# Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:14 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 3TAL |
| Title | : | Crystal structure of NurA with manganese |
| Authors | : | Chae, J.; Kim, Y.C.; Cho, Y. |
| Deposited on | : | 2011-08-04 |
| Resolution | : | 3.15 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

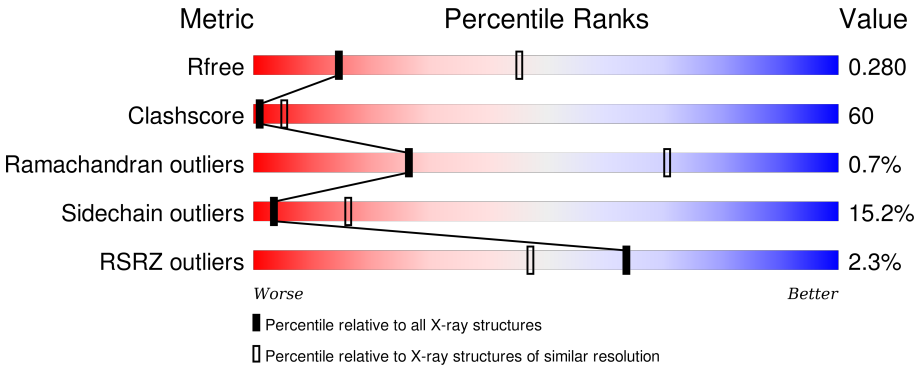
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| 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 3.15 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 1112 (3.20-3.12) |
| Clashscore | 102246 | 1249 (3.20-3.12) |
| Ramachandran outliers | 100387 | 1222 (3.20-3.12) |
| Sidechain outliers | 100360 | 1221 (3.20-3.12) |
| RSRZ outliers | 91569 | 1117 (3.20-3.12) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 | A | 471 | 2% 34% 48% 8% 10% |
| 1 | B | 471 | 2% 25% 53% 11% 11% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 3 | GOL | A | 454 | - | - | - | X |

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6861 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 DNA double-strand break repair protein nurA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 424 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 3420 | 2188 | 587 | 638 | 7 | | | |
| 1 | B | 421 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 3411 | 2186 | 584 | 634 | 7 | | | |

There are 40 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -19 | MSE | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -18 | GLY | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -17 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -16 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -15 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -14 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -13 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -12 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -11 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -10 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -9 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -8 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -7 | GLY | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -6 | LEU | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -5 | VAL | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -4 | PRO | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -3 | ARG | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -2 | GLY | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | -1 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| A | 0 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -19 | MSE | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -18 | GLY | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -17 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -16 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -15 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |

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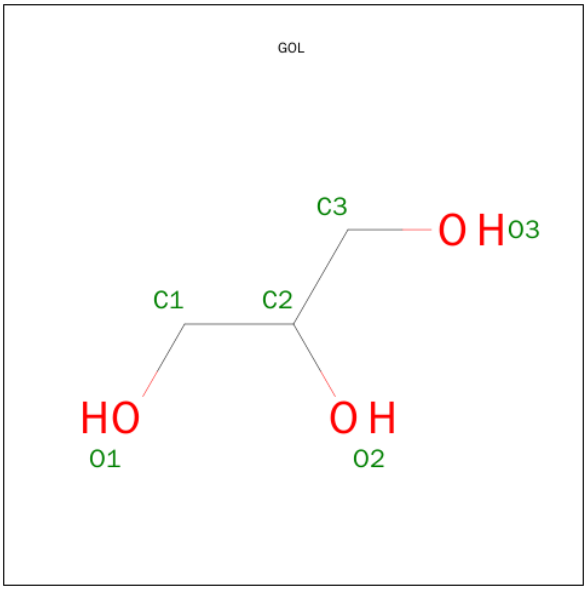
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -14 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -13 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -12 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -11 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -10 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -9 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -8 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -7 | GLY | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -6 | LEU | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -5 | VAL | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -4 | PRO | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -3 | ARG | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -2 | GLY | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | -1 | SER | - | EXPRESSION TAG | UNP Q8U1N8 |
| B | 0 | HIS | - | EXPRESSION TAG | UNP Q8U1N8 |

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | B | 2 | Total Mn<br>2 2 | 0 | 0 |
| 2 | A | 2 | Total Mn<br>2 2 | 0 | 0 |

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total C O<br>6 3 3 | 0 | 0 |

- Molecule 4 is water.

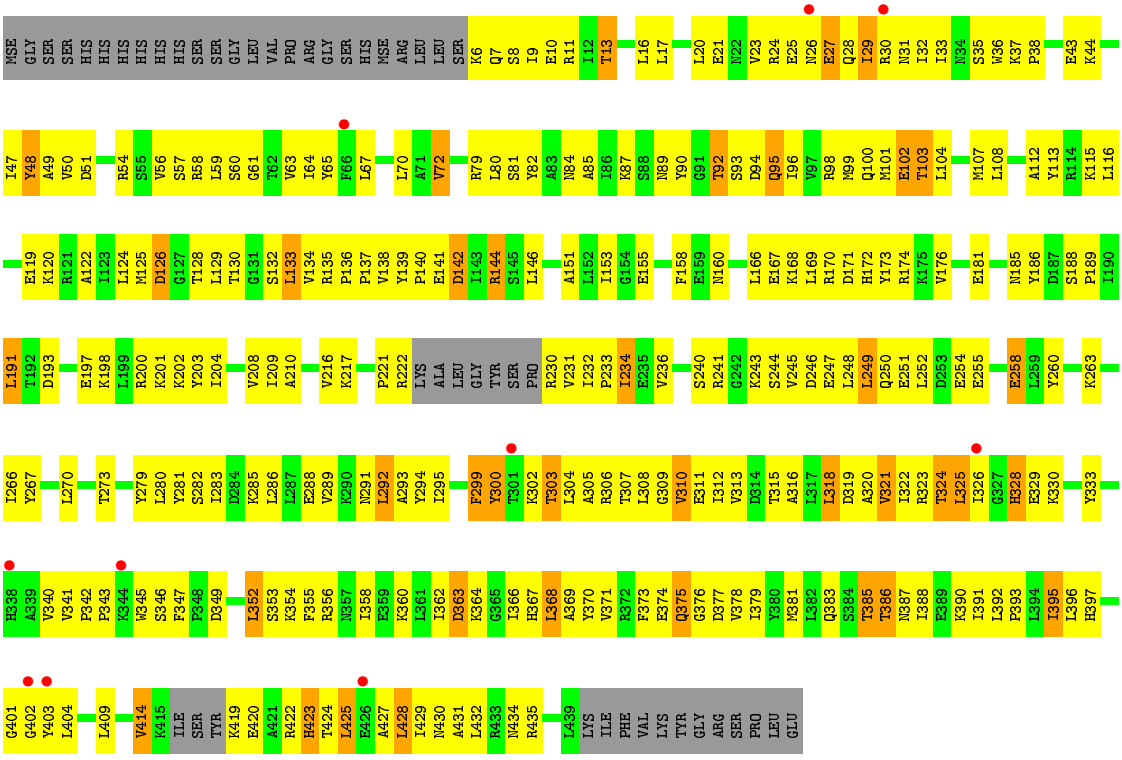
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | A | 13 | Total O<br>13 13 | 0 | 0 |
| 4 | B | 7 | Total O<br>7 7 | 0 | 0 |

