1 | O | 201 | ASP |
| 1 | O | 205 | GLU |
| 1 | O | 206 | VAL |
| 1 | O | 211 | ARG |
| 1 | O | 213 | MET |
| 1 | O | 214 | LEU |
| 1 | O | 218 | ARG |
| 1 | O | 219 | ARG |
| 1 | O | 222 | GLU |
| 1 | O | 227 | THR |
| 1 | O | 228 | ASN |
| 1 | O | 229 | ILE |
| 1 | O | 235 | THR |
| 1 | O | 236 | ARG |
| 1 | O | 237 | ILE |
| 1 | O | 239 | ILE |
| 1 | O | 240 | SER |
| 1 | O | 246 | GLN |
| 1 | O | 253 | GLN |
| 1 | O | 256 | VAL |
| 1 | O | 260 | MET |
| 1 | O | 262 | LYS |
| 1 | O | 269 | CYS |
| 1 | O | 271 | MET |
| 1 | O | 273 | MET |
| 1 | O | 278 | LYS |
| 1 | O | 280 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 281 | LYS |
| 1 | O | 290 | ILE |
| 1 | O | 295 | THR |
| 1 | O | 316 | LEU |
| 1 | O | 317 | ARG |
| 1 | O | 322 | LEU |
| 1 | O | 324 | ASN |
| 1 | O | 325 | ASP |
| 1 | O | 335 | LYS |
| 1 | O | 339 | THR |
| 1 | O | 351 | LEU |
| 1 | O | 364 | ILE |
| 1 | O | 368 | THR |
| 1 | O | 369 | ARG |
| 1 | O | 378 | ARG |
| 1 | O | 383 | SER |
| 1 | O | 389 | ARG |
| 1 | O | 391 | VAL |
| 1 | O | 392 | LEU |
| 1 | O | 402 | ARG |
| 1 | O | 406 | LEU |
| 1 | O | 407 | ARG |
| 1 | O | 415 | ASN |
| 1 | O | 418 | LEU |
| 1 | O | 423 | SER |
| 1 | O | 426 | LEU |
| 1 | O | 428 | THR |
| 1 | O | 429 | ARG |
| 1 | O | 434 | GLU |
| 1 | O | 435 | VAL |
| 1 | O | 436 | ARG |
| 1 | O | 437 | GLU |
| 1 | O | 438 | VAL |
| 1 | O | 439 | THR |
| 1 | O | 451 | VAL |
| 1 | O | 455 | GLN |
| 1 | O | 456 | ASN |
| 1 | O | 457 | LEU |
| 1 | O | 460 | LEU |
| 1 | O | 461 | GLN |
| 1 | O | 462 | GLU |
| 1 | O | 463 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 466 | ILE |
| 1 | O | 467 | GLU |
| 1 | O | 468 | ARG |
| 1 | O | 469 | GLU |
| 1 | O | 478 | GLU |
| 1 | O | 482 | ARG |
| 1 | O | 486 | TRP |
| 1 | O | 488 | LYS |
| 1 | O | 492 | ARG |
| 1 | O | 494 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Y | 11 | GLN |
| 1 | Y | 23 | HIS |
| 1 | Y | 26 | ASN |
| 1 | Y | 32 | GLN |
| 1 | Y | 73 | GLN |
| 1 | Y | 81 | ASN |
| 1 | Y | 104 | GLN |
| 1 | Y | 114 | HIS |
| 1 | Y | 127 | ASN |
| 1 | Y | 147 | HIS |
| 1 | Y | 185 | ASN |
| 1 | Y | 228 | ASN |
| 1 | Y | 253 | GLN |
| 1 | Y | 274 | ASN |
| 1 | Y | 284 | ASN |
| 1 | Y | 299 | ASN |
| 1 | Y | 324 | ASN |
| 1 | Y | 337 | GLN |
| 1 | Y | 396 | GLN |
| 1 | Y | 415 | ASN |
| 1 | Y | 420 | GLN |
| 1 | Y | 422 | GLN |
| 1 | Y | 456 | ASN |
| 1 | Y | 461 | GLN |
| 1 | O | 11 | GLN |
| 1 | O | 23 | HIS |
| 1 | O | 26 | ASN |
| 1 | O | 37 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 73 | GLN |
| 1 | O | 81 | ASN |
| 1 | O | 114 | HIS |
| 1 | O | 127 | ASN |
| 1 | O | 147 | HIS |
| 1 | O | 179 | HIS |
| 1 | O | 185 | ASN |
| 1 | O | 228 | ASN |
| 1 | O | 246 | GLN |
| 1 | O | 253 | GLN |
| 1 | O | 274 | ASN |
| 1 | O | 284 | ASN |
| 1 | O | 299 | ASN |
| 1 | O | 337 | GLN |
| 1 | O | 387 | GLN |
| 1 | O | 415 | ASN |
| 1 | O | 420 | GLN |
