# Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:40 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1BWF |
| 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 | : | 1998-09-23 |
| 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

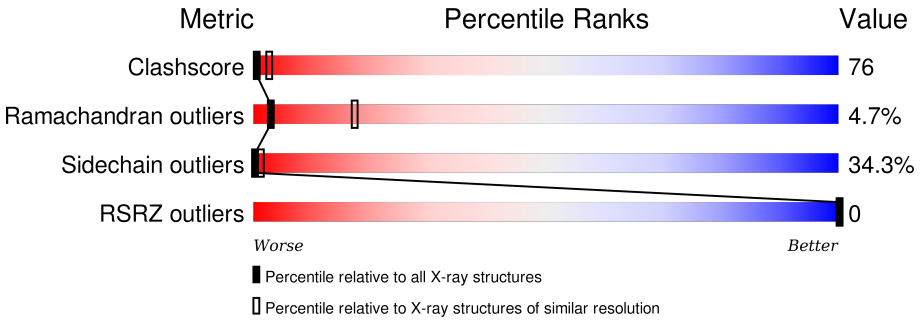
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

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 | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |
| RSRZ outliers | 91569 | 1592 (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 <=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 | 18% 40% 34% 8% |
| 1 | Y | 501 | 21% 43% 26% 9% |

# 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7900 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 | | | |

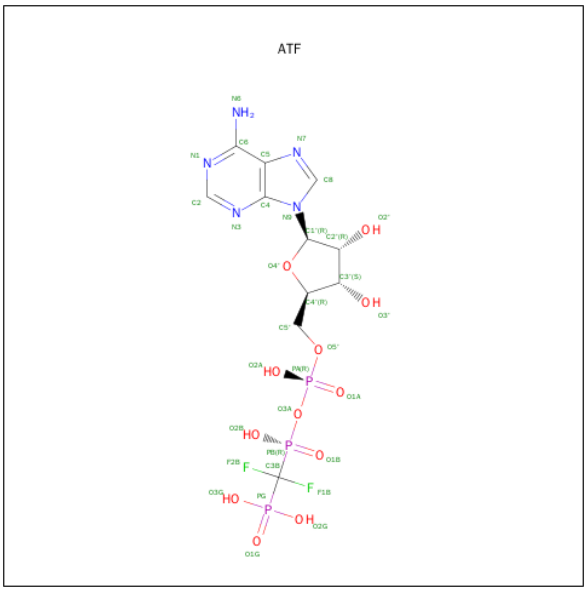
There are 2 discrepancies between the modelled and reference sequences:

| 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).

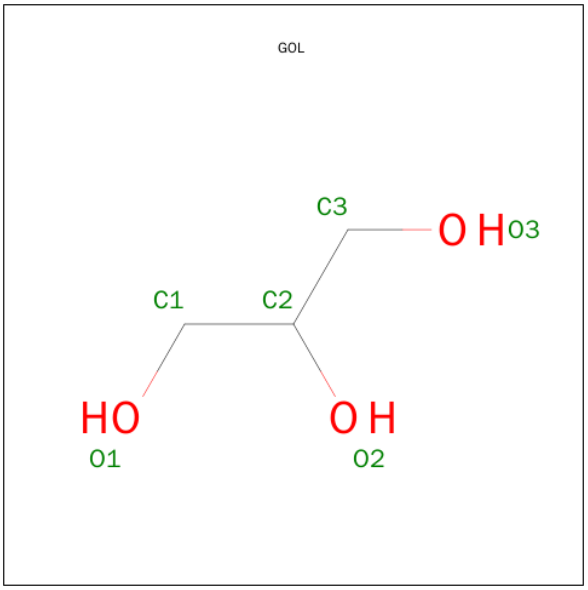
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | O | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 3 is PHOSPHODIFLUOROMETHYLPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ATF) (formula: $C_{11}H_{16}F_2N_5O_{12}P_3$).




| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | Y | 1 | Total | C | F | N | O | P | 0 | 0 |
| | | | 33 | 11 | 2 | 5 | 12 | 3 | | |
| 3 | O | 1 | Total | C | F | N | O | P | 0 | 0 |
| | | | 33 | 11 | 2 | 5 | 12 | 3 | | |

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



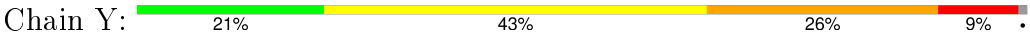

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 4 | Y | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 4 | O | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

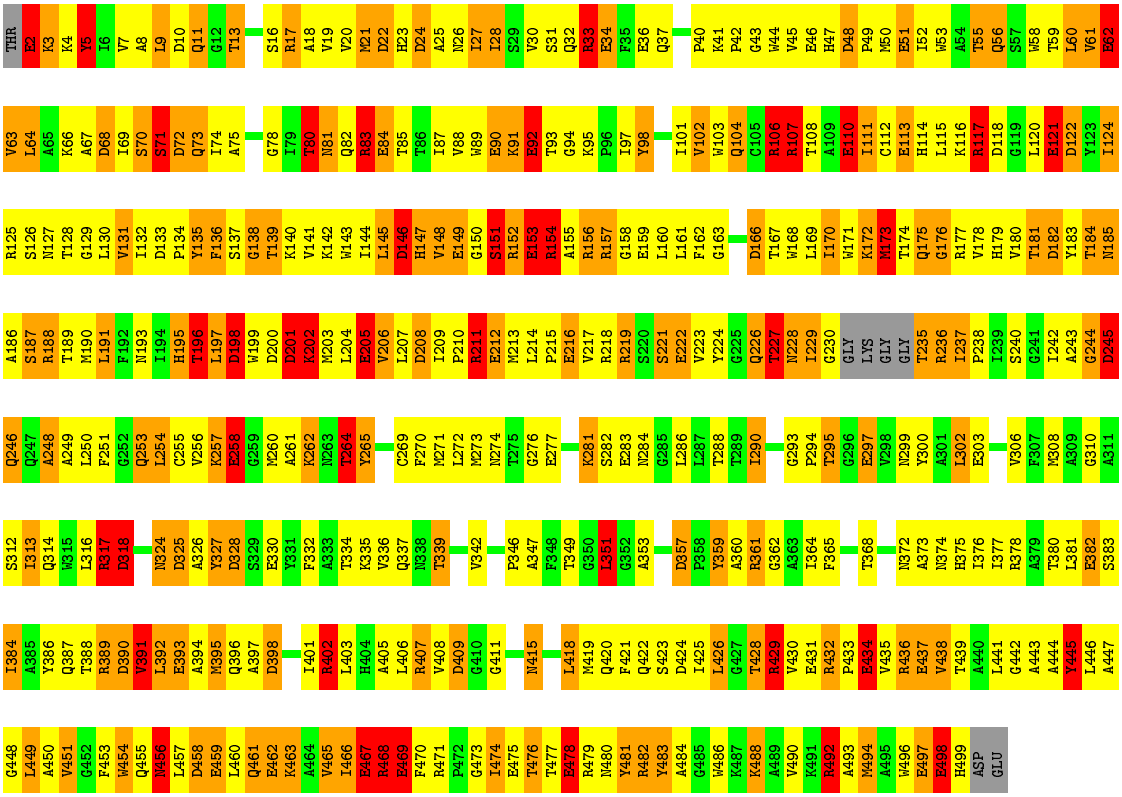
# 3 Residue-property plots (i)

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

- Molecule 1: GLYCEROL KINASE

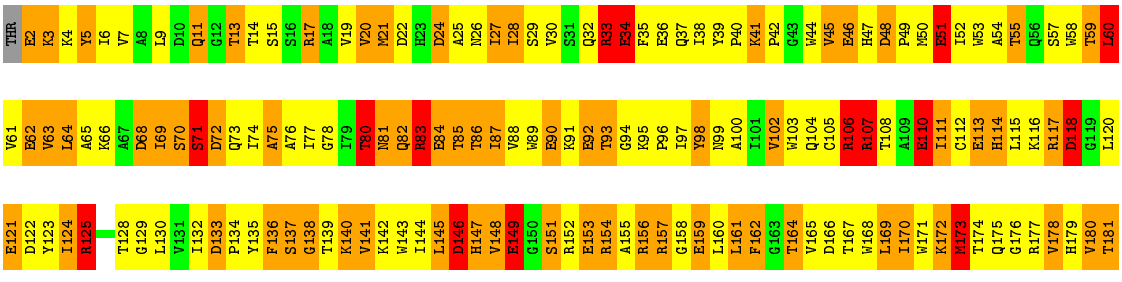
Chain Y:

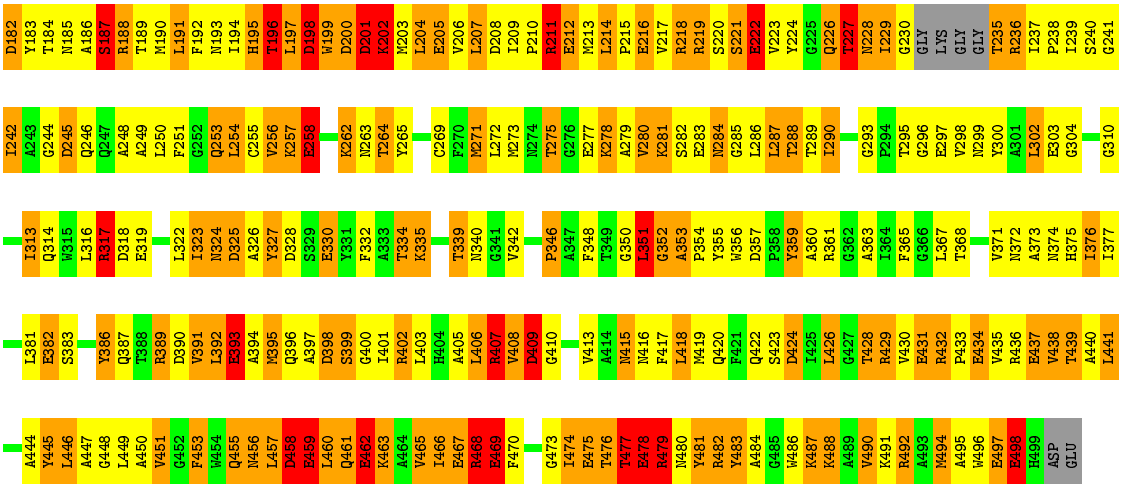


- Molecule 1: GLYCEROL KINASE

Chain O:


D182 Y183 T184 N185 A186 S187 R188 T189 M190 L191 F192 N193 I194 H195 T196 L197 D198 W199 D200 D201 K202 M203 L204 E205 V206 L207 D208 I209 P210 R211 E212 M213 L214 P215 E216 V217 R218 R219 S220 S221 E222 V223 Y224 G225 Q226 T227 N228 I229 G230 GLY LYS GLY GLY T235 R236 I237 P238 I239 S240 G241
I242 A243 G244 D245 Q246 Q247 A248 A249 L250 F251 G252 Q253 L254 C255 V256 K257 E258 K262 N263 T264 Y265 C269 F270 M271 L272 M273 N274 T275 G276 E277 K278 A279 V280 K281 S282 E283 N284 G285 L286 L287 T288 T289 I290 G293 P294 T295 G296 E297 V298 N299 Y300 A301 L302 E303 G304 G310
I313 Q314 W315 L316 R317 D318 E319 L322 I323 N324 D325 A326 Y327 D328 S329 E330 Y331 F332 A333 T334 K335 T339 N340 G341 V342 P346 A347 F348 T349 G350 L351 G352 A353 P354 Y355 W356 D357 P358 Y359 A360 R361 G362 A363 I364 F365 G366 L367 T368 V371 N372 A373 N374 H375 I376 I377
L381 E382 S383 Y386 Q387 T388 R389 D390 V391 L392 E393 A394 M395 Q396 A397 D398 S399 G400 I401 R402 L403 H404 A405 L406 R407 V408 D409 G410 V413 A414 N415 N416 F417 L418 M419 Q420 F421 Q422 S423 D424 I425 L426 G427 T428 R429 V430 E431 R432 P433 E434 V435 R436 E437 V438 T439 A440 L441
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 G473 I474 E475 T476 T477 E478 R479 N480 Y481 R482 Y483 A484 G485 W486 K487 K488 A489 V490 K491 R492 A493 M494 A495 W496 E497 E498 H499 ASP GLU

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 99.77Å 200.29Å 114.74Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.00<br>18.17 – 2.90 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 95.0 (20.00-3.00)<br>92.3 (18.17-2.90) | Depositor<br>EDS |
| $R_{merge}$ | 0.06 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 200.72 (at 2.92Å) | Xtriage |
| Refinement program | TNT V. 5-F | Depositor |
| R, $R_{free}$ | 0.168 , (Not available)<br>0.160 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | DCC |
| Wilson B-factor (Å$^2$) | 48.3 | Xtriage |
| Anisotropy | 0.104 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.22 , 123.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Outliers | 0 of 23899 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 7900 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 49.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

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 | 1.24 | 36/3991 (0.9%) | 1.72 | 77/5412 (1.4%) |
| 1 | Y | 1.30 | 36/3991 (0.9%) | 1.79 | 98/5412 (1.8%) |
| All | All | 1.27 | 72/7982 (0.9%) | 1.76 | 175/10824 (1.6%) |

All (72) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 34 | GLU | CD-OE1 | 9.50 | 1.36 | 1.25 |
| 1 | O | 121 | GLU | CD-OE2 | 8.64 | 1.35 | 1.25 |
| 1 | O | 34 | GLU | CD-OE2 | 8.52 | 1.35 | 1.25 |
| 1 | O | 84 | GLU | CD-OE1 | 8.38 | 1.34 | 1.25 |
| 1 | Y | 216 | GLU | CD-OE2 | 8.37 | 1.34 | 1.25 |
| 1 | Y | 498 | GLU | CD-OE2 | 8.19 | 1.34 | 1.25 |
| 1 | O | 62 | GLU | CD-OE1 | 8.17 | 1.34 | 1.25 |
| 1 | Y | 462 | GLU | CD-OE2 | 8.14 | 1.34 | 1.25 |
| 1 | Y | 92 | GLU | CD-OE2 | 8.12 | 1.34 | 1.25 |
| 1 | Y | 153 | GLU | CD-OE1 | 8.10 | 1.34 | 1.25 |
| 1 | Y | 205 | GLU | CD-OE1 | 8.04 | 1.34 | 1.25 |
| 1 | O | 92 | GLU | CD-OE2 | 7.76 | 1.34 | 1.25 |
| 1 | Y | 283 | GLU | CD-OE1 | 7.68 | 1.34 | 1.25 |
| 1 | O | 205 | GLU | CD-OE1 | 7.58 | 1.33 | 1.25 |
| 1 | O | 258 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | Y | 121 | GLU | CD-OE1 | 7.41 | 1.33 | 1.25 |
| 1 | O | 330 | GLU | CD-OE1 | 7.38 | 1.33 | 1.25 |
| 1 | Y | 149 | GLU | CD-OE1 | 7.30 | 1.33 | 1.25 |
| 1 | O | 283 | GLU | CD-OE1 | 7.26 | 1.33 | 1.25 |
| 1 | O | 216 | GLU | CD-OE2 | 7.24 | 1.33 | 1.25 |
| 1 | O | 113 | GLU | CD-OE2 | 7.24 | 1.33 | 1.25 |
| 1 | O | 277 | GLU | CD-OE1 | 7.18 | 1.33 | 1.25 |
| 1 | O | 462 | GLU | CD-OE1 | 7.15 | 1.33 | 1.25 |
| 1 | O | 153 | GLU | CD-OE1 | 7.09 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 110 | GLU | CD-OE1 | 7.07 | 1.33 | 1.25 |
| 1 | Y | 36 | GLU | CD-OE2 | 7.03 | 1.33 | 1.25 |
| 1 | O | 159 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | O | 51 | GLU | CD-OE1 | 6.90 | 1.33 | 1.25 |
| 1 | Y | 84 | GLU | CD-OE1 | 6.85 | 1.33 | 1.25 |
| 1 | O | 149 | GLU | CD-OE1 | 6.85 | 1.33 | 1.25 |
| 1 | O | 36 | GLU | CD-OE2 | 6.84 | 1.33 | 1.25 |
| 1 | Y | 277 | GLU | CD-OE2 | 6.80 | 1.33 | 1.25 |
| 1 | Y | 2 | GLU | CD-OE1 | 6.76 | 1.33 | 1.25 |
| 1 | Y | 431 | GLU | CD-OE1 | 6.75 | 1.33 | 1.25 |
| 1 | O | 393 | GLU | CD-OE1 | 6.75 | 1.33 | 1.25 |
| 1 | O | 469 | GLU | CD-OE2 | 6.67 | 1.32 | 1.25 |
| 1 | O | 431 | GLU | CD-OE1 | 6.63 | 1.32 | 1.25 |
| 1 | O | 353 | ALA | C-O | 6.62 | 1.35 | 1.23 |
| 1 | O | 437 | GLU | CD-OE1 | 6.61 | 1.32 | 1.25 |
| 1 | Y | 437 | GLU | CD-OE1 | 6.54 | 1.32 | 1.25 |
| 1 | O | 2 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | O | 212 | GLU | CD-OE2 | 6.40 | 1.32 | 1.25 |
| 1 | Y | 330 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | Y | 258 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 1 | O | 467 | GLU | CD-OE2 | 6.29 | 1.32 | 1.25 |
| 1 | O | 222 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | Y | 110 | GLU | CD-OE1 | 6.24 | 1.32 | 1.25 |
| 1 | Y | 382 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |
| 1 | O | 459 | GLU | CD-OE1 | 6.14 | 1.32 | 1.25 |
| 1 | O | 497 | GLU | CD-OE1 | 5.99 | 1.32 | 1.25 |
| 1 | O | 90 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | Y | 90 | GLU | CD-OE2 | 5.95 | 1.32 | 1.25 |
| 1 | O | 319 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | Y | 467 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | Y | 62 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | Y | 459 | GLU | CD-OE1 | 5.79 | 1.32 | 1.25 |
| 1 | O | 478 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | O | 382 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | Y | 51 | GLU | CD-OE2 | 5.66 | 1.31 | 1.25 |
| 1 | Y | 327 | TYR | CB-CG | -5.63 | 1.43 | 1.51 |
| 1 | Y | 297 | GLU | CD-OE2 | 5.62 | 1.31 | 1.25 |
| 1 | Y | 113 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | O | 498 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | Y | 212 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | Y | 469 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | Y | 497 | GLU | CD-OE1 | 5.38 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 434 | GLU | CD-OE1 | 5.35 | 1.31 | 1.25 |
| 1 | Y | 33 | ARG | NE-CZ | 5.34 | 1.40 | 1.33 |
| 1 | Y | 106 | ARG | CZ-NH1 | 5.33 | 1.40 | 1.33 |
| 1 | Y | 478 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 1 | O | 125 | ARG | NE-CZ | 5.18 | 1.39 | 1.33 |
| 1 | Y | 84 | GLU | CD-OE2 | -5.10 | 1.20 | 1.25 |