# 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.

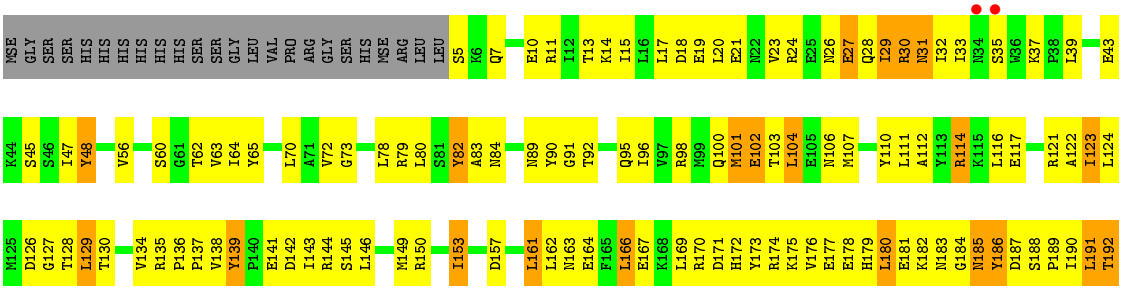
- Molecule 1: DNA double-strand break repair protein nurA

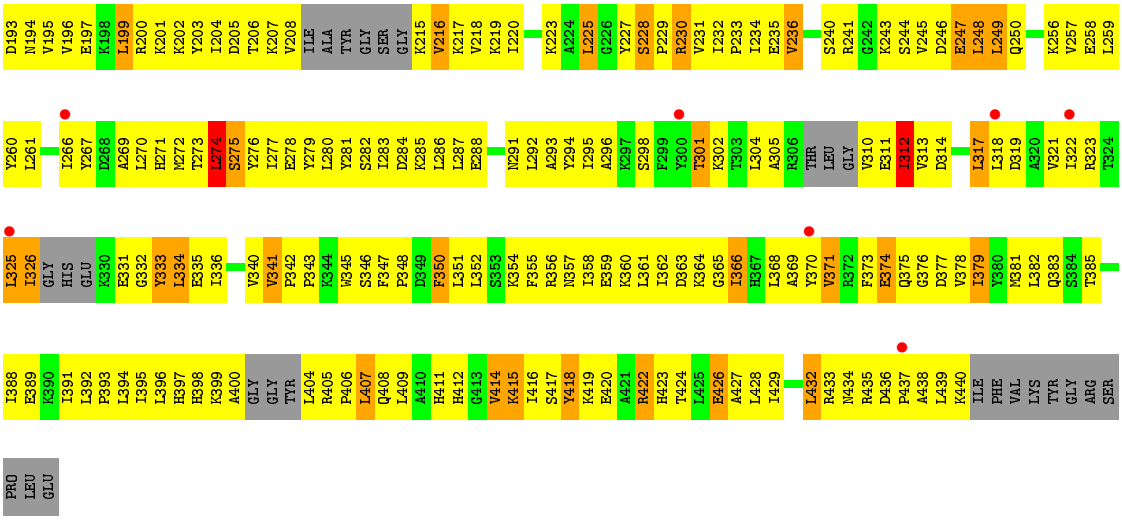
Chain A:

- Molecule 1: DNA double-strand break repair protein nurA

Chain B:


D193 N194 V195 V196 E197 K198 L199 R200 K201 K202 Y203 I204 D205 T206 K207 V208 ILE ALA TYR GLY SER GLY K215 Y216 K217 V218 K219 I220 K223 A224 L225 G226 Y227 S228 P229 R230 V231 I232 P233 I234 E235 V236 S240 R241 G242 K243 S244 V245 D246 E247 L248 L249 Q250 K256 V257 E258 L259
Y260 L261 I266 Y267 D268 A269 L270 H271 M272 T273 I274 S275 Y276 I277 E278 Y279 L280 Y281 S282 I283 D284 K285 L286 L287 E288 N291 L292 A293 Y294 I295 A296 K297 S298 F299 Y300 T301 K302 T303 L304 A305 R306 THR LEU GLY V310 E311 I312 V313 D314 L317 L318 D319 A320 V321 I322 R323 T324
L325 I326 GLY HIS GLU K330 E331 G332 Y333 L334 E335 I336 V340 V341 P342 P343 K344 W345 S346 F347 P348 D349 F350 L351 L352 S353 K354 F355 R356 N357 I358 E359 K360 L361 I362 D363 K364 G365 I366 H367 L368 A369 Y370 V371 R372 F373 E374 Q375 G376 D377 V378 I379 Y380 M381 L382 Q383 S384 T385
I388 E389 K390 I391 L392 P393 L394 I395 L396 H397 H398 K399 A400 GLY GLY TYR L404 R405 P406 I407 Q408 L409 A410 H411 H412 G413 V414 K415 I416 S417 Y418 K419 E420 A421 R422 H423 T424 L425 E426 A427 L428 I429 L432 R433 N434 R435 D436 P437 A438 L439 K440 ILE PHE VAL LYS TYR GLY ARG SER
PRO LEU GLU