| 1 | O | 499 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | GOL | O | 600 | - | 5,5,5 | 0.59 | 0 | 5,5,5 | 0.30 | 0 |
| 3 | ACP | O | 601 | 2 | 27,33,33 | 2.80 | 6 (22%) | 30,52,52 | 2.65 | 4 (13%) |
| 4 | GOL | Y | 600 | - | 5,5,5 | 0.43 | 0 | 5,5,5 | 0.72 | 0 |
| 3 | ACP | Y | 601 | 2 | 27,33,33 | 2.29 | 4 (14%) | 30,52,52 | 1.84 | 4 (13%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | GOL | O | 600 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ACP | O | 601 | 2 | - | 0/15/38/38 | 0/3/3/3 |
| 4 | GOL | Y | 600 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ACP | Y | 601 | 2 | - | 0/15/38/38 | 0/3/3/3 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3 | O | 601 | ACP | C4-N3 | -2.04 | 1.32 | 1.35 |
| 3 | O | 601 | ACP | PB-O1B | 2.22 | 1.57 | 1.51 |
| 3 | O | 601 | ACP | PB-O3A | 3.88 | 1.62 | 1.58 |
| 3 | Y | 601 | ACP | PG-O1G | 4.34 | 1.59 | 1.50 |
| 3 | Y | 601 | ACP | PB-O3A | 5.07 | 1.64 | 1.58 |
| 3 | Y | 601 | ACP | PG-O2G | 5.38 | 1.67 | 1.54 |
| 3 | O | 601 | ACP | PG-O1G | 6.07 | 1.63 | 1.50 |
| 3 | Y | 601 | ACP | PG-O3G | 7.28 | 1.72 | 1.54 |
| 3 | O | 601 | ACP | PG-O3G | 7.50 | 1.72 | 1.54 |
| 3 | O | 601 | ACP | PG-O2G | 9.18 | 1.76 | 1.54 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3 | Y | 601 | ACP | PA-O3A-PB | -3.48 | 121.17 | 132.39 |
| 3 | Y | 601 | ACP | O1G-PG-C3B | -3.27 | 104.00 | 111.22 |
| 3 | O | 601 | ACP | PA-O3A-PB | -3.14 | 122.25 | 132.39 |
| 3 | O | 601 | ACP | O1G-PG-C3B | -2.46 | 105.80 | 111.22 |
| 3 | Y | 601 | ACP | C5-C6-N6 | 2.04 | 124.64 | 120.47 |
| 3 | O | 601 | ACP | C5-C6-N6 | 2.48 | 125.53 | 120.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | Y | 601 | ACP | C1'-N9-C4 | 7.36 | 139.36 | 126.64 |
| 3 | O | 601 | ACP | C1'-N9-C4 | 13.12 | 149.31 | 126.64 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 18 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | O | 600 | GOL | 7 | 0 |
| 3 | O | 601 | ACP | 4 | 0 |
| 4 | Y | 600 | GOL | 2 | 0 |
| 3 | Y | 601 | ACP | 5 | 0 |

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, 95th 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 ²) | Q<0.9 |
|-----|-------|----------------|--------|-----------|-----------------------|-------|
| 1 | O | 494/501 (98%) | -0.79 | 0 100 100 | 13, 61, 94, 100 | 0 |
| 1 | Y | 494/501 (98%) | -0.98 | 0 100 100 | 7, 48, 81, 98 | 0 |
| All | All | 988/1002 (98%) | -0.88 | 0 100 100 | 7, 54, 88, 100 | 0 |

There are no RSRZ outliers to report.

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4 | GOL | Y | 600 | 6/6 | 0.96 | 0.13 | 1.01 | 32,32,32,32 | 0 |
| 3 | ACP | O | 601 | 31/31 | 0.96 | 0.13 | 0.58 | 60,60,60,60 | 0 |
| 3 | ACP | Y | 601 | 31/31 | 0.97 | 0.11 | 0.16 | 47,47,47,47 | 0 |
| 4 | GOL | O | 600 | 6/6 | 0.98 | 0.09 | -1.83 | 29,29,29,29 | 0 |
| 2 | MG | O | 602 | 1/1 | 0.90 | 0.56 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2 | MG | Y | 602 | 1/1 | 0.99 | 0.20 | - | 40,40,40,40 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.