All (175) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 327 | TYR | CB-CG-CD1 | -10.81 | 114.51 | 121.00 |
| 1 | O | 318 | ASP | CB-CG-OD2 | -10.45 | 108.90 | 118.30 |
| 1 | Y | 361 | ARG | NE-CZ-NH2 | -10.29 | 115.16 | 120.30 |
| 1 | Y | 106 | ARG | NE-CZ-NH2 | -10.19 | 115.21 | 120.30 |
| 1 | O | 357 | ASP | CB-CG-OD2 | -10.08 | 109.23 | 118.30 |
| 1 | O | 351 | LEU | C-N-CA | -9.90 | 101.51 | 122.30 |
| 1 | Y | 351 | LEU | C-N-CA | -9.60 | 102.14 | 122.30 |
| 1 | Y | 83 | ARG | C-N-CA | -9.45 | 98.07 | 121.70 |
| 1 | O | 409 | ASP | CB-CG-OD2 | -8.83 | 110.35 | 118.30 |
| 1 | O | 146 | ASP | CB-CG-OD2 | -8.82 | 110.37 | 118.30 |
| 1 | Y | 245 | ASP | CB-CG-OD2 | -8.75 | 110.42 | 118.30 |
| 1 | O | 357 | ASP | CB-CG-OD1 | 8.55 | 126.00 | 118.30 |
| 1 | Y | 117 | ARG | NE-CZ-NH1 | 8.53 | 124.56 | 120.30 |
| 1 | Y | 357 | ASP | CB-CG-OD1 | 8.41 | 125.87 | 118.30 |
| 1 | Y | 361 | ARG | NE-CZ-NH1 | 8.35 | 124.47 | 120.30 |
| 1 | O | 317 | ARG | NE-CZ-NH1 | 8.30 | 124.45 | 120.30 |
| 1 | O | 146 | ASP | CB-CG-OD1 | 8.08 | 125.57 | 118.30 |
| 1 | Y | 468 | ARG | NE-CZ-NH1 | 8.07 | 124.34 | 120.30 |
| 1 | O | 359 | TYR | CA-CB-CG | -8.00 | 98.20 | 113.40 |
| 1 | Y | 104 | GLN | N-CA-CB | -7.99 | 96.22 | 110.60 |
| 1 | Y | 24 | ASP | CB-CG-OD1 | -7.97 | 111.12 | 118.30 |
| 1 | O | 13 | THR | CA-CB-CG2 | -7.95 | 101.27 | 112.40 |
| 1 | Y | 334 | THR | CA-CB-CG2 | -7.92 | 101.31 | 112.40 |
| 1 | O | 106 | ARG | NE-CZ-NH2 | -7.87 | 116.37 | 120.30 |
| 1 | Y | 106 | ARG | NE-CZ-NH1 | 7.85 | 124.22 | 120.30 |
| 1 | O | 208 | ASP | CB-CG-OD2 | 7.72 | 125.25 | 118.30 |
| 1 | O | 24 | ASP | CB-CG-OD1 | -7.72 | 111.35 | 118.30 |
| 1 | Y | 353 | ALA | CB-CA-C | -7.66 | 98.62 | 110.10 |
| 1 | O | 198 | ASP | CB-CG-OD2 | -7.64 | 111.42 | 118.30 |
| 1 | O | 325 | ASP | CB-CG-OD2 | -7.59 | 111.47 | 118.30 |
| 1 | Y | 188 | ARG | NE-CZ-NH1 | 7.57 | 124.09 | 120.30 |
| 1 | Y | 353 | ALA | N-CA-CB | 7.57 | 120.69 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | O | 424 | ASP | CB-CG-OD1 | 7.55 | 125.10 | 118.30 |
| 1 | Y | 228 | ASN | N-CA-CB | 7.46 | 124.03 | 110.60 |
| 1 | Y | 200 | ASP | CB-CG-OD2 | -7.40 | 111.64 | 118.30 |
| 1 | O | 122 | ASP | CB-CG-OD2 | -7.38 | 111.65 | 118.30 |
| 1 | O | 468 | ARG | NE-CZ-NH1 | 7.37 | 123.98 | 120.30 |
| 1 | Y | 68 | ASP | CB-CG-OD1 | -7.34 | 111.69 | 118.30 |
| 1 | O | 133 | ASP | CB-CG-OD2 | -7.32 | 111.71 | 118.30 |
| 1 | O | 33 | ARG | NE-CZ-NH1 | 7.31 | 123.96 | 120.30 |
| 1 | O | 200 | ASP | CB-CG-OD2 | -7.21 | 111.81 | 118.30 |
| 1 | O | 182 | ASP | CB-CG-OD2 | -7.18 | 111.83 | 118.30 |
| 1 | Y | 398 | ASP | CB-CG-OD2 | 7.17 | 124.75 | 118.30 |
| 1 | Y | 166 | ASP | CB-CG-OD2 | -7.14 | 111.88 | 118.30 |
| 1 | Y | 10 | ASP | CB-CG-OD1 | -7.08 | 111.93 | 118.30 |
| 1 | Y | 122 | ASP | CB-CG-OD2 | -7.04 | 111.96 | 118.30 |
| 1 | O | 107 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 1 | Y | 182 | ASP | CB-CG-OD2 | -6.99 | 112.01 | 118.30 |
| 1 | Y | 390 | ASP | CB-CG-OD1 | -6.98 | 112.02 | 118.30 |
| 1 | Y | 325 | ASP | CB-CG-OD2 | -6.97 | 112.03 | 118.30 |
| 1 | O | 424 | ASP | CB-CG-OD2 | -6.96 | 112.04 | 118.30 |
| 1 | O | 334 | THR | CA-CB-CG2 | -6.95 | 102.67 | 112.40 |
| 1 | Y | 152 | ARG | NE-CZ-NH2 | -6.75 | 116.93 | 120.30 |
| 1 | Y | 227 | THR | CA-CB-CG2 | -6.69 | 103.03 | 112.40 |
| 1 | Y | 327 | TYR | CA-CB-CG | -6.65 | 100.76 | 113.40 |
| 1 | O | 228 | ASN | N-CA-CB | 6.62 | 122.51 | 110.60 |
| 1 | Y | 33 | ARG | CD-NE-CZ | 6.61 | 132.86 | 123.60 |
| 1 | Y | 248 | ALA | N-CA-CB | 6.58 | 119.32 | 110.10 |
| 1 | Y | 424 | ASP | CB-CG-OD2 | -6.58 | 112.38 | 118.30 |
| 1 | O | 328 | ASP | CB-CG-OD1 | -6.54 | 112.42 | 118.30 |
| 1 | Y | 80 | THR | N-CA-CB | 6.53 | 122.71 | 110.30 |
| 1 | O | 302 | LEU | CA-CB-CG | -6.50 | 100.36 | 115.30 |
| 1 | Y | 328 | ASP | CB-CG-OD1 | -6.41 | 112.53 | 118.30 |
| 1 | O | 245 | ASP | CB-CG-OD2 | -6.39 | 112.55 | 118.30 |
| 1 | Y | 390 | ASP | N-CA-CB | 6.38 | 122.08 | 110.60 |
| 1 | Y | 436 | ARG | NE-CZ-NH1 | 6.37 | 123.49 | 120.30 |
| 1 | Y | 152 | ARG | NE-CZ-NH1 | 6.30 | 123.45 | 120.30 |
| 1 | Y | 17 | ARG | N-CA-CB | 6.28 | 121.90 | 110.60 |
| 1 | Y | 125 | ARG | NE-CZ-NH2 | 6.26 | 123.43 | 120.30 |
| 1 | Y | 409 | ASP | CB-CG-OD1 | -6.26 | 112.66 | 118.30 |
| 1 | Y | 359 | TYR | CA-CB-CG | -6.26 | 101.51 | 113.40 |
| 1 | Y | 468 | ARG | NE-CZ-NH2 | -6.26 | 117.17 | 120.30 |
| 1 | O | 208 | ASP | CB-CG-OD1 | -6.24 | 112.68 | 118.30 |
| 1 | Y | 398 | ASP | CB-CG-OD1 | -6.24 | 112.69 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 492 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 1 | O | 83 | ARG | N-CA-C | 6.20 | 127.73 | 111.00 |
| 1 | O | 289 | THR | CA-CB-CG2 | -6.19 | 103.73 | 112.40 |
| 1 | Y | 211 | ARG | NE-CZ-NH2 | -6.15 | 117.23 | 120.30 |
| 1 | O | 83 | ARG | C-N-CA | -6.10 | 106.46 | 121.70 |
| 1 | Y | 481 | TYR | CA-CB-CG | -6.06 | 101.89 | 113.40 |
| 1 | Y | 104 | GLN | CB-CA-C | 6.05 | 122.50 | 110.40 |
| 1 | Y | 432 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 1 | O | 328 | ASP | CB-CG-OD2 | 6.02 | 123.72 | 118.30 |
| 1 | Y | 154 | ARG | NE-CZ-NH1 | 6.01 | 123.31 | 120.30 |
| 1 | Y | 432 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 1 | O | 147 | HIS | CA-CB-CG | -6.00 | 103.39 | 113.60 |
| 1 | Y | 245 | ASP | CB-CG-OD1 | 6.00 | 123.70 | 118.30 |
| 1 | O | 72 | ASP | CB-CG-OD2 | 5.98 | 123.68 | 118.30 |
| 1 | Y | 328 | ASP | CB-CG-OD2 | 5.96 | 123.67 | 118.30 |
| 1 | Y | 458 | ASP | CB-CG-OD2 | 5.96 | 123.66 | 118.30 |
| 1 | O | 72 | ASP | CB-CG-OD1 | -5.96 | 112.94 | 118.30 |
| 1 | Y | 318 | ASP | N-CA-CB | 5.94 | 121.30 | 110.60 |
| 1 | O | 80 | THR | N-CA-CB | 5.93 | 121.57 | 110.30 |
| 1 | Y | 107 | ARG | NE-CZ-NH1 | 5.93 | 123.26 | 120.30 |
| 1 | O | 327 | TYR | CB-CG-CD1 | -5.87 | 117.48 | 121.00 |
| 1 | Y | 135 | TYR | CB-CG-CD2 | -5.85 | 117.49 | 121.00 |
| 1 | Y | 166 | ASP | CB-CG-OD1 | 5.85 | 123.56 | 118.30 |
| 1 | O | 481 | TYR | CA-CB-CG | -5.82 | 102.33 | 113.40 |
| 1 | O | 200 | ASP | CB-CG-OD1 | 5.82 | 123.53 | 118.30 |
| 1 | Y | 72 | ASP | CB-CG-OD1 | -5.79 | 113.09 | 118.30 |
| 1 | Y | 5 | TYR | CB-CA-C | -5.72 | 98.97 | 110.40 |
| 1 | Y | 22 | ASP | CB-CG-OD1 | -5.69 | 113.18 | 118.30 |
| 1 | O | 20 | VAL | CB-CA-C | -5.67 | 100.62 | 111.40 |
| 1 | Y | 357 | ASP | CB-CG-OD2 | -5.65 | 113.22 | 118.30 |
| 1 | O | 204 | LEU | CA-CB-CG | -5.63 | 102.34 | 115.30 |
| 1 | O | 33 | ARG | CD-NE-CZ | 5.62 | 131.47 | 123.60 |
| 1 | O | 22 | ASP | CB-CG-OD1 | -5.60 | 113.26 | 118.30 |
| 1 | O | 275 | THR | CA-CB-CG2 | -5.59 | 104.58 | 112.40 |
| 1 | Y | 264 | THR | CA-CB-CG2 | -5.58 | 104.59 | 112.40 |
| 1 | O | 68 | ASP | CB-CG-OD1 | -5.58 | 113.28 | 118.30 |
| 1 | Y | 429 | ARG | NE-CZ-NH1 | 5.56 | 123.08 | 120.30 |
| 1 | O | 125 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | Y | 10 | ASP | CB-CG-OD2 | 5.53 | 123.28 | 118.30 |
| 1 | Y | 318 | ASP | CB-CA-C | -5.53 | 99.35 | 110.40 |
| 1 | O | 432 | ARG | NE-CZ-NH2 | -5.51 | 117.54 | 120.30 |
| 1 | Y | 48 | ASP | CB-CG-OD1 | -5.50 | 113.35 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | O | 118 | ASP | CB-CG-OD2 | -5.50 | 113.35 | 118.30 |
| 1 | O | 318 | ASP | CB-CG-OD1 | 5.47 | 123.23 | 118.30 |
| 1 | O | 398 | ASP | CB-CG-OD1 | -5.47 | 113.38 | 118.30 |
| 1 | O | 173 | MET | N-CA-CB | 5.46 | 120.42 | 110.60 |
| 1 | Y | 83 | ARG | CA-C-N | 5.43 | 129.14 | 117.20 |
| 1 | O | 201 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 1 | O | 211 | ARG | NE-CZ-NH1 | 5.41 | 123.00 | 120.30 |
| 1 | O | 242 | ILE | CB-CA-C | -5.39 | 100.82 | 111.60 |
| 1 | Y | 317 | ARG | NE-CZ-NH1 | 5.38 | 122.99 | 120.30 |
| 1 | O | 133 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 1 | O | 71 | SER | N-CA-CB | -5.34 | 102.49 | 110.50 |
| 1 | Y | 147 | HIS | CA-CB-CG | -5.34 | 104.52 | 113.60 |
| 1 | Y | 208 | ASP | CB-CG-OD2 | 5.34 | 123.11 | 118.30 |
| 1 | Y | 443 | ALA | N-CA-CB | 5.34 | 117.57 | 110.10 |
| 1 | O | 325 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | Y | 24 | ASP | CB-CG-OD2 | 5.33 | 123.09 | 118.30 |
| 1 | O | 282 | SER | N-CA-CB | 5.32 | 118.48 | 110.50 |
| 1 | O | 386 | TYR | CG-CD2-CE2 | -5.30 | 117.06 | 121.30 |
| 1 | O | 227 | THR | C-N-CA | -5.30 | 108.45 | 121.70 |
| 1 | Y | 56 | GLN | N-CA-CB | 5.30 | 120.13 | 110.60 |
| 1 | O | 468 | ARG | NE-CZ-NH2 | -5.29 | 117.66 | 120.30 |
| 1 | Y | 184 | THR | CA-CB-CG2 | -5.28 | 105.01 | 112.40 |
| 1 | Y | 146 | ASP | CB-CG-OD2 | -5.26 | 113.57 | 118.30 |
| 1 | Y | 118 | ASP | CB-CG-OD2 | -5.26 | 113.57 | 118.30 |
| 1 | O | 45 | VAL | CA-CB-CG1 | -5.24 | 103.04 | 110.90 |
| 1 | Y | 438 | VAL | CA-CB-CG2 | -5.23 | 103.05 | 110.90 |
| 1 | O | 288 | THR | CA-CB-CG2 | -5.21 | 105.11 | 112.40 |
| 1 | Y | 13 | THR | CA-CB-CG2 | -5.21 | 105.11 | 112.40 |
| 1 | Y | 125 | ARG | NE-CZ-NH1 | -5.19 | 117.70 | 120.30 |
| 1 | Y | 391 | VAL | CA-CB-CG1 | -5.19 | 103.12 | 110.90 |
| 1 | Y | 445 | TYR | CB-CG-CD2 | -5.17 | 117.90 | 121.00 |
| 1 | O | 48 | ASP | N-CA-CB | 5.16 | 119.89 | 110.60 |
| 1 | O | 86 | THR | CA-CB-CG2 | -5.15 | 105.18 | 112.40 |
| 1 | Y | 7 | VAL | CA-CB-CG2 | -5.15 | 103.18 | 110.90 |
| 1 | Y | 465 | VAL | CA-CB-CG1 | -5.13 | 103.20 | 110.90 |
| 1 | O | 257 | LYS | N-CA-CB | 5.13 | 119.84 | 110.60 |
| 1 | O | 323 | ILE | CA-CB-CG1 | -5.13 | 101.25 | 111.00 |
| 1 | Y | 208 | ASP | CB-CG-OD1 | -5.13 | 113.68 | 118.30 |
| 1 | Y | 471 | ARG | NE-CZ-NH2 | 5.13 | 122.86 | 120.30 |
| 1 | Y | 244 | GLY | N-CA-C | -5.13 | 100.28 | 113.10 |
| 1 | O | 407 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | O | 352 | GLY | C-N-CA | -5.11 | 108.93 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 198 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | O | 17 | ARG | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 1 | Y | 402 | ARG | CD-NE-CZ | 5.09 | 130.73 | 123.60 |
| 1 | Y | 390 | ASP | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | Y | 265 | TYR | CB-CG-CD2 | -5.08 | 117.95 | 121.00 |
| 1 | O | 458 | ASP | CB-CG-OD2 | 5.08 | 122.87 | 118.30 |
| 1 | O | 55 | THR | CA-CB-CG2 | -5.08 | 105.29 | 112.40 |
| 1 | O | 198 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 1 | O | 376 | ILE | CB-CA-C | -5.06 | 101.47 | 111.60 |
| 1 | Y | 107 | ARG | NE-CZ-NH2 | -5.05 | 117.77 | 120.30 |
| 1 | Y | 83 | ARG | O-C-N | -5.05 | 114.62 | 122.70 |
| 1 | Y | 454 | TRP | C-N-CA | -5.05 | 109.08 | 121.70 |
| 1 | Y | 173 | MET | CG-SD-CE | -5.05 | 92.12 | 100.20 |
| 1 | Y | 351 | LEU | CA-C-N | 5.04 | 126.29 | 116.20 |
| 1 | Y | 55 | THR | CA-CB-CG2 | -5.02 | 105.38 | 112.40 |
| 1 | Y | 201 | ASP | CB-CG-OD2 | -5.00 | 113.80 | 118.30 |
| 1 | O | 85 | THR | N-CA-CB | -5.00 | 100.79 | 110.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | O | 3910 | 0 | 3841 | 661 | 0 |
| 1 | Y | 3910 | 0 | 3841 | 537 | 1 |
| 2 | O | 1 | 0 | 0 | 0 | 0 |
| 2 | Y | 1 | 0 | 0 | 0 | 0 |
| 3 | O | 33 | 0 | 12 | 2 | 0 |
| 3 | Y | 33 | 0 | 12 | 3 | 0 |
| 4 | O | 6 | 0 | 8 | 2 | 0 |
| 4 | Y | 6 | 0 | 8 | 1 | 0 |
| All | All | 7900 | 0 | 7722 | 1195 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 76.