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 64.80Å 114.65Å 121.62Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.48 – 3.15<br>34.37 – 3.10 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 96.8 (29.48-3.15)<br>94.4 (34.37-3.10) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.39 (at 3.12Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7_650) | Depositor |
| R, $R_{free}$ | 0.218 , 0.285<br>0.214 , 0.280 | Depositor<br>DCC |
| $R_{free}$ test set | 1583 reflections (10.07%) | DCC |
| Wilson B-factor (Å$^2$) | 97.2 | Xtriage |
| Anisotropy | 0.133 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 89.1 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Outliers | 1 of 16840 reflections (0.006%) | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 6861 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 125.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: GOL, MN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.34 | 0/3470 | 0.60 | 0/4670 |
| 1 | B | 0.32 | 0/3459 | 0.62 | 1/4652 (0.0%) |
| All | All | 0.33 | 0/6929 | 0.61 | 1/9322 (0.0%) |

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 274 | LEU | CA-CB-CG | 5.97 | 129.03 | 115.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 228 | SER | Peptide |
| 1 | B | 417 | SER | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3420 | 0 | 3526 | 400 | 0 |
| 1 | B | 3411 | 0 | 3532 | 474 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 6 | 0 | 8 | 3 | 0 |
| 4 | A | 13 | 0 | 0 | 3 | 0 |
| 4 | B | 7 | 0 | 0 | 1 | 0 |
| All | All | 6861 | 0 | 7066 | 829 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All (829) 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:B:172:HIS:ND1 | 1:B:191:LEU:HD11 | 1.57 | 1.20 |
| 1:A:54:ARG:HB3 | 1:A:101:MSE:HE3 | 1.29 | 1.14 |
| 1:B:98:ARG:HH22 | 1:B:137:PRO:HB3 | 0.99 | 1.10 |
| 1:A:244:SER:HA | 1:B:244:SER:HA | 1.24 | 1.09 |
| 1:A:240:SER:HB3 | 1:A:243:LYS:HD2 | 1.31 | 1.08 |
| 1:A:310:VAL:HG12 | 1:A:311:GLU:H | 1.18 | 1.04 |
| 1:A:87:LYS:HZ3 | 1:B:19:GLU:HG3 | 1.21 | 1.02 |
| 1:A:231:VAL:HB | 1:B:231:VAL:HG11 | 1.41 | 1.02 |
| 1:B:405:ARG:HG3 | 1:B:406:PRO:HD3 | 1.43 | 0.99 |
| 1:A:135:ARG:HH22 | 1:A:140:PRO:HD3 | 1.26 | 0.99 |
| 1:A:21:GLU:HB3 | 1:A:24:ARG:HD3 | 1.43 | 0.99 |
| 1:A:87:LYS:NZ | 1:B:19:GLU:HG3 | 1.78 | 0.99 |
| 1:A:169:LEU:HD23 | 1:A:191:LEU:HD12 | 1.43 | 0.99 |
| 1:A:95:GLN:HE22 | 1:A:138:VAL:HA | 1.24 | 0.98 |
| 1:A:419:LYS:HG3 | 1:A:420:GLU:H | 1.29 | 0.98 |
| 1:A:300:TYR:HE1 | 1:A:304:LEU:H | 1.06 | 0.97 |
| 1:B:98:ARG:NH2 | 1:B:137:PRO:HB3 | 1.79 | 0.95 |
| 1:A:217:LYS:HG3 | 1:A:258:GLU:OE2 | 1.67 | 0.95 |
| 1:B:217:LYS:HG2 | 1:B:260:TYR:HE1 | 1.29 | 0.95 |
| 1:B:217:LYS:HG2 | 1:B:260:TYR:CE1 | 2.02 | 0.95 |
| 1:A:374:GLU:HB3 | 1:A:377:ASP:HB2 | 1.48 | 0.94 |
| 1:A:44:LYS:HA | 1:A:397:HIS:ND1 | 1.85 | 0.92 |
| 1:A:320:ALA:HA | 1:B:436:ASP:OD2 | 1.69 | 0.91 |