All (1195) 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 | 1.24 | 1.17 |
| 1:Y:74:ILE:HD11 | 1:Y:237:ILE:HG13 | 1.21 | 1.13 |
| 1:Y:229:ILE:HG21 | 1:Y:237:ILE:HG12 | 1.31 | 1.11 |
| 1:Y:459:GLU:HB2 | 1:Y:460:LEU:HD12 | 1.32 | 1.07 |
| 1:O:240:SER:HB2 | 1:O:450:ALA:HB3 | 1.37 | 1.05 |
| 1:Y:476:THR:O | 1:Y:480:ASN:ND2 | 1.88 | 1.04 |
| 1:O:74:ILE:HD11 | 1:O:237:ILE:HG13 | 1.39 | 1.03 |
| 1:O:313:ILE:HD11 | 1:O:381:LEU:HD23 | 1.40 | 1.02 |
| 1:O:229:ILE:HG21 | 1:O:237:ILE:HG12 | 1.41 | 1.00 |
| 1:Y:24:ASP:HB2 | 1:Y:26:ASN:HD21 | 1.27 | 0.99 |
| 1:Y:250:LEU:HD11 | 1:Y:255:CYS:HB2 | 1.43 | 0.99 |
| 1:Y:230:GLY:HA2 | 1:Y:235:THR:HB | 1.43 | 0.99 |
| 1:O:137:SER:HA | 1:O:140:LYS:HD2 | 1.44 | 0.97 |
| 1:Y:104:GLN:HG3 | 1:Y:349:THR:HG21 | 1.45 | 0.97 |
| 1:O:155:ALA:HB1 | 1:O:210:PRO:HG2 | 1.46 | 0.96 |
| 1:Y:325:ASP:HB3 | 1:Y:327:TYR:HB3 | 1.47 | 0.95 |
| 1:Y:154:ARG:HA | 1:Y:157:ARG:HG2 | 1.49 | 0.94 |
| 1:O:476:THR:O | 1:O:480:ASN:ND2 | 2.01 | 0.93 |
| 1:O:114:HIS:HA | 1:O:117:ARG:NH1 | 1.84 | 0.92 |
| 1:Y:211:ARG:HH11 | 1:Y:211:ARG:HG3 | 1.34 | 0.92 |
| 1:O:314:GLN:HG2 | 1:O:317:ARG:HH12 | 1.32 | 0.92 |
| 1:Y:492:ARG:HG2 | 1:Y:492:ARG:HH11 | 1.34 | 0.92 |
| 1:O:180:VAL:HG23 | 1:O:216:GLU:HB3 | 1.50 | 0.91 |
| 1:Y:24:ASP:HB2 | 1:Y:26:ASN:ND2 | 1.85 | 0.91 |
| 1:O:251:PHE:CE2 | 1:O:446:LEU:HD13 | 2.06 | 0.90 |
| 1:O:480:ASN:H | 1:O:480:ASN:ND2 | 1.64 | 0.90 |
| 1:O:95:LYS:HG3 | 1:O:96:PRO:HD2 | 1.53 | 0.89 |
| 1:Y:230:GLY:HA2 | 1:Y:235:THR:CB | 2.03 | 0.89 |
| 1:O:278:LYS:HZ1 | 1:O:280:VAL:HB | 1.38 | 0.89 |
| 1:O:278:LYS:NZ | 1:O:280:VAL:HB | 1.87 | 0.89 |
| 1:O:314:GLN:HG2 | 1:O:317:ARG:NH1 | 1.88 | 0.88 |
| 1:O:228:ASN:HD21 | 1:O:235:THR:N | 1.71 | 0.88 |
| 1:O:253:GLN:HG3 | 1:O:407:ARG:HD2 | 1.56 | 0.88 |
| 1:O:5:TYR:HB2 | 1:O:74:ILE:HG22 | 1.53 | 0.88 |
| 1:Y:69:ILE:HG23 | 1:Y:73:GLN:HG3 | 1.56 | 0.88 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:HG21 | 1.56 | 0.88 |
| 1:Y:468:ARG:HD2 | 1:Y:469:GLU:N | 1.89 | 0.87 |
| 1:Y:124:ILE:HD13 | 1:Y:203:MET:CE | 2.03 | 0.87 |
| 1:O:47:HIS:CB | 1:O:52:ILE:HD11 | 2.04 | 0.87 |
| 1:O:17:ARG:HH22 | 1:O:437:GLU:HG2 | 1.39 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:250:LEU:CD1 | 1:Y:255:CYS:HB2 | 2.05 | 0.86 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:CG2 | 2.03 | 0.86 |
| 1:O:415:ASN:ND2 | 1:O:418:LEU:H | 1.73 | 0.86 |
| 1:Y:460:LEU:H | 1:Y:460:LEU:HD12 | 1.41 | 0.86 |
| 1:Y:229:ILE:HG21 | 1:Y:237:ILE:CG1 | 2.06 | 0.85 |
| 1:O:183:TYR:HB3 | 1:O:290:ILE:HG21 | 1.57 | 0.85 |
| 1:Y:293:GLY:HA2 | 1:Y:299:ASN:ND2 | 1.91 | 0.85 |
| 1:Y:314:GLN:HG2 | 1:Y:317:ARG:HH12 | 1.41 | 0.84 |
| 1:O:402:ARG:HB3 | 1:O:402:ARG:HH11 | 1.41 | 0.84 |
| 1:Y:458:ASP:HA | 1:Y:461:GLN:CG | 2.05 | 0.84 |
| 1:O:115:LEU:HD12 | 1:O:115:LEU:H | 1.43 | 0.84 |
| 1:O:313:ILE:HD11 | 1:O:381:LEU:CD2 | 2.07 | 0.84 |
| 1:O:47:HIS:HB2 | 1:O:52:ILE:HD11 | 1.60 | 0.83 |
| 1:O:240:SER:HB2 | 1:O:450:ALA:CB | 2.07 | 0.83 |
| 1:O:221:SER:HB3 | 1:O:296:GLY:HA3 | 1.61 | 0.83 |
| 1:O:254:LEU:HD11 | 1:O:445:TYR:HE2 | 1.41 | 0.83 |
| 1:O:155:ALA:CB | 1:O:210:PRO:HG2 | 2.07 | 0.83 |
| 1:O:137:SER:O | 1:O:138:GLY:C | 2.12 | 0.83 |
| 1:O:389:ARG:HB2 | 1:O:426:LEU:CD1 | 2.08 | 0.83 |
| 1:O:17:ARG:HA | 1:O:59:THR:HG21 | 1.59 | 0.83 |
| 1:O:83:ARG:HB2 | 4:O:600:GOL:H12 | 1.59 | 0.82 |
| 1:Y:415:ASN:ND2 | 1:Y:418:LEU:H | 1.78 | 0.82 |
| 1:O:351:LEU:HD22 | 1:O:360:ALA:CB | 2.09 | 0.82 |
| 1:O:455:GLN:O | 1:O:456:ASN:HB2 | 1.79 | 0.81 |
| 1:Y:124:ILE:HD13 | 1:Y:203:MET:HE3 | 1.62 | 0.80 |
| 1:Y:74:ILE:CD1 | 1:Y:237:ILE:HG13 | 2.05 | 0.80 |
| 1:O:33:ARG:CZ | 1:O:58:TRP:HB3 | 2.11 | 0.80 |
| 1:Y:434:GLU:HB2 | 1:Y:465:VAL:HB | 1.63 | 0.80 |
| 1:Y:17:ARG:HG2 | 1:Y:32:GLN:HG3 | 1.64 | 0.79 |
| 1:O:59:THR:O | 1:O:63:VAL:HG23 | 1.82 | 0.79 |
| 1:O:120:LEU:O | 1:O:121:GLU:C | 2.17 | 0.79 |
| 1:O:211:ARG:HG3 | 1:O:211:ARG:HH11 | 1.45 | 0.79 |
| 1:Y:246:GLN:HG3 | 1:Y:262:LYS:NZ | 1.98 | 0.79 |
| 1:O:206:VAL:HG12 | 1:O:207:LEU:CD2 | 2.12 | 0.79 |
| 1:Y:48:ASP:O | 1:Y:52:ILE:HD12 | 1.83 | 0.79 |
| 1:O:19:VAL:CG1 | 1:O:27:ILE:HD13 | 2.12 | 0.79 |
| 1:O:199:TRP:CE2 | 1:O:214:LEU:HD23 | 2.16 | 0.79 |
| 1:O:70:SER:HB2 | 1:O:72:ASP:OD1 | 1.83 | 0.79 |
| 1:Y:60:LEU:O | 1:Y:63:VAL:HG23 | 1.84 | 0.78 |
| 1:O:463:LYS:HA | 1:O:463:LYS:HE2 | 1.65 | 0.78 |
| 1:O:199:TRP:CD1 | 1:O:214:LEU:HD23 | 2.17 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:61:VAL:O | 1:Y:62:GLU:C | 2.20 | 0.78 |
| 1:O:86:THR:OG1 | 1:O:137:SER:HB3 | 1.84 | 0.78 |
| 1:O:250:LEU:HD11 | 1:O:255:CYS:HB2 | 1.66 | 0.78 |
| 1:Y:463:LYS:CE | 1:Y:463:LYS:HA | 2.13 | 0.78 |
| 1:Y:137:SER:O | 1:Y:141:VAL:HG23 | 1.83 | 0.77 |
| 1:Y:31:SER:OG | 1:Y:59:THR:HA | 1.84 | 0.77 |
| 1:Y:261:ALA:HB2 | 1:Y:273:MET:HB2 | 1.66 | 0.77 |
| 1:O:253:GLN:CG | 1:O:407:ARG:HD2 | 2.14 | 0.77 |
| 1:O:360:ALA:O | 1:O:361:ARG:HD3 | 1.84 | 0.77 |
| 1:O:463:LYS:HA | 1:O:463:LYS:CE | 2.12 | 0.77 |
| 1:O:183:TYR:CE1 | 1:O:217:VAL:HG12 | 2.19 | 0.77 |
| 1:O:3:LYS:HA | 1:O:73:GLN:HA | 1.65 | 0.77 |
| 1:Y:84:GLU:HB2 | 1:Y:103:TRP:HB3 | 1.66 | 0.76 |
| 1:O:55:THR:HA | 1:O:58:TRP:CD1 | 2.19 | 0.76 |
| 1:Y:69:ILE:HG23 | 1:Y:73:GLN:CG | 2.15 | 0.76 |
| 1:Y:58:TRP:O | 1:Y:59:THR:C | 2.24 | 0.76 |
| 1:Y:246:GLN:HG2 | 1:Y:270:PHE:HB2 | 1.68 | 0.76 |
| 1:Y:229:ILE:HG23 | 1:Y:235:THR:O | 1.85 | 0.76 |
| 1:O:186:ALA:O | 1:O:189:THR:HG23 | 1.85 | 0.76 |
| 1:Y:154:ARG:CB | 1:Y:159:GLU:HB3 | 2.16 | 0.76 |
| 1:Y:432:ARG:HG2 | 1:Y:436:ARG:HH12 | 1.51 | 0.75 |
| 1:O:226:GLN:NE2 | 1:O:236:ARG:HB3 | 2.02 | 0.75 |
| 1:O:184:THR:HG22 | 1:O:290:ILE:O | 1.87 | 0.75 |
| 1:Y:185:ASN:HD21 | 1:Y:244:GLY:N | 1.83 | 0.75 |
| 1:Y:117:ARG:HH11 | 1:Y:117:ARG:CB | 2.00 | 0.75 |
| 1:Y:70:SER:HB2 | 1:Y:72:ASP:OD1 | 1.87 | 0.74 |
| 1:O:24:ASP:HB2 | 1:O:26:ASN:ND2 | 2.02 | 0.74 |
| 1:Y:104:GLN:CG | 1:Y:349:THR:HG21 | 2.16 | 0.74 |
| 1:O:373:ALA:O | 1:O:377:ILE:HG13 | 1.87 | 0.74 |
| 1:Y:193:ASN:HB3 | 1:Y:196:THR:HG21 | 1.69 | 0.74 |
| 1:O:17:ARG:CA | 1:O:59:THR:HG21 | 2.16 | 0.74 |
| 1:O:185:ASN:O | 1:O:188:ARG:HB2 | 1.88 | 0.74 |
| 1:Y:271:MET:C | 1:Y:272:LEU:HD12 | 2.07 | 0.74 |
| 1:Y:186:ALA:O | 1:Y:189:THR:HG23 | 1.87 | 0.74 |
| 1:Y:221:SER:HB3 | 1:Y:446:LEU:HD12 | 1.69 | 0.74 |
| 1:O:206:VAL:HG12 | 1:O:207:LEU:HD22 | 1.68 | 0.73 |
| 1:O:219:ARG:HG2 | 1:O:222:GLU:HB3 | 1.69 | 0.73 |
| 1:Y:392:LEU:HD23 | 1:Y:393:GLU:N | 2.02 | 0.73 |
| 1:O:279:ALA:HB2 | 1:O:300:TYR:CD1 | 2.23 | 0.73 |
| 1:O:181:THR:HG23 | 1:O:182:ASP:O | 1.89 | 0.73 |
| 1:O:24:ASP:HB2 | 1:O:26:ASN:HD21 | 1.53 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:271:MET:C | 1:O:272:LEU:HD12 | 2.09 | 0.73 |
| 1:Y:183:TYR:CD1 | 1:Y:217:VAL:HG12 | 2.24 | 0.73 |
| 1:Y:183:TYR:CE1 | 1:Y:217:VAL:HG12 | 2.24 | 0.73 |
| 1:O:102:VAL:HG12 | 1:O:103:TRP:CD1 | 2.23 | 0.72 |
| 1:O:325:ASP:HB3 | 1:O:327:TYR:HB3 | 1.71 | 0.72 |
| 1:O:44:TRP:CE2 | 1:O:107:ARG:HB2 | 2.24 | 0.72 |
| 1:Y:145:LEU:HD12 | 1:Y:151:SER:HB2 | 1.71 | 0.72 |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CD1 | 2.25 | 0.72 |
| 1:O:250:LEU:CD1 | 1:O:255:CYS:HB2 | 2.18 | 0.72 |
| 1:O:144:ILE:HD12 | 1:O:144:ILE:H | 1.55 | 0.72 |
| 1:Y:478:GLU:O | 1:Y:481:TYR:HB3 | 1.90 | 0.72 |
| 1:O:152:ARG:O | 1:O:155:ALA:HB3 | 1.91 | 0.71 |
| 1:Y:106:ARG:HD2 | 1:Y:349:THR:O | 1.91 | 0.71 |
| 1:O:434:GLU:HB2 | 1:O:465:VAL:HB | 1.72 | 0.71 |
| 1:Y:180:VAL:HG23 | 1:Y:216:GLU:HB3 | 1.72 | 0.71 |
| 1:Y:451:VAL:HG13 | 1:Y:453:PHE:H | 1.55 | 0.71 |
| 1:Y:456:ASN:OD1 | 1:Y:459:GLU:HG3 | 1.90 | 0.71 |
| 1:Y:324:ASN:ND2 | 1:Y:324:ASN:N | 2.38 | 0.71 |
| 1:O:332:PHE:O | 1:O:335:LYS:HB2 | 1.90 | 0.71 |
| 1:Y:458:ASP:CA | 1:Y:461:GLN:HG3 | 2.14 | 0.71 |
| 1:O:87:ILE:HD13 | 1:O:168:TRP:HB2 | 1.73 | 0.71 |
| 1:O:254:LEU:HD11 | 1:O:445:TYR:CE2 | 2.25 | 0.71 |
| 1:Y:193:ASN:HB3 | 1:Y:196:THR:CG2 | 2.20 | 0.71 |
| 1:O:435:VAL:HG22 | 1:O:436:ARG:H | 1.56 | 0.71 |
| 1:Y:459:GLU:HB2 | 1:Y:460:LEU:CD1 | 2.18 | 0.70 |
| 1:O:179:HIS:CE1 | 1:O:215:PRO:HB3 | 2.26 | 0.70 |
| 1:Y:180:VAL:CG2 | 1:Y:218:ARG:HG2 | 2.21 | 0.70 |
| 1:O:158:GLY:HA2 | 1:O:212:GLU:HB3 | 1.71 | 0.70 |
| 1:Y:51:GLU:O | 1:Y:55:THR:HG23 | 1.90 | 0.70 |
| 1:O:80:THR:HG21 | 1:O:248:ALA:CB | 2.22 | 0.70 |
| 1:O:354:PRO:HD2 | 1:O:355:TYR:CD2 | 2.27 | 0.70 |
| 1:Y:2:GLU:O | 1:Y:73:GLN:HA | 1.90 | 0.70 |
| 1:O:200:ASP:OD1 | 1:O:202:LYS:HB2 | 1.91 | 0.70 |
| 1:Y:74:ILE:HD12 | 1:Y:74:ILE:O | 1.91 | 0.70 |
| 1:O:227:THR:O | 1:O:229:ILE:HG22 | 1.92 | 0.70 |
| 1:Y:140:LYS:O | 1:Y:144:ILE:HD12 | 1.92 | 0.70 |
| 1:Y:269:CYS:HB2 | 1:Y:306:VAL:HB | 1.74 | 0.70 |
| 1:Y:45:VAL:O | 1:Y:102:VAL:HG23 | 1.92 | 0.70 |
| 1:O:199:TRP:CD2 | 1:O:214:LEU:HD23 | 2.25 | 0.70 |
| 1:O:95:LYS:HG3 | 1:O:96:PRO:CD | 2.20 | 0.70 |
| 1:Y:27:ILE:HD11 | 1:Y:30:VAL:HG23 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:435:VAL:HG22 | 1:O:436:ARG:N | 2.07 | 0.70 |
| 1:Y:253:GLN:HG3 | 1:Y:407:ARG:HD2 | 1.73 | 0.70 |
| 1:O:47:HIS:HB3 | 1:O:52:ILE:HD11 | 1.72 | 0.70 |
| 1:O:87:ILE:HD13 | 1:O:168:TRP:CB | 2.22 | 0.69 |
| 1:Y:22:ASP:OD2 | 1:Y:26:ASN:HB2 | 1.90 | 0.69 |
| 1:Y:180:VAL:HG21 | 1:Y:218:ARG:HG2 | 1.73 | 0.69 |
| 1:Y:415:ASN:HD22 | 1:Y:418:LEU:H | 1.40 | 0.69 |
| 1:O:211:ARG:NH1 | 1:O:211:ARG:HG3 | 2.03 | 0.69 |
| 1:O:415:ASN:HD21 | 1:O:417:PHE:HB3 | 1.58 | 0.69 |
| 1:O:196:THR:O | 1:O:197:LEU:C | 2.27 | 0.69 |
| 1:O:251:PHE:CE1 | 1:O:256:VAL:HG21 | 2.26 | 0.69 |
| 1:O:17:ARG:HH22 | 1:O:437:GLU:CG | 2.05 | 0.69 |
| 1:O:210:PRO:O | 1:O:213:MET:HG2 | 1.91 | 0.69 |
| 1:O:84:GLU:HB2 | 1:O:103:TRP:HB3 | 1.75 | 0.69 |
| 1:O:222:GLU:O | 1:O:240:SER:HA | 1.93 | 0.69 |
| 1:O:20:VAL:CG2 | 1:O:63:VAL:HG11 | 2.23 | 0.69 |
| 1:O:389:ARG:HB2 | 1:O:426:LEU:HD11 | 1.75 | 0.69 |
| 1:O:293:GLY:HA2 | 1:O:299:ASN:ND2 | 2.08 | 0.69 |
| 1:O:441:LEU:HD22 | 1:O:445:TYR:OH | 1.92 | 0.69 |
| 1:O:463:LYS:HZ3 | 1:O:465:VAL:HG23 | 1.57 | 0.69 |
| 1:Y:111:ILE:HG22 | 1:Y:115:LEU:CD1 | 2.23 | 0.69 |
| 1:Y:250:LEU:HD12 | 1:Y:250:LEU:O | 1.93 | 0.69 |
| 1:O:179:HIS:CD2 | 1:O:215:PRO:HB3 | 2.28 | 0.68 |
| 1:Y:48:ASP:C | 1:Y:52:ILE:HD12 | 2.13 | 0.68 |
| 1:O:227:THR:OG1 | 1:O:239:ILE:HD11 | 1.94 | 0.68 |
| 1:O:26:ASN:O | 1:O:28:ILE:HD13 | 1.93 | 0.68 |
| 1:Y:127:ASN:HB3 | 1:Y:193:ASN:ND2 | 2.07 | 0.68 |
| 1:Y:210:PRO:O | 1:Y:213:MET:HG2 | 1.94 | 0.68 |
| 1:O:340:ASN:ND2 | 1:O:371:VAL:HG22 | 2.09 | 0.68 |
| 1:Y:253:GLN:CG | 1:Y:407:ARG:HD2 | 2.24 | 0.68 |
| 1:Y:448:GLY:O | 1:Y:451:VAL:HG12 | 1.93 | 0.68 |
| 1:Y:115:LEU:H | 1:Y:115:LEU:HD12 | 1.59 | 0.68 |
| 1:Y:5:TYR:HB2 | 1:Y:74:ILE:HG22 | 1.75 | 0.67 |
| 1:O:20:VAL:HG12 | 1:O:21:MET:N | 2.09 | 0.67 |
| 1:Y:155:ALA:HA | 1:Y:160:LEU:HB2 | 1.76 | 0.67 |
| 1:Y:180:VAL:HG22 | 1:Y:181:THR:H | 1.58 | 0.67 |
| 1:Y:468:ARG:HD2 | 1:Y:469:GLU:H | 1.60 | 0.67 |
| 1:Y:202:LYS:O | 1:Y:205:GLU:HG3 | 1.93 | 0.67 |
| 1:O:230:GLY:HA2 | 1:O:235:THR:OG1 | 1.95 | 0.67 |
| 1:Y:144:ILE:O | 1:Y:148:VAL:HG23 | 1.95 | 0.67 |
| 1:Y:390:ASP:HA | 1:Y:483:TYR:OH | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:140:LYS:O | 1:O:144:ILE:HD12 | 1.95 | 0.67 |
| 1:Y:47:HIS:HB3 | 1:Y:52:ILE:HD11 | 1.77 | 0.67 |
| 1:O:47:HIS:O | 1:O:49:PRO:HD3 | 1.94 | 0.67 |
| 1:O:88:VAL:O | 1:O:97:ILE:HG12 | 1.94 | 0.67 |
| 1:O:5:TYR:HE2 | 1:O:73:GLN:HG3 | 1.60 | 0.67 |
| 1:Y:130:LEU:HD23 | 1:Y:130:LEU:N | 2.07 | 0.67 |
| 1:Y:422:GLN:NE2 | 1:Y:426:LEU:HD22 | 2.10 | 0.66 |
| 1:Y:480:ASN:ND2 | 1:Y:480:ASN:H | 1.94 | 0.66 |
| 1:Y:463:LYS:HE2 | 1:Y:463:LYS:HA | 1.75 | 0.66 |
| 1:Y:170:ILE:HA | 1:Y:173:MET:HG3 | 1.76 | 0.66 |
| 1:Y:221:SER:CB | 1:Y:450:ALA:HB2 | 2.25 | 0.66 |
| 1:O:435:VAL:HG11 | 1:O:441:LEU:HD11 | 1.76 | 0.66 |
| 1:O:90:GLU:N | 1:O:95:LYS:O | 2.29 | 0.66 |
| 1:O:154:ARG:HA | 1:O:157:ARG:CG | 2.25 | 0.66 |
| 1:O:169:LEU:O | 1:O:172:LYS:HB2 | 1.94 | 0.66 |
| 1:O:199:TRP:CG | 1:O:214:LEU:HD23 | 2.30 | 0.66 |
| 1:Y:388:THR:O | 1:Y:391:VAL:HG13 | 1.95 | 0.66 |
| 1:Y:222:GLU:O | 1:Y:240:SER:HA | 1.95 | 0.66 |
| 1:Y:9:LEU:HG | 1:Y:56:GLN:HE21 | 1.60 | 0.66 |
| 1:Y:127:ASN:HB3 | 1:Y:193:ASN:HD22 | 1.58 | 0.66 |
| 1:O:476:THR:O | 1:O:477:THR:C | 2.31 | 0.66 |
| 1:Y:449:LEU:O | 1:Y:449:LEU:HD12 | 1.95 | 0.66 |
| 1:Y:84:GLU:OE2 | 1:Y:188:ARG:HD2 | 1.96 | 0.66 |
| 1:O:279:ALA:HB2 | 1:O:300:TYR:CE1 | 2.31 | 0.66 |
| 1:O:286:LEU:C | 1:O:287:LEU:HD23 | 2.15 | 0.66 |
| 1:O:74:ILE:HD12 | 1:O:74:ILE:O | 1.96 | 0.66 |
| 1:Y:314:GLN:HG2 | 1:Y:317:ARG:NH1 | 2.11 | 0.66 |
| 1:O:460:LEU:HD12 | 1:O:460:LEU:N | 2.11 | 0.66 |
| 1:O:463:LYS:NZ | 1:O:465:VAL:HG23 | 2.10 | 0.66 |
| 1:Y:197:LEU:HD13 | 1:Y:197:LEU:H | 1.60 | 0.66 |
| 1:O:480:ASN:N | 1:O:480:ASN:ND2 | 2.40 | 0.65 |
| 1:Y:81:ASN:HD22 | 1:Y:81:ASN:N | 1.94 | 0.65 |
| 1:O:396:GLN:O | 1:O:400:GLY:N | 2.29 | 0.65 |
| 1:Y:33:ARG:HH11 | 1:Y:33:ARG:HG3 | 1.60 | 0.65 |
| 1:O:229:ILE:CG2 | 1:O:237:ILE:HG12 | 2.22 | 0.65 |
| 1:O:106:ARG:NH2 | 1:O:133:ASP:OD1 | 2.30 | 0.65 |
| 1:Y:467:GLU:HG2 | 1:Y:468:ARG:N | 2.07 | 0.65 |
| 1:O:48:ASP:HB3 | 1:O:51:GLU:HB3 | 1.78 | 0.65 |
| 1:O:275:THR:HG21 | 1:O:280:VAL:CG1 | 2.27 | 0.65 |
| 1:O:146:ASP:N | 1:O:146:ASP:OD1 | 2.29 | 0.65 |
| 1:Y:212:GLU:N | 1:Y:212:GLU:OE1 | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:184:THR:O | 1:Y:187:SER:HB3 | 1.97 | 0.65 |
| 1:Y:373:ALA:O | 1:Y:377:ILE:HG13 | 1.96 | 0.65 |
| 1:O:144:ILE:O | 1:O:148:VAL:HG23 | 1.97 | 0.65 |
| 1:Y:496:TRP:HZ3 | 1:O:492:ARG:HD3 | 1.62 | 0.65 |
| 1:Y:142:LYS:NZ | 1:Y:146:ASP:OD2 | 2.30 | 0.65 |
| 1:Y:152:ARG:O | 1:Y:155:ALA:HB3 | 1.97 | 0.65 |
| 1:O:487:LYS:HA | 1:O:490:VAL:HG23 | 1.79 | 0.65 |
| 1:O:415:ASN:O | 1:O:419:MET:HG2 | 1.97 | 0.65 |
| 1:O:177:ARG:NH1 | 1:O:226:GLN:O | 2.29 | 0.65 |
| 1:O:69:ILE:HD13 | 1:O:69:ILE:N | 2.12 | 0.65 |
| 1:O:476:THR:HG22 | 1:O:477:THR:H | 1.60 | 0.65 |
| 1:Y:180:VAL:HG21 | 1:Y:218:ARG:CG | 2.27 | 0.65 |
| 1:O:124:ILE:HD13 | 1:O:203:MET:CE | 2.27 | 0.65 |
| 1:O:170:ILE:O | 1:O:171:TRP:C | 2.35 | 0.65 |
| 1:Y:20:VAL:C | 1:Y:21:MET:HG3 | 2.17 | 0.65 |
| 1:Y:435:VAL:HG22 | 1:Y:436:ARG:N | 2.11 | 0.65 |
| 1:O:35:PHE:HB2 | 1:O:51:GLU:CG | 2.26 | 0.65 |
| 1:O:161:LEU:HD21 | 1:O:179:HIS:NE2 | 2.12 | 0.64 |
| 1:O:429:ARG:HD3 | 1:O:469:GLU:OE1 | 1.97 | 0.64 |
| 1:Y:460:LEU:H | 1:Y:460:LEU:CD1 | 2.11 | 0.64 |
| 1:Y:262:LYS:HE3 | 1:Y:270:PHE:O | 1.96 | 0.64 |
| 1:O:40:PRO:HG2 | 1:O:44:TRP:CB | 2.27 | 0.64 |
| 1:Y:161:LEU:HD22 | 1:Y:179:HIS:CE1 | 2.32 | 0.64 |
| 1:Y:460:LEU:N | 1:Y:460:LEU:HD12 | 2.11 | 0.64 |
| 1:O:89:TRP:HB2 | 1:O:95:LYS:C | 2.17 | 0.64 |
| 1:Y:111:ILE:HG21 | 1:Y:139:THR:HG22 | 1.77 | 0.64 |
| 1:O:201:ASP:O | 1:O:205:GLU:HG2 | 1.96 | 0.64 |
| 1:Y:19:VAL:HG13 | 1:Y:27:ILE:HD13 | 1.78 | 0.64 |
| 1:Y:227:THR:O | 1:Y:229:ILE:HG22 | 1.96 | 0.64 |
| 1:O:439:THR:HG22 | 1:O:440:ALA:N | 2.12 | 0.64 |
| 1:O:193:ASN:N | 1:O:198:ASP:O | 2.29 | 0.64 |
| 1:Y:246:GLN:HG3 | 1:Y:262:LYS:HZ3 | 1.61 | 0.64 |
| 1:Y:68:ASP:C | 1:Y:69:ILE:HD13 | 2.17 | 0.64 |
| 1:Y:81:ASN:N | 1:Y:81:ASN:ND2 | 2.46 | 0.64 |
| 1:O:228:ASN:HB2 | 1:O:236:ARG:HE | 1.62 | 0.64 |
| 1:O:84:GLU:OE1 | 1:O:84:GLU:N | 2.31 | 0.64 |
| 1:O:61:VAL:HA | 1:O:64:LEU:HD13 | 1.80 | 0.64 |
| 1:O:474:ILE:HG23 | 1:O:478:GLU:HB3 | 1.79 | 0.64 |
| 1:Y:419:MET:HA | 1:Y:419:MET:CE | 2.28 | 0.64 |
| 1:O:391:VAL:O | 1:O:392:LEU:C | 2.33 | 0.64 |
| 1:O:432:ARG:O | 1:O:467:GLU:N | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:262:LYS:NZ | 1:Y:264:THR:HB | 2.13 | 0.64 |
| 1:O:156:ARG:HB2 | 1:O:156:ARG:CZ | 2.27 | 0.64 |
| 1:Y:432:ARG:HD2 | 1:Y:436:ARG:NH2 | 2.13 | 0.64 |
| 1:O:455:GLN:O | 1:O:456:ASN:CB | 2.45 | 0.64 |
| 1:Y:61:VAL:HG12 | 1:Y:62:GLU:N | 2.13 | 0.64 |
| 1:O:354:PRO:HD2 | 1:O:355:TYR:CE2 | 2.33 | 0.64 |
| 1:Y:382:GLU:HG2 | 1:Y:421:PHE:CE2 | 2.32 | 0.64 |
| 1:O:63:VAL:O | 1:O:66:LYS:HG2 | 1.99 | 0.63 |
| 1:O:386:TYR:HB3 | 1:O:486:TRP:CE2 | 2.33 | 0.63 |
| 1:Y:69:ILE:HD13 | 1:Y:69:ILE:N | 2.11 | 0.63 |
| 1:Y:498:GLU:OE1 | 1:Y:498:GLU:HA | 1.99 | 0.63 |