| 1:B:28:GLN:C | 1:B:30:ARG:H | 1.64 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:5:SER:HB2 | 1:B:7:GLN:HE22 | 1.35 | 0.91 |
| 1:B:111:LEU:HD23 | 1:B:180:LEU:HD12 | 1.53 | 0.91 |
| 1:B:361:LEU:HD11 | 1:B:366:ILE:HG22 | 1.53 | 0.90 |
| 1:B:192:THR:HG21 | 1:B:275:SER:HA | 1.51 | 0.90 |
| 1:A:321:VAL:HG13 | 1:A:325:LEU:HD21 | 1.51 | 0.90 |
| 1:B:98:ARG:HH22 | 1:B:137:PRO:CB | 1.85 | 0.89 |
| 1:B:284:ASP:OD1 | 1:B:357:ASN:HB2 | 1.72 | 0.89 |
| 1:B:172:HIS:CG | 1:B:191:LEU:HD11 | 2.08 | 0.89 |
| 1:A:310:VAL:HG12 | 1:A:311:GLU:N | 1.85 | 0.89 |
| 1:B:96:ILE:HD11 | 1:B:272:MSE:HE1 | 1.53 | 0.88 |
| 1:B:232:ILE:HG12 | 1:B:236:VAL:HG11 | 1.55 | 0.88 |
| 1:A:374:GLU:HB2 | 1:A:402:GLY:HA2 | 1.53 | 0.87 |
| 1:A:99:MSE:O | 1:A:103:THR:HG22 | 1.74 | 0.87 |
| 1:B:110:TYR:HD2 | 1:B:111:LEU:HD12 | 1.39 | 0.87 |
| 1:B:172:HIS:CE1 | 1:B:191:LEU:HD11 | 2.12 | 0.85 |
| 1:A:340:VAL:HG12 | 1:A:341:VAL:H | 1.41 | 0.85 |
| 1:B:114:ARG:HH12 | 1:B:170:ARG:NH1 | 1.75 | 0.85 |
| 1:A:304:LEU:HA | 1:A:307:THR:HB | 1.59 | 0.84 |
| 1:A:300:TYR:OH | 1:A:304:LEU:HB2 | 1.78 | 0.84 |
| 1:B:370:TYR:HB3 | 1:B:379:ILE:HD11 | 1.60 | 0.84 |
| 1:B:129:LEU:HG | 1:B:294:TYR:CE2 | 2.12 | 0.83 |
| 1:A:340:VAL:CG1 | 1:A:341:VAL:H | 1.90 | 0.83 |
| 1:B:357:ASN:HA | 1:B:360:LYS:HE3 | 1.58 | 0.83 |
| 1:A:425:LEU:HD23 | 1:A:428:LEU:HD21 | 1.60 | 0.83 |
| 1:B:43:GLU:O | 1:B:397:HIS:HB2 | 1.79 | 0.83 |
| 1:B:174:ARG:HG3 | 1:B:175:LYS:N | 1.94 | 0.82 |
| 1:B:192:THR:HG22 | 1:B:274:LEU:HD13 | 1.60 | 0.82 |
| 1:A:300:TYR:CZ | 1:A:303:THR:HB | 2.14 | 0.82 |
| 1:A:299:PHE:CE1 | 1:A:304:LEU:HD22 | 2.15 | 0.82 |
| 1:A:208:VAL:HB | 1:A:216:VAL:CG1 | 2.10 | 0.82 |
| 1:B:322:ILE:HA | 1:B:325:LEU:HD23 | 1.60 | 0.81 |
| 1:A:21:GLU:HB3 | 1:A:24:ARG:NH1 | 1.96 | 0.81 |
| 1:B:426:GLU:CD | 1:B:427:ALA:H | 1.83 | 0.81 |
| 1:A:340:VAL:HG12 | 1:A:341:VAL:N | 1.96 | 0.81 |
| 1:A:107:MSE:HE1 | 1:A:189:PRO:HB2 | 1.62 | 0.81 |
| 1:B:5:SER:HB2 | 1:B:7:GLN:NE2 | 1.95 | 0.81 |
| 1:A:21:GLU:HB3 | 1:A:24:ARG:HH11 | 1.45 | 0.80 |
| 1:B:219:LYS:HB3 | 1:B:256:LYS:HD3 | 1.64 | 0.80 |
| 1:A:374:GLU:HB2 | 1:A:402:GLY:CA | 2.11 | 0.80 |
| 1:B:32:ILE:HD13 | 1:B:325:LEU:HD22 | 1.62 | 0.80 |
| 1:A:300:TYR:CE1 | 1:A:304:LEU:N | 2.49 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:32:ILE:HD12 | 1:B:33:ILE:N | 1.95 | 0.79 |
| 1:B:331:GLU:HB3 | 1:B:373:PHE:O | 1.82 | 0.79 |
| 1:A:208:VAL:HB | 1:A:216:VAL:HG11 | 1.63 | 0.79 |
| 1:A:176:VAL:HG22 | 1:A:186:TYR:HE2 | 1.48 | 0.79 |
| 1:A:321:VAL:HG13 | 1:A:325:LEU:CD2 | 2.13 | 0.78 |
| 1:B:107:MSE:O | 1:B:111:LEU:HD13 | 1.82 | 0.78 |
| 1:B:137:PRO:HG2 | 1:B:279:TYR:CZ | 2.17 | 0.78 |
| 1:B:399:LYS:HD2 | 1:B:400:ALA:N | 1.99 | 0.78 |
| 1:B:29:ILE:O | 1:B:30:ARG:HG2 | 1.82 | 0.78 |
| 1:B:205:ASP:HA | 1:B:208:VAL:HG23 | 1.66 | 0.77 |
| 1:B:146:LEU:HD12 | 1:B:273:THR:HG22 | 1.65 | 0.77 |
| 1:A:430:ASN:OD1 | 1:A:431:ALA:N | 2.15 | 0.77 |
| 1:B:230:ARG:HG3 | 1:B:231:VAL:H | 1.49 | 0.77 |
| 1:A:21:GLU:CB | 1:A:24:ARG:HD3 | 2.14 | 0.77 |
| 1:B:191:LEU:N | 1:B:191:LEU:HD12 | 2.00 | 0.77 |