| 1:O:497:GLU:HA | 1:O:497:GLU:OE1 | 1.98 | 0.63 |
| 1:O:183:TYR:CD1 | 1:O:217:VAL:HG12 | 2.33 | 0.63 |
| 1:Y:31:SER:HB2 | 1:Y:62:GLU:HB3 | 1.80 | 0.63 |
| 1:O:5:TYR:O | 1:O:75:ALA:N | 2.29 | 0.63 |
| 1:Y:4:LYS:N | 1:Y:73:GLN:O | 2.31 | 0.63 |
| 1:O:310:GLY:HA3 | 3:O:601:ATF:O3' | 1.99 | 0.63 |
| 1:Y:85:THR:HA | 1:Y:101:ILE:O | 1.98 | 0.63 |
| 1:Y:157:ARG:HG3 | 1:Y:159:GLU:OE1 | 1.98 | 0.63 |
| 1:O:123:TYR:CD2 | 1:O:203:MET:HE2 | 2.33 | 0.63 |
| 1:O:199:TRP:NE1 | 1:O:214:LEU:HD23 | 2.13 | 0.63 |
| 1:O:390:ASP:HA | 1:O:483:TYR:OH | 1.98 | 0.63 |
| 1:Y:463:LYS:HZ3 | 1:Y:465:VAL:HG23 | 1.63 | 0.63 |
| 1:O:50:MET:O | 1:O:54:ALA:N | 2.28 | 0.63 |
| 1:Y:170:ILE:HA | 1:Y:173:MET:CG | 2.29 | 0.63 |
| 1:Y:80:THR:HG21 | 1:Y:248:ALA:CB | 2.28 | 0.63 |
| 1:Y:197:LEU:N | 1:Y:197:LEU:HD13 | 2.11 | 0.63 |
| 1:Y:207:LEU:HB3 | 1:Y:209:ILE:HD12 | 1.80 | 0.63 |
| 1:O:184:THR:HA | 1:O:290:ILE:HG22 | 1.81 | 0.62 |
| 1:O:113:GLU:O | 1:O:116:LYS:HB2 | 1.98 | 0.62 |
| 1:O:456:ASN:OD1 | 1:O:458:ASP:HB2 | 2.00 | 0.62 |
| 1:Y:196:THR:HG22 | 1:Y:198:ASP:H | 1.64 | 0.62 |
| 1:Y:205:GLU:O | 1:Y:208:ASP:N | 2.31 | 0.62 |
| 1:Y:146:ASP:OD1 | 1:Y:146:ASP:N | 2.29 | 0.62 |
| 1:O:419:MET:HE2 | 1:O:419:MET:HA | 1.79 | 0.62 |
| 1:O:84:GLU:HB2 | 1:O:103:TRP:CB | 2.29 | 0.62 |
| 1:O:183:TYR:CB | 1:O:290:ILE:HG21 | 2.29 | 0.62 |
| 1:O:32:GLN:HA | 1:O:59:THR:HG23 | 1.82 | 0.62 |
| 1:O:272:LEU:HD21 | 1:O:303:GLU:OE1 | 1.99 | 0.62 |
| 1:O:133:ASP:OD1 | 1:O:135:TYR:N | 2.31 | 0.62 |
| 1:Y:22:ASP:O | 1:Y:25:ALA:N | 2.31 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:433:PRO:HA | 1:Y:466:ILE:HD13 | 1.80 | 0.62 |
| 1:Y:451:VAL:CG1 | 1:Y:453:PHE:H | 2.12 | 0.62 |
| 1:Y:156:ARG:HB2 | 1:Y:156:ARG:CZ | 2.28 | 0.62 |
| 1:O:19:VAL:HG13 | 1:O:27:ILE:HD13 | 1.82 | 0.62 |
| 1:O:202:LYS:O | 1:O:205:GLU:HG3 | 2.00 | 0.62 |
| 1:Y:179:HIS:CD2 | 1:Y:215:PRO:HA | 2.35 | 0.62 |
| 1:O:3:LYS:HA | 1:O:73:GLN:CA | 2.29 | 0.62 |
| 1:O:114:HIS:O | 1:O:117:ARG:N | 2.32 | 0.62 |
| 1:O:351:LEU:HD22 | 1:O:360:ALA:HB1 | 1.82 | 0.62 |
| 1:Y:47:HIS:O | 1:Y:49:PRO:HD3 | 2.00 | 0.61 |
| 1:O:287:LEU:O | 1:O:302:LEU:HD23 | 2.00 | 0.61 |
| 1:O:81:ASN:N | 1:O:81:ASN:HD22 | 1.97 | 0.61 |
| 1:O:69:ILE:HG23 | 1:O:73:GLN:HG3 | 1.81 | 0.61 |
| 1:Y:154:ARG:O | 1:Y:155:ALA:C | 2.33 | 0.61 |
| 1:Y:67:ALA:CB | 1:Y:69:ILE:HG12 | 2.30 | 0.61 |
| 1:Y:174:THR:O | 1:Y:176:GLY:N | 2.30 | 0.61 |
| 1:O:110:GLU:O | 1:O:113:GLU:HB2 | 2.00 | 0.61 |
| 1:O:17:ARG:NH2 | 1:O:437:GLU:HG2 | 2.13 | 0.61 |
| 1:O:207:LEU:HB3 | 1:O:209:ILE:CD1 | 2.30 | 0.61 |
| 1:O:478:GLU:OE1 | 1:O:478:GLU:HA | 2.00 | 0.61 |
| 1:Y:181:THR:HG23 | 1:Y:182:ASP:O | 2.00 | 0.61 |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:CA | 2.12 | 0.61 |
| 1:O:322:LEU:N | 1:O:322:LEU:HD23 | 2.14 | 0.61 |
| 1:O:20:VAL:C | 1:O:21:MET:HG3 | 2.20 | 0.61 |
| 1:O:113:GLU:O | 1:O:114:HIS:C | 2.38 | 0.61 |
| 1:O:47:HIS:CD2 | 1:O:82:GLN:HE22 | 2.18 | 0.61 |
| 1:Y:478:GLU:OE1 | 1:Y:478:GLU:HA | 1.98 | 0.61 |
| 1:O:297:GLU:N | 1:O:297:GLU:OE1 | 2.30 | 0.61 |
| 1:O:498:GLU:HA | 1:O:498:GLU:OE1 | 2.00 | 0.61 |
| 1:Y:71:SER:HB2 | 1:Y:235:THR:HG21 | 1.83 | 0.61 |
| 1:O:74:ILE:CD1 | 1:O:237:ILE:HG13 | 2.25 | 0.61 |
| 1:Y:211:ARG:NH1 | 1:Y:211:ARG:HG3 | 2.10 | 0.61 |
| 1:Y:222:GLU:HG3 | 1:Y:223:VAL:N | 2.15 | 0.61 |
| 1:O:90:GLU:HB3 | 1:O:93:THR:HG23 | 1.83 | 0.61 |
| 1:Y:402:ARG:HH11 | 1:Y:402:ARG:HB3 | 1.66 | 0.61 |
| 1:O:143:TRP:CE3 | 1:O:144:ILE:HA | 2.36 | 0.60 |
| 1:O:41:LYS:CG | 1:O:42:PRO:HD2 | 2.31 | 0.60 |
| 1:Y:149:GLU:OE1 | 1:Y:149:GLU:HA | 2.00 | 0.60 |
| 1:Y:310:GLY:O | 1:Y:313:ILE:HB | 2.01 | 0.60 |
| 1:O:359:TYR:HB2 | 1:O:495:ALA:HA | 1.83 | 0.60 |
| 1:Y:482:ARG:O | 1:Y:483:TYR:C | 2.39 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:432:ARG:HG2 | 1:Y:436:ARG:NH1 | 2.16 | 0.60 |
| 1:Y:196:THR:O | 1:Y:197:LEU:C | 2.38 | 0.60 |
| 1:Y:425:ILE:O | 1:Y:479:ARG:HD2 | 2.02 | 0.60 |
| 1:O:193:ASN:OD1 | 1:O:196:THR:HB | 2.00 | 0.60 |
| 1:O:108:THR:HB | 1:O:139:THR:HB | 1.83 | 0.60 |
| 1:O:124:ILE:HD13 | 1:O:203:MET:HE1 | 1.83 | 0.60 |
| 1:Y:196:THR:HG22 | 1:Y:198:ASP:N | 2.16 | 0.60 |
| 1:Y:237:ILE:HG23 | 1:Y:238:PRO:HD2 | 1.83 | 0.60 |
| 1:O:68:ASP:C | 1:O:69:ILE:HD13 | 2.22 | 0.60 |
| 1:O:154:ARG:HA | 1:O:157:ARG:HG2 | 1.84 | 0.60 |
| 1:Y:362:GLY:HA3 | 1:O:367:LEU:HB2 | 1.83 | 0.60 |
| 1:Y:456:ASN:N | 1:Y:459:GLU:OE2 | 2.35 | 0.60 |
| 1:O:90:GLU:HB3 | 1:O:93:THR:CG2 | 2.30 | 0.60 |
| 1:O:353:ALA:HB2 | 1:O:356:TRP:CZ2 | 2.37 | 0.60 |
| 1:O:88:VAL:HA | 1:O:161:LEU:O | 2.02 | 0.60 |
| 1:O:78:GLY:HA2 | 1:O:447:ALA:HB2 | 1.83 | 0.60 |
| 1:Y:432:ARG:NE | 1:Y:467:GLU:OE2 | 2.34 | 0.60 |
| 1:O:251:PHE:O | 1:O:254:LEU:N | 2.32 | 0.59 |
| 1:Y:422:GLN:HE21 | 1:Y:426:LEU:HD22 | 1.66 | 0.59 |
| 1:Y:154:ARG:HB2 | 1:Y:159:GLU:HB3 | 1.83 | 0.59 |
| 1:O:69:ILE:HG23 | 1:O:73:GLN:CG | 2.32 | 0.59 |
| 1:Y:430:VAL:HB | 1:Y:470:PHE:HB2 | 1.84 | 0.59 |
| 1:Y:246:GLN:HG3 | 1:Y:262:LYS:HZ1 | 1.67 | 0.59 |
| 1:Y:433:PRO:O | 1:Y:436:ARG:NH1 | 2.35 | 0.59 |
| 1:Y:94:GLY:HA2 | 1:Y:171:TRP:CH2 | 2.38 | 0.59 |
| 1:Y:246:GLN:H | 1:Y:246:GLN:NE2 | 1.99 | 0.59 |
| 1:O:222:GLU:HG3 | 1:O:223:VAL:N | 2.17 | 0.59 |
| 1:Y:101:ILE:HD12 | 1:Y:144:ILE:HD11 | 1.85 | 0.59 |
| 1:O:179:HIS:NE2 | 1:O:215:PRO:HB3 | 2.17 | 0.59 |
| 1:O:179:HIS:CG | 1:O:215:PRO:HB3 | 2.38 | 0.59 |
| 1:Y:237:ILE:HG22 | 1:Y:238:PRO:N | 2.18 | 0.59 |
| 1:O:251:PHE:HE1 | 1:O:256:VAL:HG21 | 1.68 | 0.59 |
| 1:O:170:ILE:HG22 | 1:O:171:TRP:N | 2.16 | 0.59 |
| 1:O:237:ILE:HG23 | 1:O:238:PRO:HD2 | 1.85 | 0.59 |
| 1:O:103:TRP:HB2 | 1:O:135:TYR:HE1 | 1.67 | 0.59 |
| 1:O:108:THR:OG1 | 1:O:134:PRO:HB3 | 2.02 | 0.59 |
| 1:O:147:HIS:ND1 | 1:O:147:HIS:N | 2.46 | 0.59 |
| 1:Y:80:THR:HG22 | 1:Y:243:ALA:O | 2.03 | 0.59 |
| 1:Y:419:MET:HA | 1:Y:419:MET:HE2 | 1.83 | 0.59 |
| 1:O:61:VAL:HA | 1:O:64:LEU:CD1 | 2.33 | 0.59 |
| 1:O:88:VAL:HG22 | 1:O:162:PHE:HB2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:111:ILE:O | 1:Y:115:LEU:HD12 | 2.03 | 0.58 |
| 1:Y:87:ILE:HG22 | 1:Y:88:VAL:N | 2.18 | 0.58 |
| 1:Y:87:ILE:HD12 | 1:Y:163:GLY:O | 2.03 | 0.58 |
| 1:O:477:THR:O | 1:O:478:GLU:C | 2.41 | 0.58 |
| 1:Y:124:ILE:HD13 | 1:Y:203:MET:HE1 | 1.84 | 0.58 |
| 1:O:166:ASP:O | 1:O:167:THR:C | 2.42 | 0.58 |
| 1:O:422:GLN:HE21 | 1:O:426:LEU:HD22 | 1.67 | 0.58 |
| 1:O:410:GLY:O | 1:O:413:VAL:HG13 | 2.03 | 0.58 |
| 1:O:387:GLN:O | 1:O:390:ASP:HB2 | 2.04 | 0.58 |
| 1:O:475:GLU:O | 1:O:478:GLU:HB2 | 2.04 | 0.58 |
| 1:O:149:GLU:HA | 1:O:149:GLU:OE1 | 2.03 | 0.58 |
| 1:Y:221:SER:OG | 1:Y:450:ALA:HB2 | 2.03 | 0.58 |
| 1:O:445:TYR:O | 1:O:447:ALA:N | 2.37 | 0.58 |
| 1:Y:435:VAL:HG22 | 1:Y:436:ARG:H | 1.68 | 0.58 |
| 1:O:401:ILE:HG22 | 1:O:402:ARG:N | 2.19 | 0.58 |
| 1:O:81:ASN:ND2 | 1:O:81:ASN:N | 2.51 | 0.58 |
| 1:O:281:LYS:HB2 | 1:O:281:LYS:NZ | 2.19 | 0.58 |
| 1:O:153:GLU:O | 1:O:157:ARG:HG2 | 2.03 | 0.58 |
| 1:O:41:LYS:CB | 1:O:42:PRO:HD2 | 2.34 | 0.58 |
| 1:O:476:THR:CG2 | 1:O:477:THR:N | 2.67 | 0.58 |
| 1:O:140:LYS:O | 1:O:143:TRP:HB3 | 2.04 | 0.58 |
| 1:O:389:ARG:HB2 | 1:O:426:LEU:HD13 | 1.84 | 0.58 |
| 1:Y:31:SER:H | 1:Y:63:VAL:HG13 | 1.68 | 0.58 |
| 1:O:207:LEU:CB | 1:O:209:ILE:HD12 | 2.34 | 0.58 |
| 1:O:5:TYR:CE2 | 1:O:73:GLN:HG3 | 2.38 | 0.58 |
| 1:Y:206:VAL:HG12 | 1:Y:207:LEU:N | 2.19 | 0.58 |
| 1:O:41:LYS:HG3 | 1:O:42:PRO:HD2 | 1.84 | 0.58 |
| 1:Y:310:GLY:HA3 | 3:Y:601:ATF:O3' | 2.04 | 0.58 |
| 1:Y:22:ASP:OD1 | 1:Y:24:ASP:N | 2.36 | 0.57 |
| 1:Y:67:ALA:HB3 | 1:Y:69:ILE:HG12 | 1.86 | 0.57 |
| 1:Y:3:LYS:HA | 1:Y:73:GLN:HA | 1.84 | 0.57 |
| 1:Y:497:GLU:OE1 | 1:Y:497:GLU:HA | 2.03 | 0.57 |
| 1:Y:226:GLN:NE2 | 1:Y:236:ARG:HB3 | 2.19 | 0.57 |
| 1:Y:18:ALA:HB1 | 1:Y:63:VAL:HG21 | 1.85 | 0.57 |
| 1:O:207:LEU:HB3 | 1:O:209:ILE:HD12 | 1.85 | 0.57 |
| 1:O:230:GLY:HA2 | 1:O:235:THR:CB | 2.33 | 0.57 |
| 1:O:402:ARG:NH1 | 1:O:402:ARG:HB3 | 2.15 | 0.57 |
| 1:O:40:PRO:HD2 | 1:O:44:TRP:O | 2.05 | 0.57 |
| 1:O:44:TRP:HA | 1:O:105:CYS:SG | 2.44 | 0.57 |
| 1:Y:104:GLN:NE2 | 1:Y:308:MET:HE2 | 2.19 | 0.57 |
| 1:O:27:ILE:HD11 | 1:O:30:VAL:HG23 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:133:ASP:OD1 | 1:Y:135:TYR:HB2 | 2.04 | 0.57 |
| 1:Y:482:ARG:HG3 | 1:Y:482:ARG:NH1 | 2.20 | 0.57 |
| 1:O:480:ASN:HD22 | 1:O:480:ASN:H | 1.49 | 0.57 |
| 1:O:473:GLY:C | 1:O:474:ILE:HD13 | 2.25 | 0.57 |
| 1:O:273:MET:HB2 | 1:O:395:MET:HE2 | 1.86 | 0.57 |
| 1:O:490:VAL:O | 1:O:494:MET:HG2 | 2.05 | 0.57 |
| 1:Y:193:ASN:OD1 | 1:Y:196:THR:HB | 2.04 | 0.57 |
| 1:O:395:MET:O | 1:O:396:GLN:C | 2.43 | 0.57 |
| 1:O:143:TRP:O | 1:O:147:HIS:ND1 | 2.38 | 0.57 |
| 1:Y:153:GLU:OE1 | 1:Y:153:GLU:HA | 2.04 | 0.57 |
| 1:O:120:LEU:O | 1:O:124:ILE:HG12 | 2.05 | 0.57 |
| 1:Y:117:ARG:CG | 1:Y:117:ARG:HH11 | 2.16 | 0.57 |
| 1:O:85:THR:HG23 | 1:O:102:VAL:HA | 1.86 | 0.57 |
| 1:Y:483:TYR:O | 1:Y:486:TRP:HB3 | 2.04 | 0.56 |
| 1:O:137:SER:O | 1:O:141:VAL:HG23 | 2.04 | 0.56 |
| 1:O:153:GLU:O | 1:O:156:ARG:HB3 | 2.05 | 0.56 |
| 1:Y:190:MET:HG2 | 1:Y:190:MET:O | 2.05 | 0.56 |
| 1:O:348:PHE:HD1 | 1:O:348:PHE:H | 1.52 | 0.56 |
| 1:Y:182:ASP:HB3 | 1:Y:242:ILE:HB | 1.87 | 0.56 |
| 1:O:123:TYR:CE2 | 1:O:203:MET:HE2 | 2.40 | 0.56 |
| 1:Y:237:ILE:N | 1:Y:237:ILE:HD13 | 2.20 | 0.56 |
| 1:O:173:MET:O | 1:O:227:THR:HG23 | 2.06 | 0.56 |
| 1:O:218:ARG:NH1 | 1:O:218:ARG:HG3 | 2.20 | 0.56 |
| 1:Y:5:TYR:O | 1:Y:74:ILE:HA | 2.05 | 0.56 |
| 1:O:419:MET:HA | 1:O:419:MET:CE | 2.35 | 0.56 |
| 1:O:17:ARG:HG2 | 1:O:32:GLN:HG3 | 1.88 | 0.56 |
| 1:O:90:GLU:O | 1:O:94:GLY:N | 2.38 | 0.56 |
| 1:O:40:PRO:HG2 | 1:O:44:TRP:HB3 | 1.87 | 0.56 |
| 1:O:487:LYS:HA | 1:O:490:VAL:CG2 | 2.35 | 0.56 |
| 1:Y:444:ALA:O | 1:Y:447:ALA:N | 2.38 | 0.56 |
| 1:Y:108:THR:OG1 | 1:Y:134:PRO:HB3 | 2.05 | 0.56 |
| 1:O:340:ASN:HD22 | 1:O:371:VAL:HG22 | 1.70 | 0.56 |
| 1:O:154:ARG:HA | 1:O:157:ARG:HG3 | 1.87 | 0.56 |
| 1:Y:27:ILE:HD12 | 1:Y:27:ILE:C | 2.27 | 0.56 |
| 1:O:240:SER:O | 1:O:447:ALA:HA | 2.06 | 0.56 |
| 1:O:254:LEU:CD1 | 1:O:445:TYR:HE2 | 2.14 | 0.56 |
| 1:Y:250:LEU:HD11 | 1:Y:255:CYS:CB | 2.27 | 0.56 |
| 1:O:433:PRO:O | 1:O:436:ARG:NH1 | 2.38 | 0.56 |
| 1:O:476:THR:HG22 | 1:O:477:THR:N | 2.21 | 0.56 |
| 1:Y:246:GLN:NE2 | 1:Y:246:GLN:N | 2.54 | 0.56 |
| 1:Y:445:TYR:O | 1:Y:449:LEU:HB2 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:154:ARG:CA | 1:O:157:ARG:HG2 | 2.36 | 0.56 |
| 1:O:80:THR:HG21 | 1:O:248:ALA:HB2 | 1.87 | 0.56 |
| 1:Y:359:TYR:HD2 | 1:Y:497:GLU:HB3 | 1.70 | 0.56 |
| 1:O:408:VAL:HG23 | 1:O:409:ASP:N | 2.21 | 0.55 |
| 1:Y:20:VAL:HG12 | 1:Y:21:MET:N | 2.20 | 0.55 |
| 1:O:245:ASP:OD1 | 1:O:246:GLN:N | 2.39 | 0.55 |
| 1:O:142:LYS:O | 1:O:143:TRP:C | 2.44 | 0.55 |
| 1:Y:153:GLU:O | 1:Y:156:ARG:N | 2.39 | 0.55 |
| 1:O:114:HIS:O | 1:O:117:ARG:HB2 | 2.06 | 0.55 |
| 1:Y:70:SER:O | 1:Y:72:ASP:N | 2.40 | 0.55 |
| 1:O:219:ARG:HD3 | 1:O:222:GLU:HB2 | 1.88 | 0.55 |
| 1:O:115:LEU:CD1 | 1:O:115:LEU:H | 2.16 | 0.55 |
| 1:Y:492:ARG:HG2 | 1:Y:492:ARG:NH1 | 2.11 | 0.55 |
| 1:O:55:THR:HA | 1:O:58:TRP:HD1 | 1.68 | 0.55 |
| 1:O:64:LEU:H | 1:O:64:LEU:HD12 | 1.70 | 0.55 |
| 1:Y:83:ARG:HB2 | 4:Y:600:GOL:O2 | 2.05 | 0.55 |
| 1:O:179:HIS:CD2 | 1:O:215:PRO:HA | 2.42 | 0.55 |
| 1:O:441:LEU:HD23 | 1:O:445:TYR:HE1 | 1.71 | 0.55 |
| 1:O:63:VAL:O | 1:O:66:LYS:N | 2.40 | 0.55 |
| 1:Y:188:ARG:HH22 | 1:Y:303:GLU:CD | 2.10 | 0.55 |
| 1:O:275:THR:HB | 1:O:278:LYS:O | 2.07 | 0.55 |
| 1:Y:463:LYS:NZ | 1:Y:465:VAL:HG23 | 2.22 | 0.55 |
| 1:Y:488:LYS:HD2 | 1:O:496:TRP:CH2 | 2.41 | 0.55 |
| 1:O:103:TRP:HB2 | 1:O:135:TYR:CE1 | 2.41 | 0.55 |
| 1:Y:150:GLY:O | 1:Y:153:GLU:N | 2.39 | 0.55 |
| 1:Y:272:LEU:HD21 | 1:Y:303:GLU:OE1 | 2.07 | 0.55 |
| 1:Y:396:GLN:O | 1:Y:397:ALA:C | 2.45 | 0.55 |
| 1:O:482:ARG:NH1 | 1:O:482:ARG:HG3 | 2.21 | 0.55 |
| 1:O:144:ILE:O | 1:O:145:LEU:C | 2.44 | 0.55 |
| 1:Y:420:GLN:O | 1:Y:420:GLN:NE2 | 2.39 | 0.55 |
| 1:Y:308:MET:HB2 | 1:Y:346:PRO:HB2 | 1.88 | 0.55 |
| 1:Y:325:ASP:O | 1:Y:326:ALA:C | 2.42 | 0.55 |
| 1:O:180:VAL:CG2 | 1:O:218:ARG:HG2 | 2.37 | 0.55 |
| 1:O:340:ASN:HB2 | 1:O:375:HIS:CD2 | 2.40 | 0.55 |
| 1:Y:405:ALA:HB2 | 1:Y:429:ARG:HD2 | 1.88 | 0.55 |
| 1:O:14:THR:O | 1:O:34:GLU:HG2 | 2.07 | 0.55 |
| 1:Y:325:ASP:HB3 | 1:Y:327:TYR:CB | 2.29 | 0.54 |
| 1:O:206:VAL:HG12 | 1:O:207:LEU:HD23 | 1.89 | 0.54 |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CE1 | 2.41 | 0.54 |
| 1:Y:282:SER:HA | 1:Y:398:ASP:OD2 | 2.06 | 0.54 |
| 1:Y:219:ARG:HG2 | 1:Y:222:GLU:HB3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:80:THR:HG21 | 1:Y:248:ALA:HB3 | 1.89 | 0.54 |
| 1:O:41:LYS:HG3 | 1:O:42:PRO:CD | 2.38 | 0.54 |
| 1:O:3:LYS:HG2 | 1:O:72:ASP:O | 2.07 | 0.54 |
| 1:O:473:GLY:O | 1:O:474:ILE:HD13 | 2.08 | 0.54 |
| 1:Y:463:LYS:HZ3 | 1:Y:463:LYS:HA | 1.72 | 0.54 |
| 1:O:6:ILE:HG13 | 1:O:7:VAL:H | 1.71 | 0.54 |
| 1:O:219:ARG:NH2 | 1:O:295:THR:OG1 | 2.40 | 0.54 |
| 1:O:164:THR:H | 1:O:167:THR:HB | 1.72 | 0.54 |
| 1:O:424:ASP:OD1 | 1:O:473:GLY:N | 2.36 | 0.54 |
| 1:O:4:LYS:N | 1:O:73:GLN:O | 2.40 | 0.54 |
| 1:Y:251:PHE:CE2 | 1:Y:446:LEU:HD22 | 2.43 | 0.54 |
| 1:Y:480:ASN:O | 1:Y:481:TYR:C | 2.44 | 0.54 |
| 1:O:166:ASP:OD1 | 1:O:166:ASP:N | 2.38 | 0.54 |
| 1:Y:20:VAL:O | 1:Y:28:ILE:N | 2.30 | 0.54 |
| 1:Y:120:LEU:O | 1:Y:124:ILE:HG12 | 2.06 | 0.54 |
| 1:Y:227:THR:N | 1:Y:237:ILE:O | 2.29 | 0.54 |
| 1:O:180:VAL:HG21 | 1:O:218:ARG:HG3 | 1.90 | 0.54 |
| 1:O:80:THR:CG2 | 1:O:248:ALA:HB2 | 2.38 | 0.54 |
| 1:Y:113:GLU:O | 1:Y:116:LYS:HB2 | 2.08 | 0.54 |
| 1:O:244:GLY:O | 1:O:245:ASP:C | 2.41 | 0.54 |
| 1:Y:31:SER:N | 1:Y:63:VAL:HG13 | 2.23 | 0.54 |
| 1:Y:201:ASP:O | 1:Y:202:LYS:C | 2.46 | 0.54 |
| 1:O:468:ARG:HH11 | 1:O:468:ARG:HG3 | 1.73 | 0.54 |
| 1:Y:221:SER:HB3 | 1:Y:446:LEU:CD1 | 2.36 | 0.53 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:CB | 2.38 | 0.53 |
| 1:O:90:GLU:OE1 | 1:O:95:LYS:NZ | 2.38 | 0.53 |
| 1:O:422:GLN:NE2 | 1:O:426:LEU:HD22 | 2.23 | 0.53 |
| 1:O:229:ILE:O | 1:O:230:GLY:C | 2.46 | 0.53 |
| 1:Y:18:ALA:HB1 | 1:Y:63:VAL:CG2 | 2.38 | 0.53 |
| 1:Y:117:ARG:CA | 1:Y:117:ARG:HH11 | 2.21 | 0.53 |
| 1:O:20:VAL:HG23 | 1:O:63:VAL:HG11 | 1.90 | 0.53 |
| 1:Y:468:ARG:CG | 1:Y:468:ARG:HH11 | 2.21 | 0.53 |
| 1:O:40:PRO:HD2 | 1:O:44:TRP:HB2 | 1.91 | 0.53 |
| 1:Y:40:PRO:HG3 | 1:Y:46:GLU:OE2 | 2.09 | 0.53 |
| 1:Y:31:SER:CB | 1:Y:62:GLU:HB3 | 2.39 | 0.53 |
| 1:Y:63:VAL:O | 1:Y:64:LEU:C | 2.46 | 0.53 |
| 1:Y:360:ALA:HB2 | 1:Y:494:MET:HA | 1.91 | 0.53 |
| 1:O:118:ASP:N | 1:O:118:ASP:OD1 | 2.40 | 0.53 |
| 1:Y:74:ILE:CD1 | 1:Y:237:ILE:HG21 | 2.39 | 0.53 |
| 1:O:415:ASN:HD22 | 1:O:418:LEU:H | 1.50 | 0.53 |
| 1:Y:272:LEU:HD12 | 1:Y:272:LEU:N | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:398:ASP:O | 1:O:399:SER:C | 2.44 | 0.53 |
| 1:O:451:VAL:HG13 | 1:O:451:VAL:O | 2.09 | 0.53 |
| 1:O:71:SER:O | 1:O:237:ILE:HD11 | 2.09 | 0.53 |
| 1:Y:473:GLY:O | 1:Y:474:ILE:HD13 | 2.09 | 0.53 |
| 1:Y:481:TYR:O | 1:Y:484:ALA:HB3 | 2.09 | 0.53 |
| 1:Y:114:HIS:O | 1:Y:115:LEU:C | 2.47 | 0.53 |
| 1:O:249:ALA:HB2 | 1:O:439:THR:OG1 | 2.09 | 0.53 |
| 1:O:192:PHE:CE2 | 1:O:217:VAL:HG11 | 2.44 | 0.53 |
| 1:O:346:PRO:HA | 1:O:348:PHE:CE1 | 2.44 | 0.53 |
| 1:O:180:VAL:HG21 | 1:O:218:ARG:CG | 2.39 | 0.52 |
| 1:Y:387:GLN:O | 1:Y:391:VAL:HG12 | 2.09 | 0.52 |
| 1:Y:61:VAL:O | 1:Y:63:VAL:N | 2.43 | 0.52 |
| 1:O:21:MET:HB3 | 1:O:26:ASN:O | 2.09 | 0.52 |
| 1:O:188:ARG:HH22 | 1:O:303:GLU:CD | 2.12 | 0.52 |
| 1:Y:463:LYS:NZ | 1:Y:463:LYS:HA | 2.25 | 0.52 |
| 1:O:488:LYS:O | 1:O:492:ARG:HD2 | 2.09 | 0.52 |
| 1:O:123:TYR:HD2 | 1:O:203:MET:CE | 2.23 | 0.52 |
| 1:O:35:PHE:HB2 | 1:O:51:GLU:HG3 | 1.91 | 0.52 |
| 1:O:330:GLU:O | 1:O:334:THR:HG23 | 2.10 | 0.52 |
| 1:O:181:THR:HG23 | 1:O:182:ASP:N | 2.25 | 0.52 |
| 1:O:108:THR:HG21 | 1:O:140:LYS:N | 2.25 | 0.52 |
| 1:Y:236:ARG:C | 1:Y:237:ILE:HD13 | 2.29 | 0.52 |
| 1:Y:364:ILE:O | 1:O:363:ALA:HB1 | 2.09 | 0.52 |
| 1:Y:80:THR:CG2 | 1:Y:248:ALA:HB2 | 2.39 | 0.52 |
| 1:Y:8:ALA:O | 1:Y:9:LEU:HD12 | 2.09 | 0.52 |
| 1:O:33:ARG:NH1 | 1:O:62:GLU:OE1 | 2.43 | 0.52 |
| 1:Y:18:ALA:CB | 1:Y:59:THR:HB | 2.40 | 0.52 |
| 1:Y:129:GLY:C | 1:Y:130:LEU:HD23 | 2.29 | 0.52 |
| 1:Y:177:ARG:NH1 | 1:Y:226:GLN:O | 2.43 | 0.52 |
| 1:Y:143:TRP:CD2 | 1:Y:147:HIS:HD2 | 2.27 | 0.52 |
| 1:O:39:TYR:HA | 1:O:44:TRP:O | 2.10 | 0.52 |
| 1:O:445:TYR:O | 1:O:448:GLY:N | 2.43 | 0.52 |
| 1:O:97:ILE:O | 1:O:98:TYR:HB2 | 2.08 | 0.52 |
| 1:Y:74:ILE:C | 1:Y:74:ILE:HD12 | 2.30 | 0.51 |
| 1:Y:246:GLN:HG2 | 1:Y:270:PHE:CB | 2.40 | 0.51 |
| 1:Y:240:SER:HB2 | 1:Y:450:ALA:HB3 | 1.92 | 0.51 |
| 1:O:237:ILE:CG2 | 1:O:238:PRO:HD2 | 2.40 | 0.51 |
| 1:Y:293:GLY:HA3 | 1:Y:297:GLU:CD | 2.30 | 0.51 |
| 1:O:351:LEU:HD22 | 1:O:360:ALA:HB2 | 1.92 | 0.51 |
| 1:Y:44:TRP:CE2 | 1:Y:107:ARG:HB2 | 2.45 | 0.51 |
| 1:Y:480:ASN:H | 1:Y:480:ASN:HD22 | 1.57 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:59:THR:O | 1:Y:63:VAL:HG22 | 2.10 | 0.51 |
| 1:O:445:TYR:O | 1:O:446:LEU:C | 2.48 | 0.51 |
| 1:O:173:MET:HB3 | 1:O:227:THR:HG21 | 1.93 | 0.51 |
| 1:O:476:THR:O | 1:O:477:THR:O | 2.28 | 0.51 |
| 1:Y:271:MET:HE1 | 1:Y:392:LEU:HB2 | 1.92 | 0.51 |
| 1:Y:49:PRO:HA | 1:Y:52:ILE:HD13 | 1.93 | 0.51 |
| 1:O:286:LEU:O | 1:O:287:LEU:HD23 | 2.11 | 0.51 |
| 1:Y:401:ILE:HG22 | 1:Y:402:ARG:N | 2.24 | 0.51 |
| 1:Y:78:GLY:HA2 | 1:Y:447:ALA:HB2 | 1.92 | 0.51 |
| 1:O:154:ARG:CA | 1:O:159:GLU:HB3 | 2.41 | 0.51 |
| 1:Y:143:TRP:CE2 | 1:Y:147:HIS:CD2 | 2.99 | 0.51 |
| 1:Y:142:LYS:O | 1:Y:145:LEU:N | 2.44 | 0.51 |
| 1:O:183:TYR:O | 1:O:187:SER:HB3 | 2.11 | 0.51 |
| 1:Y:26:ASN:O | 1:Y:28:ILE:HD13 | 2.10 | 0.51 |
| 1:O:278:LYS:HG2 | 1:O:279:ALA:N | 2.25 | 0.51 |
| 1:O:125:ARG:HG2 | 1:O:130:LEU:O | 2.11 | 0.51 |
| 1:Y:43:GLY:C | 1:Y:44:TRP:HD1 | 2.14 | 0.51 |
| 1:Y:395:MET:O | 1:Y:396:GLN:C | 2.48 | 0.51 |
| 1:O:406:LEU:HD23 | 1:O:407:ARG:N | 2.25 | 0.51 |
| 1:O:281:LYS:HZ2 | 1:O:281:LYS:HB2 | 1.75 | 0.51 |
| 1:Y:75:ALA:O | 1:Y:238:PRO:HD2 | 2.11 | 0.51 |
| 1:O:251:PHE:CZ | 1:O:446:LEU:HD13 | 2.46 | 0.51 |
| 1:O:53:TRP:HE3 | 1:O:169:LEU:CD1 | 2.24 | 0.51 |
| 1:Y:185:ASN:ND2 | 1:Y:244:GLY:N | 2.55 | 0.51 |
| 1:Y:137:SER:O | 1:Y:138:GLY:C | 2.49 | 0.51 |
| 1:Y:56:GLN:O | 1:Y:56:GLN:HG3 | 2.11 | 0.51 |
| 1:O:346:PRO:HA | 1:O:348:PHE:HE1 | 1.75 | 0.51 |
| 1:O:220:SER:O | 1:O:224:TYR:OH | 2.29 | 0.51 |
| 1:Y:71:SER:HB2 | 1:Y:235:THR:CG2 | 2.40 | 0.50 |
| 1:O:352:GLY:O | 1:O:356:TRP:N | 2.34 | 0.50 |
| 1:O:466:ILE:O | 1:O:466:ILE:HG22 | 2.08 | 0.50 |
| 1:Y:389:ARG:O | 1:Y:390:ASP:C | 2.48 | 0.50 |
| 1:O:158:GLY:CA | 1:O:212:GLU:HB3 | 2.39 | 0.50 |
| 1:Y:466:ILE:O | 1:Y:466:ILE:HG22 | 2.11 | 0.50 |
| 1:Y:273:MET:CB | 1:Y:395:MET:HE3 | 2.41 | 0.50 |
| 1:Y:117:ARG:HB2 | 1:Y:117:ARG:HH11 | 1.77 | 0.50 |
| 1:O:395:MET:O | 1:O:399:SER:N | 2.44 | 0.50 |
| 1:O:196:THR:HG22 | 1:O:198:ASP:H | 1.77 | 0.50 |
| 1:Y:40:PRO:HG3 | 1:Y:46:GLU:CD | 2.32 | 0.50 |
| 1:O:228:ASN:HB2 | 1:O:236:ARG:NE | 2.26 | 0.50 |
| 1:O:477:THR:O | 1:O:480:ASN:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:137:SER:O | 1:O:138:GLY:O | 2.29 | 0.50 |
| 1:Y:314:GLN:O | 1:Y:318:ASP:N | 2.35 | 0.50 |
| 1:O:408:VAL:O | 1:O:409:ASP:HB3 | 2.11 | 0.50 |
| 1:O:174:THR:HB | 1:O:177:ARG:HB2 | 1.93 | 0.50 |
| 1:O:144:ILE:CG2 | 1:O:148:VAL:HG21 | 2.41 | 0.50 |
| 1:O:317:ARG:HB2 | 1:O:323:ILE:HG13 | 1.94 | 0.50 |
| 1:Y:47:HIS:CD2 | 1:Y:82:GLN:HE22 | 2.30 | 0.50 |
| 1:Y:242:ILE:HG22 | 1:Y:243:ALA:N | 2.26 | 0.50 |
| 1:O:113:GLU:O | 1:O:114:HIS:O | 2.30 | 0.50 |
| 1:O:35:PHE:HB2 | 1:O:51:GLU:CD | 2.32 | 0.50 |
| 1:O:28:ILE:HG22 | 1:O:29:SER:N | 2.27 | 0.50 |
| 1:O:15:SER:CB | 1:O:34:GLU:HA | 2.41 | 0.50 |
| 1:O:418:LEU:O | 1:O:419:MET:C | 2.50 | 0.50 |
| 1:O:444:ALA:O | 1:O:445:TYR:O | 2.29 | 0.50 |
| 1:Y:393:GLU:O | 1:Y:394:ALA:C | 2.50 | 0.50 |
| 1:O:129:GLY:C | 1:O:130:LEU:HD23 | 2.32 | 0.50 |
| 1:Y:94:GLY:CA | 1:Y:171:TRP:HH2 | 2.25 | 0.50 |
| 1:O:218:ARG:HH11 | 1:O:218:ARG:CG | 2.25 | 0.49 |
| 1:O:342:VAL:HA | 1:O:365:PHE:O | 2.12 | 0.49 |
| 1:O:216:GLU:OE2 | 1:O:218:ARG:HD3 | 2.11 | 0.49 |
| 1:O:303:GLU:HG3 | 1:O:304:GLY:N | 2.28 | 0.49 |
| 1:Y:197:LEU:N | 1:Y:197:LEU:HD22 | 2.27 | 0.49 |
| 1:O:201:ASP:O | 1:O:202:LYS:C | 2.48 | 0.49 |
| 1:O:89:TRP:HB2 | 1:O:95:LYS:O | 2.12 | 0.49 |
| 1:Y:156:ARG:C | 1:Y:158:GLY:H | 2.15 | 0.49 |
| 1:Y:33:ARG:NH2 | 1:Y:58:TRP:HB3 | 2.27 | 0.49 |
| 1:O:438:VAL:HA | 1:O:441:LEU:HD12 | 1.93 | 0.49 |
| 1:O:166:ASP:CG | 1:O:167:THR:H | 2.14 | 0.49 |
| 1:O:273:MET:HB2 | 1:O:395:MET:CE | 2.42 | 0.49 |
| 1:O:431:GLU:HB3 | 1:O:466:ILE:HG13 | 1.93 | 0.49 |
| 1:Y:89:TRP:HD1 | 1:Y:90:GLU:O | 1.95 | 0.49 |
| 1:O:103:TRP:N | 1:O:103:TRP:CD1 | 2.80 | 0.49 |
| 1:Y:124:ILE:HG21 | 1:Y:190:MET:CE | 2.43 | 0.49 |
| 1:O:44:TRP:N | 1:O:44:TRP:CD1 | 2.80 | 0.49 |
| 1:Y:170:ILE:HG22 | 1:Y:171:TRP:N | 2.27 | 0.49 |
| 1:O:284:ASN:OD1 | 1:O:398:ASP:OD1 | 2.30 | 0.49 |
| 1:Y:71:SER:HB3 | 1:Y:229:ILE:HG13 | 1.95 | 0.49 |
| 1:Y:389:ARG:HB2 | 1:Y:426:LEU:CD1 | 2.42 | 0.49 |
| 1:O:196:THR:HG22 | 1:O:198:ASP:N | 2.28 | 0.49 |
| 1:O:3:LYS:HA | 1:O:73:GLN:C | 2.32 | 0.49 |
| 1:O:478:GLU:O | 1:O:482:ARG:HG2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:154:ARG:O | 1:O:155:ALA:C | 2.51 | 0.49 |
| 1:O:324:ASN:N | 1:O:324:ASN:ND2 | 2.61 | 0.49 |
| 1:O:415:ASN:HD22 | 1:O:415:ASN:C | 2.15 | 0.49 |
| 1:O:413:VAL:HA | 1:O:419:MET:SD | 2.53 | 0.49 |
| 1:O:50:MET:O | 1:O:53:TRP:HB3 | 2.12 | 0.49 |
| 1:Y:80:THR:HG21 | 1:Y:248:ALA:HB2 | 1.94 | 0.49 |
| 1:O:111:ILE:O | 1:O:112:CYS:C | 2.51 | 0.49 |
| 1:Y:237:ILE:CG2 | 1:Y:238:PRO:HD2 | 2.42 | 0.49 |
| 1:O:137:SER:HA | 1:O:140:LYS:HB2 | 1.94 | 0.49 |
| 1:O:389:ARG:O | 1:O:393:GLU:HG2 | 2.11 | 0.49 |
| 1:O:80:THR:HG21 | 1:O:245:ASP:HA | 1.94 | 0.49 |
| 1:Y:253:GLN:CD | 1:Y:407:ARG:HD2 | 2.33 | 0.49 |
| 1:O:415:ASN:ND2 | 1:O:418:LEU:HB2 | 2.28 | 0.49 |
| 1:O:182:ASP:OD2 | 1:O:184:THR:OG1 | 2.29 | 0.49 |
| 1:Y:262:LYS:HZ1 | 1:Y:264:THR:HB | 1.77 | 0.49 |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:HA2 | 1.77 | 0.49 |
| 1:Y:221:SER:HB2 | 1:Y:450:ALA:HB2 | 1.93 | 0.49 |
| 1:O:448:GLY:O | 1:O:451:VAL:HG12 | 2.13 | 0.49 |
| 1:O:143:TRP:HE3 | 1:O:144:ILE:HA | 1.75 | 0.49 |
| 1:Y:249:ALA:HB2 | 1:Y:439:THR:OG1 | 2.13 | 0.49 |
| 1:O:402:ARG:HH12 | 1:O:403:LEU:C | 2.15 | 0.49 |
| 1:Y:415:ASN:O | 1:Y:419:MET:HG2 | 2.13 | 0.49 |
| 1:Y:339:THR:OG1 | 1:Y:339:THR:O | 2.31 | 0.49 |
| 1:Y:445:TYR:O | 1:Y:446:LEU:C | 2.49 | 0.48 |
| 1:O:162:PHE:O | 1:O:179:HIS:HE1 | 1.96 | 0.48 |
| 1:O:272:LEU:HG | 1:O:303:GLU:HB2 | 1.94 | 0.48 |
| 1:O:348:PHE:CD1 | 1:O:348:PHE:N | 2.78 | 0.48 |
| 1:Y:221:SER:HB2 | 1:Y:446:LEU:O | 2.13 | 0.48 |
| 1:O:173:MET:HB3 | 1:O:227:THR:CG2 | 2.43 | 0.48 |
| 1:O:154:ARG:HA | 1:O:159:GLU:HB3 | 1.95 | 0.48 |
| 1:Y:143:TRP:CD2 | 1:Y:147:HIS:CD2 | 3.01 | 0.48 |
| 1:Y:392:LEU:HD23 | 1:Y:393:GLU:HG2 | 1.94 | 0.48 |
| 1:O:61:VAL:O | 1:O:62:GLU:C | 2.52 | 0.48 |
| 1:Y:174:THR:C | 1:Y:176:GLY:H | 2.16 | 0.48 |
| 1:O:199:TRP:CZ2 | 1:O:215:PRO:HD2 | 2.48 | 0.48 |
| 1:Y:250:LEU:HD12 | 1:Y:250:LEU:C | 2.28 | 0.48 |
| 1:O:132:ILE:O | 1:O:133:ASP:HB2 | 2.13 | 0.48 |
| 1:O:440:ALA:O | 1:O:441:LEU:C | 2.51 | 0.48 |
| 1:O:229:ILE:HG23 | 1:O:235:THR:O | 2.13 | 0.48 |
| 1:O:17:ARG:C | 1:O:59:THR:HG21 | 2.34 | 0.48 |
| 1:O:144:ILE:HG22 | 1:O:148:VAL:CG2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:185:ASN:HD21 | 1:Y:244:GLY:CA | 2.25 | 0.48 |
| 1:Y:18:ALA:HB2 | 1:Y:59:THR:HB | 1.95 | 0.48 |
| 1:Y:245:ASP:O | 1:Y:249:ALA:N | 2.41 | 0.48 |
| 1:Y:167:THR:HG21 | 1:Y:215:PRO:HG3 | 1.94 | 0.48 |
| 1:O:457:LEU:C | 1:O:459:GLU:H | 2.17 | 0.48 |
| 1:O:172:LYS:HA | 1:O:172:LYS:HD2 | 1.45 | 0.48 |
| 1:O:75:ALA:CB | 1:O:453:PHE:HD2 | 2.26 | 0.48 |
| 1:O:156:ARG:C | 1:O:158:GLY:H | 2.17 | 0.48 |
| 1:Y:172:LYS:HA | 1:Y:172:LYS:HD2 | 1.58 | 0.48 |
| 1:Y:328:ASP:HB3 | 1:Y:332:PHE:HE2 | 1.79 | 0.48 |
| 1:O:441:LEU:HD23 | 1:O:445:TYR:CE1 | 2.48 | 0.48 |
| 1:Y:153:GLU:O | 1:Y:154:ARG:C | 2.49 | 0.48 |
| 1:Y:184:THR:HA | 1:Y:290:ILE:HG22 | 1.94 | 0.48 |
| 1:Y:91:LYS:O | 1:Y:92:GLU:C | 2.51 | 0.48 |
| 1:O:161:LEU:CD2 | 1:O:162:PHE:H | 2.27 | 0.48 |
| 1:O:184:THR:CA | 1:O:290:ILE:HG22 | 2.43 | 0.48 |
| 1:O:151:SER:O | 1:O:154:ARG:HG3 | 2.13 | 0.48 |
| 1:Y:193:ASN:OD1 | 1:Y:195:HIS:N | 2.44 | 0.48 |
| 1:O:293:GLY:HA2 | 1:O:299:ASN:HD22 | 1.78 | 0.48 |
| 1:O:241:GLY:HA3 | 1:O:447:ALA:HB2 | 1.96 | 0.48 |
| 1:O:193:ASN:HB3 | 1:O:196:THR:HB | 1.95 | 0.48 |
| 1:O:24:ASP:O | 1:O:25:ALA:HB3 | 2.14 | 0.48 |
| 1:Y:246:GLN:CG | 1:Y:270:PHE:HB2 | 2.41 | 0.48 |
| 1:Y:154:ARG:CA | 1:Y:159:GLU:HB3 | 2.44 | 0.48 |
| 1:O:406:LEU:HD23 | 1:O:407:ARG:H | 1.79 | 0.48 |
| 1:Y:3:LYS:HA | 1:Y:73:GLN:C | 2.33 | 0.48 |
| 1:O:462:GLU:O | 1:O:465:VAL:HG22 | 2.14 | 0.48 |
| 1:O:191:LEU:O | 1:O:199:TRP:HE3 | 1.97 | 0.48 |
| 1:O:5:TYR:CB | 1:O:74:ILE:HG22 | 2.35 | 0.48 |
| 1:Y:3:LYS:HA | 1:Y:73:GLN:CA | 2.43 | 0.48 |
| 1:Y:205:GLU:O | 1:Y:206:VAL:C | 2.50 | 0.48 |
| 1:O:408:VAL:HG23 | 1:O:413:VAL:HG11 | 1.95 | 0.47 |
| 1:O:60:LEU:HD12 | 1:O:60:LEU:C | 2.33 | 0.47 |
| 1:O:437:GLU:OE1 | 1:O:437:GLU:N | 2.48 | 0.47 |
| 1:Y:124:ILE:O | 1:Y:128:THR:OG1 | 2.29 | 0.47 |
| 1:Y:33:ARG:CZ | 1:Y:58:TRP:HB3 | 2.44 | 0.47 |
| 1:O:449:LEU:HA | 1:O:449:LEU:HD12 | 1.72 | 0.47 |
| 1:Y:152:ARG:O | 1:Y:153:GLU:C | 2.53 | 0.47 |
| 1:Y:169:LEU:O | 1:Y:173:MET:HG2 | 2.14 | 0.47 |
| 1:Y:425:ILE:HA | 1:Y:479:ARG:HG2 | 1.96 | 0.47 |
| 1:O:199:TRP:HZ2 | 1:O:215:PRO:HD2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:32:GLN:HA | 1:Y:59:THR:CG2 | 2.45 | 0.47 |
| 1:O:392:LEU:O | 1:O:392:LEU:HG | 2.15 | 0.47 |
| 1:O:141:VAL:O | 1:O:142:LYS:C | 2.53 | 0.47 |
| 1:Y:207:LEU:CB | 1:Y:209:ILE:HD12 | 2.44 | 0.47 |
| 1:O:405:ALA:HB2 | 1:O:429:ARG:HD2 | 1.96 | 0.47 |
| 1:O:359:TYR:CD2 | 1:O:359:TYR:N | 2.79 | 0.47 |
| 1:O:468:ARG:HG3 | 1:O:468:ARG:NH1 | 2.28 | 0.47 |
| 1:Y:37:GLN:OE1 | 1:Y:47:HIS:HE1 | 1.97 | 0.47 |
| 1:O:41:LYS:HG3 | 1:O:42:PRO:N | 2.28 | 0.47 |
| 1:Y:477:THR:O | 1:Y:478:GLU:C | 2.52 | 0.47 |
| 1:O:5:TYR:O | 1:O:74:ILE:HA | 2.14 | 0.47 |
| 1:O:420:GLN:HE21 | 1:O:424:ASP:CG | 2.18 | 0.47 |
| 1:Y:264:THR:HG23 | 1:Y:265:TYR:N | 2.28 | 0.47 |
| 1:O:137:SER:CA | 1:O:140:LYS:HD2 | 2.32 | 0.47 |
| 1:Y:144:ILE:O | 1:Y:145:LEU:C | 2.52 | 0.47 |
| 1:O:250:LEU:HD11 | 1:O:255:CYS:CB | 2.42 | 0.47 |
| 1:O:354:PRO:O | 1:O:356:TRP:HD1 | 1.97 | 0.47 |
| 1:O:287:LEU:HD23 | 1:O:287:LEU:N | 2.28 | 0.47 |
| 1:Y:313:ILE:CD1 | 1:Y:380:THR:HG22 | 2.44 | 0.47 |
| 1:Y:429:ARG:HA | 1:Y:470:PHE:O | 2.15 | 0.47 |
| 1:Y:336:VAL:HG11 | 1:Y:375:HIS:CD2 | 2.49 | 0.47 |
| 1:Y:222:GLU:HG2 | 1:Y:224:TYR:CE1 | 2.49 | 0.47 |
| 1:O:94:GLY:HA2 | 1:O:171:TRP:CH2 | 2.49 | 0.47 |
| 1:O:281:LYS:HG3 | 1:O:281:LYS:O | 2.15 | 0.47 |
| 1:O:193:ASN:CG | 1:O:196:THR:HB | 2.35 | 0.47 |
| 1:O:482:ARG:CG | 1:O:482:ARG:HH11 | 2.27 | 0.47 |
| 1:Y:21:MET:HB3 | 1:Y:26:ASN:O | 2.14 | 0.47 |
| 1:O:123:TYR:CD2 | 1:O:203:MET:CE | 2.98 | 0.47 |
| 1:O:105:CYS:SG | 1:O:107:ARG:NH1 | 2.87 | 0.47 |
| 1:O:20:VAL:HG21 | 1:O:63:VAL:HG11 | 1.96 | 0.47 |
| 1:O:124:ILE:HG21 | 1:O:190:MET:CE | 2.44 | 0.47 |
| 1:Y:48:ASP:O | 1:Y:52:ILE:N | 2.44 | 0.47 |
| 1:O:340:ASN:ND2 | 1:O:371:VAL:CG2 | 2.77 | 0.47 |
| 3:Y:601:ATF:O2B | 3:Y:601:ATF:O3G | 2.33 | 0.47 |
| 1:Y:13:THR:N | 3:Y:601:ATF:O2G | 2.39 | 0.47 |
| 1:Y:454:TRP:CD1 | 1:Y:460:LEU:HD11 | 2.50 | 0.46 |
| 1:O:186:ALA:C | 1:O:188:ARG:H | 2.17 | 0.46 |
| 1:O:272:LEU:N | 1:O:272:LEU:HD12 | 2.30 | 0.46 |
| 1:Y:253:GLN:HE22 | 1:Y:409:ASP:HB3 | 1.80 | 0.46 |
| 1:O:386:TYR:HB3 | 1:O:486:TRP:CD2 | 2.49 | 0.46 |
| 1:O:197:LEU:H | 1:O:197:LEU:HD13 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:197:LEU:HD13 | 1:O:197:LEU:N | 2.30 | 0.46 |
| 1:O:156:ARG:CB | 1:O:156:ARG:NH1 | 2.79 | 0.46 |
| 1:O:218:ARG:HH11 | 1:O:218:ARG:HG3 | 1.81 | 0.46 |
| 1:O:161:LEU:HD23 | 1:O:162:PHE:H | 1.80 | 0.46 |
| 1:O:263:ASN:HB2 | 1:O:271:MET:HG3 | 1.96 | 0.46 |
| 1:Y:434:GLU:CB | 1:Y:465:VAL:HB | 2.41 | 0.46 |
| 1:O:124:ILE:HG12 | 1:O:124:ILE:H | 1.37 | 0.46 |
| 1:Y:41:LYS:HG3 | 1:Y:42:PRO:HD2 | 1.97 | 0.46 |
| 1:Y:44:TRP:CD1 | 1:Y:44:TRP:N | 2.80 | 0.46 |
| 1:Y:74:ILE:HD11 | 1:Y:237:ILE:CG1 | 2.15 | 0.46 |
| 1:O:183:TYR:CD2 | 1:O:298:VAL:CG2 | 2.98 | 0.46 |
| 1:Y:47:HIS:CB | 1:Y:52:ILE:HD11 | 2.45 | 0.46 |
| 1:Y:115:LEU:HD21 | 1:Y:207:LEU:HD21 | 1.97 | 0.46 |
| 1:Y:16:SER:HB3 | 1:Y:56:GLN:HA | 1.98 | 0.46 |
| 1:Y:293:GLY:N | 1:Y:297:GLU:O | 2.36 | 0.46 |
| 1:O:403:LEU:N | 1:O:403:LEU:CD1 | 2.79 | 0.46 |
| 1:Y:87:ILE:HD13 | 1:Y:168:TRP:HB2 | 1.98 | 0.46 |
| 1:Y:458:ASP:HA | 1:Y:461:GLN:CB | 2.44 | 0.46 |
| 1:O:144:ILE:HD12 | 1:O:144:ILE:N | 2.27 | 0.46 |
| 1:Y:151:SER:O | 1:Y:155:ALA:N | 2.37 | 0.46 |
| 1:O:264:THR:CG2 | 1:O:265:TYR:N | 2.78 | 0.46 |
| 1:O:214:LEU:CD1 | 1:O:214:LEU:N | 2.78 | 0.46 |
| 1:O:113:GLU:O | 1:O:117:ARG:HD3 | 2.15 | 0.46 |
| 1:Y:284:ASN:OD1 | 1:Y:398:ASP:OD1 | 2.33 | 0.46 |
| 1:Y:281:LYS:HG3 | 1:Y:281:LYS:O | 2.16 | 0.46 |
| 1:O:161:LEU:CD2 | 1:O:162:PHE:N | 2.79 | 0.46 |
| 1:O:4:LYS:HB3 | 1:O:4:LYS:HE2 | 1.68 | 0.46 |
| 1:Y:11:GLN:HE22 | 1:Y:82:GLN:HE21 | 1.62 | 0.46 |
| 1:Y:313:ILE:HD11 | 1:Y:381:LEU:HD23 | 1.98 | 0.46 |
| 1:O:53:TRP:HZ3 | 1:O:173:MET:CE | 2.29 | 0.46 |
| 1:Y:142:LYS:O | 1:Y:145:LEU:HB2 | 2.16 | 0.46 |
| 1:O:293:GLY:CA | 1:O:299:ASN:ND2 | 2.78 | 0.46 |
| 1:Y:201:ASP:O | 1:Y:204:LEU:HB2 | 2.16 | 0.46 |
| 1:O:81:ASN:OD1 | 1:O:165:VAL:HB | 2.15 | 0.46 |
| 1:Y:401:ILE:CG2 | 1:Y:402:ARG:N | 2.79 | 0.46 |
| 1:O:6:ILE:HG13 | 1:O:7:VAL:N | 2.30 | 0.46 |
| 1:O:161:LEU:CD2 | 1:O:179:HIS:CE1 | 2.99 | 0.46 |
| 1:O:194:ILE:HB | 1:O:290:ILE:HD11 | 1.98 | 0.46 |
| 1:O:145:LEU:HD12 | 1:O:145:LEU:HA | 1.78 | 0.46 |
| 1:Y:150:GLY:O | 1:Y:151:SER:C | 2.54 | 0.46 |
| 1:Y:111:ILE:HG22 | 1:Y:115:LEU:HD11 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:457:LEU:HA | 1:O:457:LEU:HD12 | 1.82 | 0.46 |
| 1:O:53:TRP:CE3 | 1:O:169:LEU:CD1 | 3.00 | 0.45 |
| 1:Y:156:ARG:CB | 1:Y:156:ARG:NH1 | 2.79 | 0.45 |
| 1:O:401:ILE:CG2 | 1:O:402:ARG:N | 2.79 | 0.45 |
| 1:Y:41:LYS:O | 1:Y:44:TRP:HB2 | 2.16 | 0.45 |
| 1:Y:104:GLN:NE2 | 1:Y:308:MET:CE | 2.79 | 0.45 |
| 1:O:460:LEU:C | 1:O:462:GLU:H | 2.19 | 0.45 |
| 1:Y:94:GLY:CA | 1:Y:171:TRP:CH2 | 2.99 | 0.45 |
| 1:O:6:ILE:HD12 | 1:O:76:ALA:HB3 | 1.97 | 0.45 |
| 1:Y:110:GLU:O | 1:Y:113:GLU:N | 2.49 | 0.45 |
| 1:Y:237:ILE:CG2 | 1:Y:238:PRO:N | 2.79 | 0.45 |
| 1:Y:422:GLN:NE2 | 1:Y:426:LEU:CD2 | 2.79 | 0.45 |
| 1:O:69:ILE:N | 1:O:69:ILE:CD1 | 2.80 | 0.45 |
| 1:O:144:ILE:HG22 | 1:O:148:VAL:HG21 | 1.97 | 0.45 |
| 1:Y:48:ASP:HB3 | 1:Y:51:GLU:HB3 | 1.98 | 0.45 |
| 1:Y:111:ILE:O | 1:Y:112:CYS:C | 2.51 | 0.45 |
| 1:Y:372:ASN:OD1 | 1:Y:374:ASN:HB2 | 2.16 | 0.45 |
| 1:Y:449:LEU:HD13 | 1:Y:454:TRP:O | 2.15 | 0.45 |
| 1:Y:391:VAL:O | 1:Y:392:LEU:C | 2.55 | 0.45 |
| 1:Y:433:PRO:HA | 1:Y:466:ILE:CD1 | 2.44 | 0.45 |
| 1:Y:199:TRP:CD2 | 1:Y:214:LEU:HD23 | 2.52 | 0.45 |
| 1:Y:214:LEU:CD1 | 1:Y:214:LEU:N | 2.79 | 0.45 |
| 1:O:325:ASP:HB3 | 1:O:327:TYR:CB | 2.45 | 0.45 |
| 1:O:44:TRP:CZ2 | 1:O:107:ARG:HB2 | 2.49 | 0.45 |
| 1:O:40:PRO:HG2 | 1:O:44:TRP:HB2 | 1.95 | 0.45 |
| 1:Y:382:GLU:HG2 | 1:Y:421:PHE:CZ | 2.51 | 0.45 |
| 1:O:6:ILE:CD1 | 1:O:76:ALA:HB3 | 2.46 | 0.45 |
| 1:Y:316:LEU:HD23 | 1:Y:316:LEU:HA | 1.49 | 0.45 |
| 1:Y:226:GLN:HB3 | 1:Y:237:ILE:O | 2.17 | 0.45 |
| 1:O:230:GLY:HA2 | 1:O:235:THR:HB | 1.96 | 0.45 |
| 1:O:226:GLN:HE21 | 1:O:236:ARG:HG2 | 1.80 | 0.45 |
| 1:O:482:ARG:HG3 | 1:O:482:ARG:HH11 | 1.81 | 0.45 |
| 1:O:108:THR:HG21 | 1:O:139:THR:C | 2.37 | 0.45 |
| 1:O:125:ARG:NH2 | 1:O:285:GLY:H | 2.15 | 0.45 |
| 1:O:207:LEU:CD2 | 1:O:207:LEU:N | 2.79 | 0.45 |
| 1:Y:161:LEU:CD2 | 1:Y:179:HIS:NE2 | 2.80 | 0.45 |
| 1:O:20:VAL:O | 1:O:28:ILE:HB | 2.17 | 0.45 |
| 1:O:218:ARG:NH1 | 1:O:218:ARG:CG | 2.80 | 0.45 |
| 1:O:58:TRP:CA | 1:O:58:TRP:CE3 | 2.99 | 0.45 |
| 1:O:428:THR:HG23 | 1:O:429:ARG:N | 2.32 | 0.45 |