| 1:B:342:PRO:HD2 | 1:B:362:ILE:HA | 1.67 | 0.76 |
| 1:A:428:LEU:N | 1:A:435:ARG:HH22 | 1.83 | 0.76 |
| 1:B:32:ILE:HD13 | 1:B:325:LEU:CD2 | 2.16 | 0.76 |
| 1:A:144:ARG:HH12 | 1:B:229:PRO:HG2 | 1.48 | 0.76 |
| 1:B:420:GLU:HA | 1:B:423:HIS:CD2 | 2.21 | 0.76 |
| 1:B:47:ILE:HD12 | 1:B:122:ALA:HB3 | 1.66 | 0.76 |
| 1:A:133:LEU:HD11 | 1:A:347:PHE:CZ | 2.20 | 0.76 |
| 1:B:228:SER:O | 1:B:230:ARG:HG2 | 1.85 | 0.76 |
| 1:B:179:HIS:HA | 1:B:182:LYS:HG2 | 1.66 | 0.75 |
| 1:A:378:VAL:HG13 | 1:B:440:LYS:HE3 | 1.66 | 0.75 |
| 1:A:304:LEU:CD2 | 1:A:312:ILE:HD12 | 2.16 | 0.75 |
| 1:A:24:ARG:HG2 | 1:A:25:GLU:N | 2.02 | 0.75 |
| 1:A:307:THR:HG23 | 1:A:309:GLY:H | 1.51 | 0.75 |
| 1:A:245:VAL:HG22 | 1:B:243:LYS:O | 1.87 | 0.75 |
| 1:B:370:TYR:HD1 | 1:B:379:ILE:HD11 | 1.52 | 0.75 |
| 1:B:362:ILE:HG13 | 1:B:363:ASP:N | 2.00 | 0.74 |
| 1:B:123:ILE:HG22 | 1:B:292:LEU:HD13 | 1.68 | 0.74 |
| 1:A:428:LEU:H | 1:A:428:LEU:HD12 | 1.51 | 0.74 |
| 1:B:301:THR:HG21 | 1:B:314:ASP:HB2 | 1.69 | 0.74 |
| 1:B:426:GLU:N | 1:B:426:GLU:OE1 | 2.20 | 0.74 |
| 1:B:373:PHE:CE2 | 1:B:399:LYS:HE3 | 2.23 | 0.74 |
| 1:A:20:LEU:O | 1:A:23:VAL:HB | 1.88 | 0.73 |
| 1:A:37:LYS:HG2 | 1:A:38:PRO:HD2 | 1.69 | 0.73 |
| 1:B:114:ARG:HH12 | 1:B:170:ARG:HH12 | 1.36 | 0.73 |
| 1:A:44:LYS:HG3 | 1:A:397:HIS:HE1 | 1.53 | 0.73 |
| 1:B:433:ARG:HG3 | 1:B:434:ASN:H | 1.52 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:325:LEU:HG | 1:B:326:ILE:H | 1.54 | 0.73 |
| 1:B:89:ASN:OD1 | 1:B:92:THR:HB | 1.88 | 0.73 |
| 1:B:244:SER:N | 1:B:247:GLU:OE2 | 2.22 | 0.73 |
| 1:A:302:LYS:CE | 1:A:306:ARG:NH2 | 2.52 | 0.73 |
| 1:B:207:LYS:HD2 | 1:B:207:LYS:N | 2.03 | 0.73 |
| 1:A:135:ARG:NH2 | 1:A:140:PRO:HD3 | 2.03 | 0.73 |
| 1:B:21:GLU:HA | 1:B:24:ARG:HG3 | 1.71 | 0.73 |
| 1:B:348:PRO:HG2 | 1:B:351:LEU:HD13 | 1.70 | 0.72 |
| 1:B:433:ARG:HG3 | 1:B:434:ASN:N | 2.04 | 0.72 |
| 1:A:176:VAL:HG22 | 1:A:186:TYR:CE2 | 2.25 | 0.72 |
| 1:B:325:LEU:HG | 1:B:326:ILE:N | 2.04 | 0.72 |
| 1:A:395:ILE:HD12 | 1:A:404:LEU:HD13 | 1.72 | 0.72 |
| 1:B:48:TYR:CD1 | 1:B:112:ALA:HB1 | 2.25 | 0.72 |
| 1:A:248:LEU:HD12 | 1:A:248:LEU:O | 1.90 | 0.72 |
| 1:A:129:LEU:HD23 | 1:A:366:ILE:HG12 | 1.71 | 0.71 |
| 1:B:240:SER:HB3 | 1:B:243:LYS:HD2 | 1.72 | 0.71 |
| 1:B:243:LYS:HB3 | 1:B:247:GLU:OE2 | 1.90 | 0.71 |
| 1:B:373:PHE:CZ | 1:B:399:LYS:HE3 | 2.26 | 0.71 |
| 1:A:29:ILE:O | 1:A:32:ILE:HG22 | 1.89 | 0.71 |
| 1:A:95:GLN:OE1 | 1:A:137:PRO:O | 2.08 | 0.71 |
| 1:A:113:TYR:CG | 1:A:289:VAL:HG22 | 2.25 | 0.71 |
| 1:B:191:LEU:N | 1:B:191:LEU:CD1 | 2.53 | 0.71 |
| 1:A:126:ASP:O | 1:A:126:ASP:OD1 | 2.08 | 0.70 |
| 1:B:172:HIS:HB2 | 1:B:191:LEU:HD21 | 1.72 | 0.70 |
| 1:B:172:HIS:O | 1:B:176:VAL:HG13 | 1.91 | 0.70 |
| 1:A:28:GLN:OE1 | 1:A:28:GLN:HA | 1.91 | 0.70 |
| 1:A:231:VAL:HB | 1:B:231:VAL:CG1 | 2.19 | 0.70 |
| 1:B:216:VAL:O | 1:B:260:TYR:HA | 1.91 | 0.70 |
| 1:B:370:TYR:HB3 | 1:B:379:ILE:CD1 | 2.20 | 0.70 |
| 1:B:124:LEU:HD13 | 1:B:395:ILE:HD11 | 1.74 | 0.70 |
| 1:A:134:VAL:O | 1:A:345:TRP:HH2 | 1.74 | 0.70 |