| 1:Y:351:LEU:HD22 | 1:Y:360:ALA:CB | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:53:TRP:CZ3 | 1:O:173:MET:CE | 3.00 | 0.45 |
| 1:O:204:LEU:HA | 1:O:204:LEU:HD23 | 1.51 | 0.45 |
| 1:O:422:GLN:NE2 | 1:O:426:LEU:CD2 | 2.80 | 0.45 |
| 1:O:188:ARG:HA | 1:O:188:ARG:HD3 | 1.28 | 0.45 |
| 1:O:170:ILE:CG2 | 1:O:171:TRP:N | 2.80 | 0.45 |
| 1:O:179:HIS:CD2 | 1:O:215:PRO:CA | 3.00 | 0.45 |
| 1:O:191:LEU:O | 1:O:192:PHE:HB2 | 2.17 | 0.45 |
| 1:Y:189:THR:OG1 | 1:Y:191:LEU:HD12 | 2.17 | 0.45 |
| 1:Y:108:THR:HB | 1:Y:139:THR:HB | 1.99 | 0.45 |
| 1:O:430:VAL:HB | 1:O:470:PHE:HB2 | 1.97 | 0.45 |
| 1:Y:251:PHE:CD2 | 1:Y:446:LEU:CD2 | 3.00 | 0.45 |
| 1:O:170:ILE:HA | 1:O:173:MET:CG | 2.47 | 0.45 |
| 1:Y:211:ARG:NH1 | 1:Y:211:ARG:CG | 2.80 | 0.45 |
| 1:O:58:TRP:N | 1:O:58:TRP:CD2 | 2.80 | 0.45 |
| 1:O:58:TRP:O | 1:O:62:GLU:N | 2.42 | 0.45 |
| 1:Y:17:ARG:HH22 | 1:Y:437:GLU:HG2 | 1.81 | 0.45 |
| 1:Y:498:GLU:OE2 | 1:O:488:LYS:HE2 | 2.17 | 0.45 |
| 1:Y:256:VAL:HG12 | 1:Y:294:PRO:HG3 | 1.97 | 0.44 |
| 1:O:168:TRP:O | 1:O:169:LEU:C | 2.54 | 0.44 |
| 1:O:179:HIS:CD2 | 1:O:215:PRO:CB | 2.99 | 0.44 |
| 1:Y:468:ARG:CG | 1:Y:468:ARG:NH1 | 2.80 | 0.44 |
| 1:O:403:LEU:N | 1:O:403:LEU:HD12 | 2.31 | 0.44 |
| 1:O:264:THR:HG23 | 1:O:265:TYR:N | 2.32 | 0.44 |
| 1:O:350:GLY:HA2 | 1:O:360:ALA:HB3 | 1.99 | 0.44 |
| 1:Y:193:ASN:HB3 | 1:Y:196:THR:HB | 1.99 | 0.44 |
| 1:O:372:ASN:OD1 | 1:O:374:ASN:N | 2.50 | 0.44 |
| 1:O:13:THR:HG22 | 1:O:13:THR:O | 2.15 | 0.44 |
| 1:O:199:TRP:CZ2 | 1:O:214:LEU:HB3 | 2.52 | 0.44 |
| 1:O:70:SER:O | 1:O:72:ASP:N | 2.50 | 0.44 |
| 1:O:90:GLU:CD | 1:O:93:THR:HG21 | 2.37 | 0.44 |
| 1:O:37:GLN:OE1 | 1:O:47:HIS:HE1 | 1.99 | 0.44 |
| 1:O:58:TRP:N | 1:O:58:TRP:CE3 | 2.85 | 0.44 |
| 1:Y:195:HIS:ND1 | 1:Y:195:HIS:N | 2.65 | 0.44 |
| 1:Y:108:THR:CB | 1:Y:139:THR:HB | 2.47 | 0.44 |
| 3:O:601:ATF:O2B | 3:O:601:ATF:O1G | 2.35 | 0.44 |
| 1:O:41:LYS:HB3 | 1:O:41:LYS:HE2 | 1.78 | 0.44 |
| 1:Y:403:LEU:CD1 | 1:Y:403:LEU:N | 2.80 | 0.44 |
| 1:Y:342:VAL:HA | 1:Y:365:PHE:O | 2.18 | 0.44 |
| 1:O:409:ASP:CA | 1:O:413:VAL:HG11 | 2.47 | 0.44 |
| 1:Y:480:ASN:N | 1:Y:480:ASN:ND2 | 2.64 | 0.44 |
| 1:Y:361:ARG:HD3 | 1:Y:361:ARG:HA | 1.74 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:115:LEU:O | 1:O:116:LYS:C | 2.56 | 0.44 |
| 1:O:251:PHE:CE1 | 1:O:256:VAL:CG2 | 2.99 | 0.44 |
| 1:O:444:ALA:O | 1:O:445:TYR:C | 2.53 | 0.44 |
| 1:Y:24:ASP:CB | 1:Y:26:ASN:HD21 | 2.14 | 0.44 |
| 1:Y:142:LYS:O | 1:Y:143:TRP:C | 2.55 | 0.44 |
| 1:Y:185:ASN:O | 1:Y:188:ARG:HB2 | 2.16 | 0.44 |
| 1:O:494:MET:HB3 | 1:O:494:MET:HE3 | 1.48 | 0.44 |
| 1:O:394:ALA:O | 1:O:397:ALA:HB3 | 2.16 | 0.44 |
| 1:O:199:TRP:HB3 | 1:O:204:LEU:HD11 | 2.00 | 0.44 |
| 1:Y:150:GLY:O | 1:Y:153:GLU:HB2 | 2.18 | 0.44 |
| 1:Y:393:GLU:H | 1:Y:393:GLU:HG2 | 1.21 | 0.44 |
| 1:Y:191:LEU:O | 1:Y:199:TRP:HE3 | 2.01 | 0.44 |
| 1:Y:117:ARG:H | 1:Y:117:ARG:HG3 | 1.68 | 0.44 |
| 1:O:78:GLY:CA | 1:O:447:ALA:HB2 | 2.48 | 0.44 |
| 1:O:183:TYR:CD1 | 1:O:217:VAL:CG1 | 3.00 | 0.44 |
| 1:O:237:ILE:HG22 | 1:O:238:PRO:N | 2.33 | 0.44 |
| 1:O:179:HIS:NE2 | 1:O:215:PRO:CB | 2.80 | 0.44 |
| 1:O:192:PHE:HE2 | 1:O:217:VAL:HG11 | 1.83 | 0.44 |
| 1:Y:142:LYS:O | 1:Y:146:ASP:OD1 | 2.36 | 0.44 |
| 1:O:278:LYS:HZ2 | 1:O:280:VAL:HB | 1.77 | 0.44 |
| 1:Y:67:ALA:HB1 | 1:Y:69:ILE:HG12 | 1.99 | 0.44 |
| 1:Y:466:ILE:HA | 1:Y:466:ILE:HD13 | 1.51 | 0.44 |
| 1:O:219:ARG:HG2 | 1:O:222:GLU:CB | 2.44 | 0.44 |
| 1:O:166:ASP:O | 1:O:169:LEU:N | 2.51 | 0.44 |
| 1:O:20:VAL:CG1 | 1:O:21:MET:N | 2.80 | 0.44 |
| 1:Y:27:ILE:HD11 | 1:Y:30:VAL:CG2 | 2.45 | 0.44 |
| 1:Y:9:LEU:HD12 | 1:Y:9:LEU:HA | 1.87 | 0.44 |
| 1:Y:166:ASP:O | 1:Y:167:THR:C | 2.56 | 0.44 |
| 1:O:428:THR:CG2 | 1:O:429:ARG:N | 2.80 | 0.43 |
| 1:Y:40:PRO:HD2 | 1:Y:44:TRP:HB2 | 1.99 | 0.43 |
| 1:O:316:LEU:HD23 | 1:O:316:LEU:HA | 1.43 | 0.43 |
| 1:Y:383:SER:O | 1:Y:384:ILE:C | 2.52 | 0.43 |
| 1:Y:221:SER:OG | 1:Y:221:SER:O | 2.34 | 0.43 |
| 1:O:156:ARG:O | 1:O:212:GLU:HG2 | 2.18 | 0.43 |
| 1:Y:44:TRP:CZ2 | 1:Y:107:ARG:HB2 | 2.52 | 0.43 |
| 1:Y:482:ARG:CG | 1:Y:482:ARG:NH1 | 2.79 | 0.43 |
| 1:Y:324:ASN:N | 1:Y:324:ASN:HD22 | 2.14 | 0.43 |
| 1:Y:347:ALA:HB2 | 1:Y:351:LEU:HD13 | 2.01 | 0.43 |
| 1:Y:328:ASP:HB3 | 1:Y:332:PHE:CE2 | 2.53 | 0.43 |
| 1:O:339:THR:O | 1:O:339:THR:OG1 | 2.34 | 0.43 |
| 1:Y:240:SER:HB2 | 1:Y:450:ALA:CB | 2.47 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:251:PHE:CD2 | 1:O:446:LEU:HD13 | 2.51 | 0.43 |
| 1:O:148:VAL:HB | 1:O:151:SER:HB3 | 1.99 | 0.43 |
| 1:Y:308:MET:HE3 | 1:Y:349:THR:HG23 | 2.00 | 0.43 |
| 1:Y:32:GLN:N | 1:Y:59:THR:HG22 | 2.34 | 0.43 |
| 1:O:183:TYR:CD2 | 1:O:298:VAL:HG22 | 2.53 | 0.43 |
| 1:Y:286:LEU:HD11 | 1:Y:394:ALA:CB | 2.48 | 0.43 |
| 1:Y:435:VAL:HG21 | 1:Y:441:LEU:HD11 | 2.01 | 0.43 |
| 1:Y:170:ILE:O | 1:Y:171:TRP:C | 2.55 | 0.43 |
| 1:Y:386:TYR:HB3 | 1:Y:486:TRP:CE2 | 2.53 | 0.43 |
| 1:O:88:VAL:HG12 | 1:O:97:ILE:HG12 | 2.01 | 0.43 |
| 1:Y:264:THR:CG2 | 1:Y:265:TYR:N | 2.80 | 0.43 |
| 1:O:137:SER:O | 1:O:140:LYS:N | 2.52 | 0.43 |
| 1:O:84:GLU:OE1 | 1:O:103:TRP:HB3 | 2.19 | 0.43 |
| 1:O:11:GLN:NE2 | 1:O:82:GLN:HE21 | 2.17 | 0.43 |
| 1:O:130:LEU:HD13 | 1:O:136:PHE:CD1 | 2.54 | 0.43 |
| 1:O:33:ARG:NH2 | 1:O:58:TRP:HB3 | 2.31 | 0.43 |
| 1:Y:276:GLY:O | 1:Y:300:TYR:N | 2.51 | 0.43 |
| 1:O:108:THR:CB | 1:O:139:THR:HB | 2.48 | 0.43 |
| 1:O:142:LYS:O | 1:O:145:LEU:N | 2.52 | 0.43 |
| 1:Y:156:ARG:CG | 1:Y:156:ARG:HH11 | 2.31 | 0.43 |
| 1:Y:432:ARG:CG | 1:Y:436:ARG:NH1 | 2.81 | 0.43 |
| 1:O:271:MET:O | 1:O:272:LEU:HD12 | 2.19 | 0.43 |
| 1:O:463:LYS:NZ | 1:O:465:VAL:CG2 | 2.80 | 0.43 |
| 1:Y:408:VAL:HG23 | 1:Y:409:ASP:N | 2.33 | 0.43 |
| 1:Y:169:LEU:O | 1:Y:172:LYS:HB2 | 2.18 | 0.43 |
| 1:Y:228:ASN:HD21 | 1:Y:235:THR:N | 2.16 | 0.43 |
| 1:Y:250:LEU:HD12 | 1:Y:255:CYS:HB2 | 1.97 | 0.43 |
| 1:Y:326:ALA:O | 1:Y:327:TYR:C | 2.57 | 0.43 |
| 1:O:180:VAL:HG21 | 1:O:218:ARG:HH11 | 1.84 | 0.43 |
| 1:O:406:LEU:CD2 | 1:O:407:ARG:N | 2.82 | 0.43 |
| 1:O:49:PRO:HA | 1:O:52:ILE:HD12 | 2.00 | 0.43 |
| 1:O:83:ARG:CZ | 1:O:246:GLN:HG2 | 2.49 | 0.43 |
| 1:O:386:TYR:CB | 1:O:486:TRP:CD2 | 3.01 | 0.43 |
| 1:Y:91:LYS:HE3 | 1:Y:91:LYS:HB3 | 1.80 | 0.43 |
| 1:O:170:ILE:HA | 1:O:173:MET:HG2 | 2.01 | 0.43 |
| 1:O:87:ILE:O | 1:O:88:VAL:HG23 | 2.19 | 0.43 |
| 1:O:95:LYS:HG3 | 1:O:96:PRO:N | 2.33 | 0.43 |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:N | 2.17 | 0.43 |
| 1:O:78:GLY:HA2 | 1:O:241:GLY:HA3 | 2.00 | 0.43 |
| 1:O:475:GLU:O | 1:O:478:GLU:CB | 2.67 | 0.43 |
| 1:Y:468:ARG:HD2 | 1:Y:468:ARG:C | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:389:ARG:HG3 | 1:O:389:ARG:O | 2.19 | 0.43 |
| 1:O:263:ASN:HB2 | 1:O:271:MET:CG | 2.48 | 0.43 |
| 1:Y:262:LYS:HZ2 | 1:Y:264:THR:HB | 1.84 | 0.42 |
| 1:O:278:LYS:HD3 | 1:O:279:ALA:C | 2.40 | 0.42 |
| 1:O:136:PHE:HB3 | 1:O:188:ARG:O | 2.19 | 0.42 |
| 1:O:250:LEU:HD12 | 1:O:255:CYS:HB2 | 2.01 | 0.42 |
| 1:Y:170:ILE:HA | 1:Y:173:MET:HG2 | 2.01 | 0.42 |
| 1:O:491:LYS:O | 1:O:494:MET:HG3 | 2.19 | 0.42 |
| 1:O:466:ILE:HD13 | 1:O:466:ILE:HA | 1.61 | 0.42 |
| 1:Y:302:LEU:HD23 | 1:Y:302:LEU:HA | 1.10 | 0.42 |
| 1:O:240:SER:C | 1:O:447:ALA:HA | 2.40 | 0.42 |
| 1:O:413:VAL:HG23 | 1:O:432:ARG:HD2 | 2.01 | 0.42 |
| 1:O:161:LEU:HA | 1:O:161:LEU:HD23 | 1.67 | 0.42 |
| 1:Y:144:ILE:O | 1:Y:147:HIS:N | 2.33 | 0.42 |
| 1:Y:415:ASN:ND2 | 1:Y:418:LEU:HB2 | 2.34 | 0.42 |
| 1:O:40:PRO:CG | 1:O:44:TRP:HB3 | 2.49 | 0.42 |
| 1:Y:81:ASN:H | 1:Y:81:ASN:ND2 | 2.16 | 0.42 |
| 1:Y:357:ASP:OD2 | 1:Y:494:MET:HB3 | 2.19 | 0.42 |
| 1:O:53:TRP:CH2 | 1:O:172:LYS:HB3 | 2.54 | 0.42 |
| 1:O:383:SER:O | 1:O:387:GLN:HB2 | 2.19 | 0.42 |
| 1:O:482:ARG:O | 1:O:483:TYR:C | 2.58 | 0.42 |
| 1:Y:23:HIS:ND1 | 1:Y:453:PHE:CE1 | 2.88 | 0.42 |
| 1:O:48:ASP:O | 1:O:51:GLU:HB3 | 2.19 | 0.42 |
| 1:O:359:TYR:HD1 | 1:O:497:GLU:HB3 | 1.85 | 0.42 |
| 1:O:90:GLU:HB3 | 1:O:93:THR:OG1 | 2.19 | 0.42 |
| 1:O:381:LEU:O | 1:O:382:GLU:C | 2.55 | 0.42 |
| 1:O:102:VAL:O | 1:O:103:TRP:C | 2.57 | 0.42 |
| 1:Y:144:ILE:HG23 | 1:Y:148:VAL:CG2 | 2.49 | 0.42 |
| 1:O:278:LYS:O | 1:O:278:LYS:HD2 | 2.18 | 0.42 |
| 1:Y:467:GLU:OE2 | 1:Y:468:ARG:HB2 | 2.20 | 0.42 |
| 1:Y:184:THR:HG22 | 1:Y:290:ILE:HG22 | 2.00 | 0.42 |
| 1:O:108:THR:CG2 | 1:O:139:THR:HB | 2.50 | 0.42 |
| 1:O:144:ILE:CG2 | 1:O:148:VAL:CG2 | 2.97 | 0.42 |
| 1:Y:124:ILE:H | 1:Y:124:ILE:HG12 | 1.68 | 0.42 |
| 1:O:389:ARG:HD2 | 1:O:393:GLU:OE2 | 2.20 | 0.42 |
| 1:O:398:ASP:O | 1:O:400:GLY:N | 2.52 | 0.42 |
| 1:Y:359:TYR:CD1 | 1:Y:359:TYR:N | 2.87 | 0.42 |
| 1:Y:40:PRO:HD2 | 1:Y:44:TRP:CB | 2.49 | 0.42 |
| 1:Y:50:MET:O | 1:Y:53:TRP:HB3 | 2.19 | 0.42 |
| 1:O:5:TYR:N | 1:O:73:GLN:O | 2.35 | 0.42 |
| 1:O:157:ARG:H | 1:O:157:ARG:HG2 | 1.61 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:435:VAL:CG2 | 1:Y:436:ARG:N | 2.80 | 0.42 |
| 1:Y:441:LEU:HD23 | 1:Y:441:LEU:HA | 1.89 | 0.42 |
| 1:O:130:LEU:N | 1:O:130:LEU:HD23 | 2.33 | 0.42 |
| 1:Y:122:ASP:O | 1:Y:126:SER:N | 2.47 | 0.42 |
| 1:O:193:ASN:CB | 1:O:196:THR:HB | 2.50 | 0.42 |
| 1:O:5:TYR:HE2 | 1:O:69:ILE:HG23 | 1.84 | 0.42 |
| 1:O:382:GLU:O | 1:O:383:SER:C | 2.55 | 0.42 |
| 1:Y:325:ASP:CB | 1:Y:327:TYR:HB3 | 2.33 | 0.42 |
| 1:Y:151:SER:O | 1:Y:152:ARG:C | 2.55 | 0.42 |
| 1:O:262:LYS:HA | 1:O:407:ARG:O | 2.19 | 0.42 |
| 1:Y:124:ILE:HG21 | 1:Y:190:MET:HE1 | 2.01 | 0.42 |
| 1:O:11:GLN:HE22 | 1:O:82:GLN:HE21 | 1.66 | 0.42 |
| 1:O:83:ARG:HE | 4:O:600:GOL:H2 | 1.85 | 0.42 |
| 1:Y:375:HIS:O | 1:Y:376:ILE:C | 2.56 | 0.42 |
| 1:O:161:LEU:HD22 | 1:O:179:HIS:CE1 | 2.55 | 0.42 |
| 1:O:161:LEU:HD22 | 1:O:162:PHE:N | 2.35 | 0.42 |
| 1:O:77:ILE:HB | 1:O:238:PRO:O | 2.20 | 0.42 |
| 1:O:5:TYR:HB3 | 1:O:21:MET:O | 2.20 | 0.42 |
| 1:O:188:ARG:HD2 | 1:O:188:ARG:HH11 | 1.60 | 0.42 |
| 1:Y:47:HIS:HD2 | 1:Y:82:GLN:HE22 | 1.68 | 0.42 |
| 1:Y:111:ILE:CG2 | 1:Y:115:LEU:HD11 | 2.50 | 0.42 |
| 1:Y:111:ILE:CG2 | 1:Y:139:THR:HG22 | 2.46 | 0.42 |
| 1:O:229:ILE:HG21 | 1:O:237:ILE:CG1 | 2.31 | 0.42 |
| 1:O:137:SER:O | 1:O:140:LYS:HB2 | 2.20 | 0.42 |
| 1:O:351:LEU:HD13 | 1:O:351:LEU:HA | 1.74 | 0.42 |
| 1:O:64:LEU:N | 1:O:64:LEU:HD12 | 2.35 | 0.42 |
| 1:Y:253:GLN:OE1 | 1:Y:407:ARG:HD2 | 2.20 | 0.42 |
| 1:Y:408:VAL:O | 1:Y:409:ASP:HB3 | 2.20 | 0.42 |
| 1:O:187:SER:CB | 1:O:290:ILE:HB | 2.50 | 0.42 |
| 1:Y:17:ARG:HH22 | 1:Y:437:GLU:CG | 2.32 | 0.42 |
| 1:Y:60:LEU:HA | 1:Y:60:LEU:HD12 | 1.80 | 0.42 |
| 1:Y:117:ARG:HH11 | 1:Y:117:ARG:HG3 | 1.85 | 0.42 |
| 1:Y:127:ASN:CB | 1:Y:193:ASN:ND2 | 2.80 | 0.42 |
| 1:Y:254:LEU:C | 1:Y:256:VAL:H | 2.23 | 0.41 |
| 1:O:32:GLN:HA | 1:O:59:THR:CG2 | 2.50 | 0.41 |
| 1:O:60:LEU:O | 1:O:63:VAL:HB | 2.20 | 0.41 |
| 1:Y:103:TRP:HA | 1:Y:140:LYS:HE3 | 2.02 | 0.41 |
| 1:O:393:GLU:HG2 | 1:O:393:GLU:H | 1.63 | 0.41 |
| 1:Y:360:ALA:HA | 1:Y:493:ALA:O | 2.19 | 0.41 |
| 1:O:46:GLU:HB3 | 1:O:100:ALA:O | 2.20 | 0.41 |
| 1:Y:458:ASP:HA | 1:Y:461:GLN:HB2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:251:PHE:CD2 | 1:Y:446:LEU:HD22 | 2.55 | 0.41 |
| 1:O:416:ASN:O | 1:O:417:PHE:C | 2.59 | 0.41 |
| 1:O:441:LEU:CD2 | 1:O:445:TYR:CE1 | 3.03 | 0.41 |
| 1:O:133:ASP:HA | 1:O:134:PRO:HD3 | 1.92 | 0.41 |
| 1:O:487:LYS:O | 1:O:488:LYS:C | 2.56 | 0.41 |
| 1:Y:87:ILE:HD13 | 1:Y:168:TRP:CB | 2.50 | 0.41 |
| 1:Y:132:ILE:HD13 | 1:Y:132:ILE:HG21 | 1.86 | 0.41 |
| 1:Y:103:TRP:N | 1:Y:103:TRP:CD1 | 2.88 | 0.41 |
| 1:Y:130:LEU:HB3 | 1:Y:131:VAL:H | 1.51 | 0.41 |
| 1:Y:490:VAL:H | 1:Y:490:VAL:HG23 | 1.60 | 0.41 |
| 1:Y:97:ILE:O | 1:Y:98:TYR:HB2 | 2.21 | 0.41 |
| 1:O:263:ASN:ND2 | 1:O:265:TYR:CZ | 2.88 | 0.41 |
| 1:O:128:THR:HG21 | 1:O:190:MET:HA | 2.02 | 0.41 |
| 1:O:38:ILE:O | 1:O:45:VAL:HA | 2.20 | 0.41 |
| 1:O:376:ILE:HG22 | 1:O:376:ILE:O | 2.20 | 0.41 |
| 1:O:28:ILE:HD12 | 1:O:28:ILE:HA | 1.85 | 0.41 |
| 1:Y:145:LEU:HA | 1:Y:145:LEU:HD12 | 1.59 | 0.41 |
| 1:Y:244:GLY:O | 1:Y:245:ASP:C | 2.59 | 0.41 |
| 1:O:113:GLU:HA | 1:O:113:GLU:OE1 | 2.20 | 0.41 |
| 1:Y:120:LEU:O | 1:Y:121:GLU:C | 2.54 | 0.41 |
| 1:O:64:LEU:O | 1:O:65:ALA:C | 2.57 | 0.41 |
| 1:Y:114:HIS:H | 1:Y:114:HIS:CD2 | 2.38 | 0.41 |
| 1:Y:377:ILE:O | 1:Y:378:ARG:C | 2.58 | 0.41 |
| 1:Y:256:VAL:HG11 | 1:Y:294:PRO:HB3 | 2.02 | 0.41 |
| 1:O:89:TRP:CZ2 | 1:O:161:LEU:HD13 | 2.56 | 0.41 |
| 1:O:174:THR:HG21 | 1:O:178:VAL:HG23 | 2.02 | 0.41 |
| 1:Y:185:ASN:HD21 | 1:Y:243:ALA:C | 2.24 | 0.41 |
| 1:Y:189:THR:O | 1:Y:190:MET:HB3 | 2.21 | 0.41 |
| 1:O:458:ASP:HA | 1:O:461:GLN:HB2 | 2.01 | 0.41 |
| 1:O:55:THR:O | 1:O:58:TRP:HB2 | 2.21 | 0.41 |
| 1:Y:23:HIS:HA | 1:Y:453:PHE:HE1 | 1.86 | 0.41 |
| 1:Y:16:SER:HB3 | 1:Y:56:GLN:OE1 | 2.21 | 0.41 |
| 1:O:273:MET:CB | 1:O:395:MET:CE | 2.99 | 0.41 |
| 1:O:484:ALA:O | 1:O:487:LYS:N | 2.54 | 0.41 |
| 1:Y:428:THR:HG23 | 1:Y:429:ARG:N | 2.36 | 0.41 |
| 1:Y:445:TYR:O | 1:Y:449:LEU:N | 2.39 | 0.41 |
| 1:O:441:LEU:HD22 | 1:O:445:TYR:CZ | 2.55 | 0.41 |
| 1:O:156:ARG:CG | 1:O:156:ARG:HH11 | 2.34 | 0.41 |
| 1:Y:257:LYS:HG3 | 1:Y:260:MET:SD | 2.61 | 0.41 |
| 1:Y:258:GLU:N | 1:Y:274:ASN:OD1 | 2.54 | 0.41 |
| 1:Y:222:GLU:HG2 | 1:Y:224:TYR:CD1 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:251:PHE:O | 1:Y:254:LEU:HD12 | 2.21 | 0.41 |
| 1:O:192:PHE:CE1 | 1:O:197:LEU:HA | 2.56 | 0.41 |
| 1:O:226:GLN:NE2 | 1:O:236:ARG:CB | 2.79 | 0.41 |
| 1:O:53:TRP:O | 1:O:54:ALA:C | 2.58 | 0.41 |
| 1:Y:250:LEU:HD13 | 1:Y:262:LYS:HG2 | 2.03 | 0.41 |
| 1:Y:3:LYS:HG2 | 1:Y:72:ASP:O | 2.21 | 0.41 |
| 1:Y:117:ARG:NH1 | 1:Y:117:ARG:CG | 2.80 | 0.41 |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CG | 2.56 | 0.41 |
| 1:Y:23:HIS:HE1 | 1:Y:453:PHE:O | 2.04 | 0.41 |
| 1:Y:169:LEU:N | 1:Y:169:LEU:HD22 | 2.36 | 0.41 |
| 1:O:487:LYS:O | 1:O:490:VAL:HG23 | 2.21 | 0.41 |
| 1:O:195:HIS:N | 1:O:195:HIS:HD1 | 2.19 | 0.41 |
| 1:Y:183:TYR:CD1 | 1:Y:217:VAL:CG1 | 2.98 | 0.41 |
| 1:Y:237:ILE:CG2 | 1:Y:238:PRO:CD | 2.99 | 0.40 |
| 1:O:419:MET:CE | 1:O:419:MET:CA | 2.99 | 0.40 |
| 1:O:86:THR:HG1 | 1:O:137:SER:HB3 | 1.83 | 0.40 |
| 1:Y:84:GLU:HB2 | 1:Y:103:TRP:CB | 2.42 | 0.40 |
| 1:O:262:LYS:C | 1:O:262:LYS:HD2 | 2.42 | 0.40 |
| 1:Y:11:GLN:NE2 | 1:Y:82:GLN:HG2 | 2.36 | 0.40 |
| 1:O:6:ILE:CG1 | 1:O:7:VAL:N | 2.84 | 0.40 |
| 1:O:439:THR:CG2 | 1:O:440:ALA:N | 2.82 | 0.40 |
| 1:O:480:ASN:O | 1:O:481:TYR:C | 2.58 | 0.40 |
| 1:O:155:ALA:O | 1:O:212:GLU:HB2 | 2.20 | 0.40 |
| 1:Y:180:VAL:HG21 | 1:Y:218:ARG:HG3 | 2.03 | 0.40 |
| 1:O:180:VAL:CG2 | 1:O:218:ARG:CG | 2.99 | 0.40 |
| 1:O:45:VAL:HG12 | 1:O:46:GLU:N | 2.36 | 0.40 |
| 1:Y:226:GLN:HE21 | 1:Y:236:ARG:HB3 | 1.85 | 0.40 |
| 1:Y:256:VAL:CG1 | 1:Y:294:PRO:CB | 3.00 | 0.40 |
| 1:O:251:PHE:CD1 | 1:O:256:VAL:CG2 | 3.04 | 0.40 |
| 1:Y:481:TYR:HD2 | 1:Y:482:ARG:HD2 | 1.86 | 0.40 |
| 1:O:474:ILE:HA | 1:O:474:ILE:HD12 | 1.60 | 0.40 |
| 1:Y:295:THR:N | 1:Y:297:GLU:OE1 | 2.50 | 0.40 |
| 1:O:41:LYS:CB | 1:O:42:PRO:CD | 2.99 | 0.40 |
| 1:O:457:LEU:O | 1:O:459:GLU:N | 2.54 | 0.40 |
| 1:Y:74:ILE:HD13 | 1:Y:237:ILE:HG21 | 2.02 | 0.40 |
| 1:Y:256:VAL:CG1 | 1:Y:294:PRO:CG | 2.99 | 0.40 |
| 1:Y:457:LEU:C | 1:Y:459:GLU:H | 2.24 | 0.40 |
| 1:O:477:THR:O | 1:O:479:ARG:N | 2.55 | 0.40 |
| 1:Y:169:LEU:HD13 | 1:Y:169:LEU:HA | 1.50 | 0.40 |
| 1:Y:41:LYS:CB | 1:Y:42:PRO:CD | 3.00 | 0.40 |
| 1:Y:229:ILE:HG13 | 1:Y:230:GLY:N | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:409:ASP:HB2 | 1:O:438:VAL:HG21 | 2.04 | 0.40 |
| 1:O:160:LEU:O | 1:O:213:MET:HB3 | 2.22 | 0.40 |
| 1:Y:432:ARG:CD | 1:Y:436:ARG:NH2 | 2.82 | 0.40 |
| 1:O:326:ALA:O | 1:O:327:TYR:C | 2.57 | 0.40 |
| 1:Y:133:ASP:HA | 1:Y:134:PRO:HD3 | 1.91 | 0.40 |
| 1:Y:201:ASP:O | 1:Y:205:GLU:HG2 | 2.21 | 0.40 |
| 1:Y:87:ILE:CG2 | 1:Y:88:VAL:N | 2.83 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:58:TRP:CZ2 | 1:Y:58:TRP:CZ2[3_655] | 2.10 | 0.10 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%) | 375 (76%) | 87 (18%) | 28 (6%) | 2 12 |
| 1 | Y | 490/501 (98%) | 404 (82%) | 68 (14%) | 18 (4%) | 4 23 |
| All | All | 980/1002 (98%) | 779 (80%) | 155 (16%) | 46 (5%) | 3 17 |