| 1:A:300:TYR:CZ | 1:A:304:LEU:HB2 | 2.27 | 0.70 |
| 1:B:101:MSE:HA | 1:B:101:MSE:HE3 | 1.74 | 0.70 |
| 1:B:370:TYR:CD1 | 1:B:379:ILE:HD11 | 2.27 | 0.70 |
| 1:A:21:GLU:HB3 | 1:A:24:ARG:CD | 2.21 | 0.69 |
| 1:A:136:PRO:HB2 | 1:A:138:VAL:HG13 | 1.73 | 0.69 |
| 1:A:230:ARG:HG3 | 1:B:234:ILE:CG1 | 2.22 | 0.69 |
| 1:B:204:ILE:HD11 | 1:B:270:LEU:HD12 | 1.75 | 0.69 |
| 1:A:428:LEU:CD1 | 1:A:429:ILE:H | 2.06 | 0.69 |
| 1:A:64:ILE:HD11 | 1:A:425:LEU:HD22 | 1.74 | 0.69 |
| 1:A:300:TYR:HE1 | 1:A:304:LEU:N | 1.85 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:285:LYS:O | 1:A:288:GLU:HB2 | 1.91 | 0.69 |
| 1:A:21:GLU:CB | 1:A:24:ARG:HH11 | 2.06 | 0.69 |
| 1:A:302:LYS:HE3 | 1:A:306:ARG:NH2 | 2.08 | 0.69 |
| 1:A:217:LYS:CG | 1:A:258:GLU:OE2 | 2.40 | 0.69 |
| 1:A:378:VAL:HG13 | 1:B:440:LYS:CE | 2.22 | 0.69 |
| 1:B:416:ILE:O | 1:B:416:ILE:HG22 | 1.92 | 0.69 |
| 1:A:230:ARG:HG3 | 1:B:234:ILE:HG12 | 1.75 | 0.69 |
| 1:A:134:VAL:O | 1:A:345:TRP:CH2 | 2.46 | 0.68 |
| 1:B:163:ASN:O | 1:B:167:GLU:HG3 | 1.94 | 0.68 |
| 1:A:315:THR:HG22 | 1:A:370:TYR:CD1 | 2.29 | 0.68 |
| 1:B:182:LYS:HG3 | 1:B:183:ASN:H | 1.59 | 0.68 |
| 1:B:30:ARG:O | 1:B:33:ILE:HG22 | 1.94 | 0.68 |
| 1:A:313:VAL:HG12 | 1:A:318:LEU:HB2 | 1.75 | 0.68 |
| 1:A:364:LYS:HE3 | 4:A:461:HOH:O | 1.94 | 0.68 |
| 1:B:368:LEU:HB3 | 1:B:381:MSE:HE1 | 1.74 | 0.68 |
| 1:B:21:GLU:HG3 | 1:B:24:ARG:HD2 | 1.74 | 0.68 |
| 1:B:104:LEU:HA | 1:B:107:MSE:HE2 | 1.75 | 0.68 |
| 1:B:28:GLN:C | 1:B:30:ARG:N | 2.39 | 0.68 |
| 1:A:363:ASP:OD1 | 1:A:363:ASP:C | 2.32 | 0.67 |
| 1:A:302:LYS:HE3 | 1:A:306:ARG:CZ | 2.24 | 0.67 |
| 1:B:325:LEU:HG | 1:B:326:ILE:HG22 | 1.76 | 0.67 |
| 1:B:269:ALA:O | 1:B:273:THR:HG23 | 1.94 | 0.67 |
| 1:A:299:PHE:CZ | 1:A:304:LEU:HD22 | 2.29 | 0.67 |
| 1:A:304:LEU:HD23 | 1:A:312:ILE:HD12 | 1.77 | 0.67 |
| 1:B:106:ASN:HB2 | 1:B:282:SER:HB2 | 1.76 | 0.67 |
| 1:B:334:LEU:HD12 | 1:B:335:GLU:O | 1.95 | 0.67 |
| 1:B:439:LEU:HD12 | 1:B:440:LYS:N | 2.09 | 0.67 |
| 1:B:127:GLY:O | 1:B:296:ALA:HB2 | 1.95 | 0.66 |
| 1:A:419:LYS:HG3 | 1:A:420:GLU:N | 2.07 | 0.66 |
| 1:A:302:LYS:HG2 | 1:A:306:ARG:CZ | 2.25 | 0.66 |
| 1:B:294:TYR:HB2 | 1:B:383:GLN:HB2 | 1.77 | 0.66 |
| 1:A:24:ARG:HG2 | 1:A:25:GLU:H | 1.60 | 0.66 |
| 1:A:355:PHE:HB3 | 1:A:358:ILE:HD12 | 1.78 | 0.66 |
| 1:A:302:LYS:HE2 | 1:A:306:ARG:NH2 | 2.11 | 0.66 |
| 1:A:307:THR:O | 1:A:308:LEU:HB2 | 1.95 | 0.66 |
| 1:A:32:ILE:O | 1:A:35:SER:HB3 | 1.96 | 0.66 |
| 1:A:304:LEU:O | 1:A:307:THR:HG22 | 1.96 | 0.65 |
| 1:A:29:ILE:HA | 1:A:32:ILE:HG22 | 1.77 | 0.65 |
| 1:B:336:ILE:HD11 | 1:B:370:TYR:HE2 | 1.61 | 0.65 |
| 1:A:64:ILE:CD1 | 1:A:425:LEU:HD22 | 2.27 | 0.65 |
| 1:B:311:GLU:O | 1:B:312:ILE:HG23 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:48:TYR:CD1 | 1:A:116:LEU:HD13 | 2.31 | 0.65 |
| 1:B:161:LEU:HA | 1:B:203:TYR:CZ | 2.32 | 0.65 |
| 1:B:283:ILE:HG22 | 1:B:287:LEU:HD11 | 1.78 | 0.65 |
| 1:B:248:LEU:HD12 | 1:B:248:LEU:O | 1.97 | 0.65 |
| 1:A:300:TYR:CE1 | 1:A:304:LEU:HB2 | 2.32 | 0.65 |
| 1:A:26:ASN:HB2 | 1:A:30:ARG:CG | 2.26 | 0.65 |
| 1:A:310:VAL:CG1 | 1:A:311:GLU:N | 2.58 | 0.65 |
| 1:A:209:ILE:O | 1:A:216:VAL:HG13 | 1.97 | 0.64 |
| 1:B:172:HIS:ND1 | 1:B:191:LEU:CD1 | 2.48 | 0.64 |
| 1:B:231:VAL:HG12 | 1:B:232:ILE:N | 2.13 | 0.64 |
| 1:B:56:VAL:HG22 | 1:B:65:TYR:HB3 | 1.78 | 0.64 |
| 1:A:29:ILE:HD11 | 1:A:33:ILE:HG12 | 1.80 | 0.64 |
| 1:B:172:HIS:CE1 | 1:B:191:LEU:CD1 | 2.81 | 0.64 |
| 1:B:174:ARG:HG3 | 1:B:175:LYS:H | 1.63 | 0.64 |
| 1:A:87:LYS:NZ | 1:B:19:GLU:CG | 2.58 | 0.64 |
| 1:A:24:ARG:CG | 1:A:25:GLU:N | 2.61 | 0.64 |
| 1:B:420:GLU:HA | 1:B:423:HIS:NE2 | 2.13 | 0.63 |
| 1:B:411:HIS:O | 1:B:414:VAL:HG12 | 1.99 | 0.63 |
| 1:B:336:ILE:HD11 | 1:B:370:TYR:CE2 | 2.34 | 0.63 |
| 1:A:21:GLU:CD | 1:A:24:ARG:HD3 | 2.19 | 0.63 |
| 1:A:100:GLN:HA | 1:A:103:THR:HG23 | 1.81 | 0.63 |
| 1:B:375:GLN:HG3 | 1:B:376:GLY:N | 2.13 | 0.63 |
| 1:B:142:ASP:OD1 | 1:B:143:ILE:N | 2.31 | 0.63 |
| 1:A:176:VAL:HG13 | 1:A:186:TYR:HD2 | 1.62 | 0.63 |
| 1:B:347:PHE:CB | 1:B:352:LEU:HD11 | 2.28 | 0.63 |
| 1:B:123:ILE:HG22 | 1:B:292:LEU:CD1 | 2.29 | 0.62 |
| 1:B:215:LYS:HA | 1:B:261:LEU:O | 1.99 | 0.62 |
| 1:A:65:TYR:CZ | 1:A:84:ASN:HB3 | 2.34 | 0.62 |
| 1:B:182:LYS:HG3 | 1:B:183:ASN:N | 2.14 | 0.62 |
| 1:A:151:ALA:HB1 | 1:A:233:PRO:HD3 | 1.80 | 0.62 |
| 1:B:138:VAL:O | 1:B:139:TYR:HB2 | 1.99 | 0.62 |
| 1:A:28:GLN:O | 1:A:31:ASN:OD1 | 2.18 | 0.62 |
| 1:A:115:LYS:HZ3 | 1:A:181:GLU:HA | 1.64 | 0.62 |
| 1:A:95:GLN:HE22 | 1:A:138:VAL:CA | 2.08 | 0.62 |
| 1:A:304:LEU:HD21 | 1:A:312:ILE:HD12 | 1.82 | 0.62 |
| 1:B:357:ASN:CA | 1:B:360:LYS:HE3 | 2.30 | 0.62 |
| 1:B:89:ASN:CG | 1:B:92:THR:HB | 2.20 | 0.62 |
| 1:A:16:LEU:HD21 | 1:B:62:THR:HG21 | 1.82 | 0.62 |
| 1:B:92:THR:HG22 | 1:B:96:ILE:HD13 | 1.82 | 0.61 |
| 1:B:391:ILE:O | 1:B:394:LEU:HB2 | 2.00 | 0.61 |
| 1:B:179:HIS:HA | 1:B:182:LYS:CG | 2.28 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:177:GLU:HA | 1:B:180:LEU:HB2 | 1.82 | 0.61 |
| 1:A:428:LEU:HD13 | 1:A:429:ILE:H | 1.66 | 0.61 |
| 1:A:202:LYS:HE2 | 1:A:203:TYR:CE1 | 2.36 | 0.61 |
| 1:B:341:VAL:HG23 | 1:B:342:PRO:O | 2.00 | 0.61 |
| 1:B:398:HIS:O | 1:B:405:ARG:HG2 | 2.00 | 0.61 |
| 1:B:405:ARG:HG3 | 1:B:406:PRO:CD | 2.25 | 0.61 |
| 1:A:430:ASN:HB3 | 1:A:435:ARG:CZ | 2.29 | 0.61 |
| 1:A:43:GLU:HG2 | 1:A:120:LYS:NZ | 2.14 | 0.61 |
| 1:B:95:GLN:HB3 | 1:B:138:VAL:HG23 | 1.81 | 0.61 |
| 1:B:439:LEU:HD12 | 1:B:440:LYS:HG3 | 1.82 | 0.61 |
| 1:A:171:ASP:HA | 1:A:174:ARG:HD3 | 1.82 | 0.61 |
| 1:B:232:ILE:CG1 | 1:B:236:VAL:HG11 | 2.30 | 0.61 |
| 1:B:11:ARG:O | 1:B:15:ILE:HG13 | 2.01 | 0.61 |
| 1:B:378:VAL:HG12 | 1:B:379:ILE:H | 1.66 | 0.61 |
| 1:A:240:SER:HB3 | 1:A:243:LYS:CD | 2.21 | 0.60 |
| 1:A:245:VAL:HG21 | 1:B:241:ARG:HA | 1.82 | 0.60 |
| 1:A:200:ARG:HD3 | 1:A:267:TYR:CE1 | 2.36 | 0.60 |
| 1:B:355:PHE:O | 1:B:359:GLU:HB2 | 2.01 | 0.60 |
| 1:A:346:SER:O | 1:A:347:PHE:CD1 | 2.55 | 0.60 |
| 1:A:306:ARG:O | 1:A:308:LEU:HD12 | 2.01 | 0.60 |
| 1:B:26:ASN:O | 1:B:28:GLN:HG2 | 2.01 | 0.60 |