All (46) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 71 | SER |
| 1 | Y | 151 | SER |
| 1 | Y | 153 | GLU |
| 1 | Y | 175 | GLN |
| 1 | O | 60 | LEU |
| 1 | O | 445 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 446 | LEU |
| 1 | O | 456 | ASN |
| 1 | Y | 61 | VAL |
| 1 | Y | 196 | THR |
| 1 | O | 63 | VAL |
| 1 | O | 75 | ALA |
| 1 | O | 111 | ILE |
| 1 | O | 118 | ASP |
| 1 | O | 151 | SER |
| 1 | O | 199 | TRP |
| 1 | O | 477 | THR |
| 1 | O | 478 | GLU |
| 1 | Y | 111 | ILE |
| 1 | Y | 456 | ASN |
| 1 | O | 71 | SER |
| 1 | O | 98 | TYR |
| 1 | Y | 60 | LEU |
| 1 | Y | 62 | GLU |
| 1 | Y | 64 | LEU |
| 1 | Y | 98 | TYR |
| 1 | O | 110 | GLU |
| 1 | O | 114 | HIS |
| 1 | O | 138 | GLY |
| 1 | O | 176 | GLY |
| 1 | O | 202 | LYS |
| 1 | O | 441 | LEU |
| 1 | Y | 202 | LYS |
| 1 | Y | 258 | GLU |
| 1 | O | 99 | ASN |
| 1 | O | 149 | GLU |
| 1 | O | 196 | THR |
| 1 | O | 479 | ARG |
| 1 | Y | 138 | GLY |
| 1 | Y | 411 | GLY |
| 1 | O | 187 | SER |
| 1 | O | 242 | ILE |
| 1 | O | 258 | GLU |
| 1 | O | 458 | ASP |
| 1 | Y | 176 | GLY |
| 1 | Y | 442 | GLY |

### 5.3.2 Protein sidechains (i)

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%) | 259 (64%) | 149 (36%) | 0 1 |
| 1 | Y | 408/412 (99%) | 277 (68%) | 131 (32%) | 0 1 |
| All | All | 816/824 (99%) | 536 (66%) | 280 (34%) | 0 1 |

All (280) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 2 | GLU |
| 1 | Y | 3 | LYS |
| 1 | Y | 5 | TYR |
| 1 | Y | 9 | LEU |
| 1 | Y | 11 | GLN |
| 1 | Y | 21 | MET |
| 1 | Y | 27 | ILE |
| 1 | Y | 28 | ILE |
| 1 | Y | 33 | ARG |
| 1 | Y | 34 | GLU |
| 1 | Y | 62 | GLU |
| 1 | Y | 63 | VAL |
| 1 | Y | 66 | LYS |
| 1 | Y | 70 | SER |
| 1 | Y | 71 | SER |
| 1 | Y | 73 | GLN |
| 1 | Y | 80 | THR |
| 1 | Y | 81 | ASN |
| 1 | Y | 83 | ARG |
| 1 | Y | 91 | LYS |
| 1 | Y | 92 | GLU |
| 1 | Y | 93 | THR |
| 1 | Y | 95 | LYS |
| 1 | Y | 102 | VAL |
| 1 | Y | 106 | ARG |
| 1 | Y | 107 | ARG |
| 1 | Y | 110 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 117 | ARG |
| 1 | Y | 121 | GLU |
| 1 | Y | 124 | ILE |
| 1 | Y | 131 | VAL |
| 1 | Y | 136 | PHE |
| 1 | Y | 139 | THR |
| 1 | Y | 145 | LEU |
| 1 | Y | 146 | ASP |
| 1 | Y | 148 | VAL |
| 1 | Y | 151 | SER |
| 1 | Y | 154 | ARG |
| 1 | Y | 156 | ARG |
| 1 | Y | 157 | ARG |
| 1 | Y | 162 | PHE |
| 1 | Y | 170 | ILE |
| 1 | Y | 172 | LYS |
| 1 | Y | 173 | MET |
| 1 | Y | 175 | GLN |
| 1 | Y | 178 | VAL |
| 1 | Y | 181 | THR |
| 1 | Y | 185 | ASN |
| 1 | Y | 187 | SER |
| 1 | Y | 191 | LEU |
| 1 | Y | 195 | HIS |
| 1 | Y | 196 | THR |
| 1 | Y | 197 | LEU |
| 1 | Y | 198 | ASP |
| 1 | Y | 201 | ASP |
| 1 | Y | 202 | LYS |
| 1 | Y | 205 | GLU |
| 1 | Y | 206 | VAL |
| 1 | Y | 211 | ARG |
| 1 | Y | 219 | ARG |
| 1 | Y | 221 | SER |
| 1 | Y | 222 | GLU |
| 1 | Y | 226 | GLN |
| 1 | Y | 227 | THR |
| 1 | Y | 229 | ILE |
| 1 | Y | 235 | THR |
| 1 | Y | 236 | ARG |
| 1 | Y | 237 | ILE |
| 1 | Y | 245 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 246 | GLN |
| 1 | Y | 253 | GLN |
| 1 | Y | 254 | LEU |
| 1 | Y | 257 | LYS |
| 1 | Y | 258 | GLU |
| 1 | Y | 262 | LYS |
| 1 | Y | 264 | THR |
| 1 | Y | 281 | LYS |
| 1 | Y | 288 | THR |
| 1 | Y | 290 | ILE |
| 1 | Y | 295 | THR |
| 1 | Y | 302 | LEU |
| 1 | Y | 312 | SER |
| 1 | Y | 313 | ILE |
| 1 | Y | 317 | ARG |
| 1 | Y | 318 | ASP |
| 1 | Y | 324 | ASN |
| 1 | Y | 335 | LYS |
| 1 | Y | 337 | GLN |
| 1 | Y | 339 | THR |
| 1 | Y | 351 | LEU |
| 1 | Y | 368 | THR |
| 1 | Y | 384 | ILE |
| 1 | Y | 389 | ARG |
| 1 | Y | 391 | VAL |
| 1 | Y | 392 | LEU |
| 1 | Y | 393 | GLU |
| 1 | Y | 395 | MET |
| 1 | Y | 402 | ARG |
| 1 | Y | 406 | LEU |
| 1 | Y | 407 | ARG |
| 1 | Y | 415 | ASN |
| 1 | Y | 418 | LEU |
| 1 | Y | 423 | SER |
| 1 | Y | 426 | LEU |
| 1 | Y | 428 | THR |
| 1 | Y | 429 | ARG |
| 1 | Y | 434 | GLU |
| 1 | Y | 438 | VAL |
| 1 | Y | 445 | TYR |
| 1 | Y | 449 | LEU |
| 1 | Y | 451 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 455 | GLN |
| 1 | Y | 456 | ASN |
| 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 | 475 | GLU |
| 1 | Y | 476 | THR |
| 1 | Y | 478 | GLU |
| 1 | Y | 482 | ARG |
| 1 | Y | 483 | TYR |
| 1 | Y | 488 | LYS |
| 1 | Y | 492 | ARG |
| 1 | Y | 494 | MET |
| 1 | Y | 498 | GLU |
| 1 | Y | 499 | HIS |
| 1 | O | 2 | GLU |
| 1 | O | 3 | LYS |
| 1 | O | 5 | TYR |
| 1 | O | 9 | LEU |
| 1 | O | 11 | GLN |
| 1 | O | 21 | MET |
| 1 | O | 27 | ILE |
| 1 | O | 28 | ILE |
| 1 | O | 33 | ARG |
| 1 | O | 34 | GLU |
| 1 | O | 41 | LYS |
| 1 | O | 46 | GLU |
| 1 | O | 51 | GLU |
| 1 | O | 57 | SER |
| 1 | O | 59 | THR |
| 1 | O | 60 | LEU |
| 1 | O | 64 | LEU |
| 1 | O | 69 | ILE |
| 1 | O | 70 | SER |
| 1 | O | 71 | SER |
| 1 | O | 80 | THR |
| 1 | O | 81 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 82 | GLN |
| 1 | O | 83 | ARG |
| 1 | O | 87 | ILE |
| 1 | O | 91 | LYS |
| 1 | O | 92 | GLU |
| 1 | O | 93 | THR |
| 1 | O | 102 | VAL |
| 1 | O | 104 | GLN |
| 1 | O | 106 | ARG |
| 1 | O | 107 | ARG |
| 1 | O | 110 | GLU |
| 1 | O | 117 | ARG |
| 1 | O | 124 | ILE |
| 1 | O | 125 | ARG |
| 1 | O | 136 | PHE |
| 1 | O | 137 | SER |
| 1 | O | 140 | LYS |
| 1 | O | 141 | VAL |
| 1 | O | 145 | LEU |
| 1 | O | 146 | ASP |
| 1 | O | 148 | VAL |
| 1 | O | 154 | ARG |
| 1 | O | 156 | ARG |
| 1 | O | 157 | ARG |
| 1 | O | 161 | LEU |
| 1 | O | 162 | PHE |
| 1 | O | 164 | THR |
| 1 | O | 169 | LEU |
| 1 | O | 170 | ILE |
| 1 | O | 172 | LYS |
| 1 | O | 173 | MET |
| 1 | O | 175 | GLN |
| 1 | O | 178 | VAL |
| 1 | O | 180 | VAL |
| 1 | O | 181 | THR |
| 1 | O | 187 | SER |
| 1 | O | 188 | ARG |
| 1 | O | 191 | LEU |
| 1 | O | 195 | HIS |
| 1 | O | 196 | THR |
| 1 | O | 197 | LEU |
| 1 | O | 198 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 201 | ASP |
| 1 | O | 202 | LYS |
| 1 | O | 207 | LEU |
| 1 | O | 211 | ARG |
| 1 | O | 214 | LEU |
| 1 | O | 218 | ARG |
| 1 | O | 219 | ARG |
| 1 | O | 221 | SER |
| 1 | O | 222 | GLU |
| 1 | O | 226 | GLN |
| 1 | O | 227 | THR |
| 1 | O | 229 | ILE |
| 1 | O | 235 | THR |
| 1 | O | 236 | ARG |
| 1 | O | 253 | GLN |
| 1 | O | 254 | LEU |
| 1 | O | 256 | VAL |
| 1 | O | 257 | LYS |
| 1 | O | 258 | GLU |
| 1 | O | 262 | LYS |
| 1 | O | 264 | THR |
| 1 | O | 269 | CYS |
| 1 | O | 271 | MET |
| 1 | O | 278 | LYS |
| 1 | O | 280 | VAL |
| 1 | O | 281 | LYS |
| 1 | O | 284 | ASN |
| 1 | O | 287 | LEU |
| 1 | O | 288 | THR |
| 1 | O | 290 | ILE |
| 1 | O | 313 | ILE |
| 1 | O | 317 | ARG |
| 1 | O | 324 | ASN |
| 1 | O | 335 | LYS |
| 1 | O | 339 | THR |
| 1 | O | 346 | PRO |
| 1 | O | 351 | LEU |
| 1 | O | 368 | THR |
| 1 | O | 389 | ARG |
| 1 | O | 391 | VAL |
| 1 | O | 392 | LEU |
| 1 | O | 393 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 395 | MET |
| 1 | O | 399 | SER |
| 1 | O | 402 | ARG |
| 1 | O | 406 | LEU |
| 1 | O | 407 | ARG |
| 1 | O | 408 | VAL |
| 1 | O | 409 | ASP |
| 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 | 438 | VAL |
| 1 | O | 439 | THR |
| 1 | O | 451 | VAL |
| 1 | O | 453 | PHE |
| 1 | O | 455 | GLN |
| 1 | O | 457 | LEU |
| 1 | O | 459 | GLU |
| 1 | O | 460 | LEU |
| 1 | O | 461 | GLN |
| 1 | O | 462 | GLU |
| 1 | O | 463 | LYS |
| 1 | O | 465 | VAL |
| 1 | O | 466 | ILE |
| 1 | O | 468 | ARG |
| 1 | O | 469 | GLU |
| 1 | O | 474 | ILE |
| 1 | O | 475 | GLU |
| 1 | O | 476 | THR |
| 1 | O | 477 | THR |
| 1 | O | 478 | GLU |
| 1 | O | 479 | ARG |
| 1 | O | 482 | ARG |
| 1 | O | 483 | TYR |
| 1 | O | 487 | LYS |
| 1 | O | 488 | LYS |
| 1 | O | 490 | VAL |
| 1 | O | 492 | ARG |
| 1 | O | 494 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 498 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 11 | GLN |
| 1 | Y | 26 | ASN |
| 1 | Y | 47 | HIS |
| 1 | Y | 56 | 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 | 226 | GLN |
| 1 | Y | 246 | GLN |
| 1 | Y | 253 | GLN |
| 1 | Y | 324 | ASN |
| 1 | Y | 340 | ASN |
| 1 | Y | 396 | GLN |
| 1 | Y | 404 | HIS |
| 1 | Y | 415 | ASN |
| 1 | Y | 461 | GLN |
| 1 | Y | 480 | ASN |
| 1 | Y | 499 | HIS |
| 1 | O | 11 | GLN |
| 1 | O | 26 | ASN |
| 1 | O | 47 | HIS |
| 1 | O | 81 | ASN |
| 1 | O | 114 | HIS |
| 1 | O | 179 | HIS |
| 1 | O | 185 | ASN |
| 1 | O | 226 | GLN |
| 1 | O | 314 | GLN |
| 1 | O | 324 | ASN |
| 1 | O | 340 | ASN |
| 1 | O | 396 | GLN |
| 1 | O | 404 | HIS |
| 1 | O | 415 | ASN |
| 1 | O | 420 | GLN |
| 1 | O | 461 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 480 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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 | 0.55 | 0 |
| 3 | ATF | O | 601 | 2 | 29,35,35 | 5.10 | 10 (34%) | 27,57,57 | 1.74 | 6 (22%) |
| 4 | GOL | Y | 600 | - | 5,5,5 | 0.57 | 0 | 5,5,5 | 0.86 | 0 |
| 3 | ATF | Y | 601 | 2 | 29,35,35 | 5.90 | 9 (31%) | 27,57,57 | 2.07 | 8 (29%) |

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 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | ATF | O | 601 | 2 | - | 0/13/50/50 | 0/3/3/3 |
| 4 | GOL | Y | 600 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ATF | Y | 601 | 2 | - | 0/13/50/50 | 0/3/3/3 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | Y | 601 | ATF | PG-C3B | -21.60 | 1.65 | 1.85 |
| 3 | O | 601 | ATF | PB-C3B | -19.03 | 1.67 | 1.85 |
| 3 | Y | 601 | ATF | PB-C3B | -18.38 | 1.68 | 1.85 |
| 3 | O | 601 | ATF | PG-C3B | -14.55 | 1.71 | 1.85 |
| 3 | O | 601 | ATF | PB-O1B | -3.62 | 1.44 | 1.51 |
| 3 | O | 601 | ATF | C4-N3 | -3.42 | 1.30 | 1.35 |
| 3 | Y | 601 | ATF | PA-O1A | -2.05 | 1.43 | 1.51 |
| 3 | O | 601 | ATF | O2'-C2' | 2.48 | 1.48 | 1.43 |
| 3 | O | 601 | ATF | PA-O2A | 2.51 | 1.65 | 1.54 |
| 3 | Y | 601 | ATF | O4'-C1' | 2.51 | 1.44 | 1.41 |
| 3 | O | 601 | ATF | O4'-C1' | 2.80 | 1.44 | 1.41 |
| 3 | Y | 601 | ATF | PB-O3A | 2.85 | 1.61 | 1.58 |
| 3 | Y | 601 | ATF | F2B-C3B | 4.56 | 1.41 | 1.36 |
| 3 | O | 601 | ATF | PB-O2B | 5.38 | 1.67 | 1.56 |
| 3 | O | 601 | ATF | PG-O3G | 5.51 | 1.65 | 1.54 |
| 3 | Y | 601 | ATF | PB-O2B | 6.32 | 1.69 | 1.56 |
| 3 | Y | 601 | ATF | PG-O2G | 7.00 | 1.68 | 1.54 |
| 3 | O | 601 | ATF | PG-O2G | 7.38 | 1.68 | 1.54 |
| 3 | Y | 601 | ATF | PG-O3G | 7.74 | 1.69 | 1.54 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | Y | 601 | ATF | PA-O3A-PB | -6.73 | 113.82 | 132.73 |
| 3 | O | 601 | ATF | PA-O3A-PB | -4.36 | 120.49 | 132.73 |
| 3 | Y | 601 | ATF | C5'-C4'-C3' | -2.48 | 105.36 | 115.21 |
| 3 | Y | 601 | ATF | N6-C6-N1 | -2.18 | 114.52 | 119.20 |
| 3 | Y | 601 | ATF | PB-C3B-PG | 2.08 | 118.28 | 113.38 |
| 3 | Y | 601 | ATF | O3G-PG-O2G | 2.22 | 114.51 | 108.24 |
| 3 | O | 601 | ATF | O3A-PA-O5' | 2.23 | 108.85 | 102.94 |
| 3 | O | 601 | ATF | O3'-C3'-C2' | 2.27 | 119.20 | 111.83 |
| 3 | O | 601 | ATF | C2'-C1'-N9 | 2.56 | 118.21 | 114.29 |
| 3 | O | 601 | ATF | C4-C5-N7 | 2.65 | 111.92 | 109.48 |
| 3 | Y | 601 | ATF | O5'-C5'-C4' | 2.93 | 119.91 | 109.12 |
| 3 | Y | 601 | ATF | O4'-C1'-N9 | 3.22 | 114.84 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | Y | 601 | ATF | O3A-PA-O5' | 3.44 | 112.05 | 102.94 |
| 3 | O | 601 | ATF | C1'-N9-C4 | 3.80 | 132.67 | 126.94 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | O | 600 | GOL | 2 | 0 |
| 3 | O | 601 | ATF | 2 | 0 |
| 4 | Y | 600 | GOL | 1 | 0 |
| 3 | Y | 601 | ATF | 3 | 0 |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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%) | -0.75 | 0 | 100 | 100 | 9, 52, 92, 100 | 0 |
| 1 | Y | 494/501 (98%) | -0.92 | 0 | 100 | 100 | 7, 41, 80, 100 | 0 |
| All | All | 988/1002 (98%) | -0.84 | 0 | 100 | 100 | 7, 47, 88, 100 | 0 |

There are no RSRZ outliers to report.

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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, $95^{th}$ 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 |
|---|---|---|---|---|---|---|---|---|---|
| 3 | ATF | Y | 601 | 33/33 | 0.94 | 0.15 | 1.99 | 42,42,42,42 | 0 |
| 3 | ATF | O | 601 | 33/33 | 0.96 | 0.12 | 0.30 | 56,56,56,56 | 0 |
| 4 | GOL | Y | 600 | 6/6 | 0.98 | 0.10 | -1.08 | 14,14,14,14 | 0 |
| 4 | GOL | O | 600 | 6/6 | 0.97 | 0.10 | -2.00 | 31,31,31,31 | 0 |
| 2 | MG | O | 602 | 1/1 | 0.92 | 0.38 | - | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 2 | MG | Y | 602 | 1/1 | 0.95 | 0.42 | - | 43,43,43,43 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.