| 1:B:435:ARG:O | 1:B:438:ALA:HB3 | 2.01 | 0.60 |
| 1:B:375:GLN:HG3 | 1:B:376:GLY:H | 1.67 | 0.60 |
| 1:A:323:ARG:HG2 | 1:A:329:GLU:HB2 | 1.83 | 0.60 |
| 1:B:373:PHE:CD2 | 1:B:374:GLU:N | 2.70 | 0.60 |
| 1:A:419:LYS:CG | 1:A:420:GLU:H | 2.11 | 0.60 |
| 1:A:104:LEU:HD11 | 1:A:189:PRO:HG2 | 1.82 | 0.60 |
| 1:A:130:THR:HG23 | 1:A:383:GLN:OE1 | 2.01 | 0.60 |
| 1:B:439:LEU:CD1 | 1:B:440:LYS:HG3 | 2.32 | 0.60 |
| 1:B:173:TYR:O | 1:B:176:VAL:HG22 | 2.02 | 0.60 |
| 1:B:172:HIS:CD2 | 1:B:176:VAL:HG12 | 2.36 | 0.60 |
| 1:A:427:ALA:C | 1:A:435:ARG:HH22 | 2.04 | 0.60 |
| 1:A:92:THR:HA | 1:A:95:GLN:HB3 | 1.84 | 0.60 |
| 1:B:407:LEU:HD23 | 1:B:408:GLN:N | 2.17 | 0.59 |
| 1:A:17:LEU:HD21 | 1:B:432:LEU:CD2 | 2.32 | 0.59 |
| 1:B:31:ASN:O | 1:B:35:SER:N | 2.36 | 0.59 |
| 1:A:422:ARG:O | 1:A:425:LEU:N | 2.35 | 0.59 |
| 1:A:29:ILE:CD1 | 1:A:33:ILE:HG12 | 2.32 | 0.59 |
| 1:B:110:TYR:CD2 | 1:B:111:LEU:HD12 | 2.30 | 0.59 |
| 1:B:27:GLU:O | 1:B:29:ILE:HG13 | 2.02 | 0.59 |
| 1:A:302:LYS:HE3 | 1:A:306:ARG:NH1 | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:425:LEU:O | 1:A:428:LEU:HD11 | 2.02 | 0.59 |
| 1:A:142:ASP:OD1 | 1:A:142:ASP:C | 2.40 | 0.59 |
| 1:B:191:LEU:CD1 | 1:B:191:LEU:H | 2.16 | 0.59 |
| 1:B:149:MSE:HE3 | 1:B:270:LEU:N | 2.18 | 0.59 |
| 1:A:243:LYS:HB2 | 1:A:247:GLU:OE1 | 2.02 | 0.59 |
| 1:A:432:LEU:HD22 | 1:B:13:THR:HG21 | 1.84 | 0.59 |
| 1:A:234:ILE:HB | 1:B:229:PRO:O | 2.02 | 0.58 |
| 1:A:422:ARG:HG3 | 1:A:423:HIS:N | 2.18 | 0.58 |
| 1:B:271:HIS:HA | 1:B:274:LEU:HD11 | 1.85 | 0.58 |
| 1:A:130:THR:OG1 | 1:A:299:PHE:CZ | 2.57 | 0.58 |
| 1:A:113:TYR:CD2 | 1:A:289:VAL:HG22 | 2.37 | 0.58 |
| 1:B:392:LEU:C | 1:B:392:LEU:HD23 | 2.24 | 0.58 |
| 1:B:405:ARG:CG | 1:B:406:PRO:HD3 | 2.23 | 0.58 |
| 1:A:378:VAL:HG13 | 1:B:440:LYS:NZ | 2.18 | 0.58 |
| 1:B:19:GLU:O | 1:B:23:VAL:HG23 | 2.03 | 0.58 |
| 1:B:436:ASP:HB2 | 1:B:437:PRO:HD3 | 1.85 | 0.58 |
| 1:A:366:ILE:HG22 | 1:A:368:LEU:HD22 | 1.85 | 0.58 |
| 1:B:388:ILE:CG2 | 1:B:389:GLU:N | 2.65 | 0.58 |
| 1:B:138:VAL:CG1 | 1:B:142:ASP:HB3 | 2.34 | 0.58 |
| 1:B:235:GLU:HA | 1:B:235:GLU:OE1 | 2.04 | 0.58 |
| 1:A:428:LEU:H | 1:A:428:LEU:CD1 | 2.12 | 0.57 |
| 1:A:320:ALA:HB1 | 1:B:434:ASN:ND2 | 2.19 | 0.57 |
| 1:A:104:LEU:HD11 | 1:A:189:PRO:CG | 2.34 | 0.57 |
| 1:A:202:LYS:HE2 | 1:A:203:TYR:CZ | 2.40 | 0.57 |
| 1:A:176:VAL:HG13 | 1:A:186:TYR:CD2 | 2.39 | 0.57 |
| 1:B:172:HIS:CD2 | 1:B:176:VAL:CG1 | 2.87 | 0.57 |
| 1:B:192:THR:HG21 | 1:B:275:SER:CA | 2.31 | 0.57 |
| 1:A:21:GLU:CB | 1:A:24:ARG:NH1 | 2.64 | 0.57 |
| 1:A:172:HIS:O | 1:A:176:VAL:HG23 | 2.03 | 0.57 |
| 1:A:141:GLU:HA | 1:A:144:ARG:HE | 1.68 | 0.57 |
| 1:A:99:MSE:O | 1:A:103:THR:CG2 | 2.51 | 0.57 |
| 1:B:110:TYR:CD1 | 1:B:285:LYS:HB3 | 2.39 | 0.57 |
| 1:A:169:LEU:CD2 | 1:A:191:LEU:HD12 | 2.26 | 0.57 |
| 1:A:428:LEU:N | 1:A:428:LEU:HD12 | 2.19 | 0.57 |
| 1:B:82:TYR:CD2 | 1:B:190:ILE:HD12 | 2.40 | 0.57 |
| 1:B:225:LEU:CD1 | 1:B:227:TYR:HB2 | 2.35 | 0.57 |
| 1:A:79:ARG:HB3 | 1:A:185:ASN:HB2 | 1.86 | 0.57 |
| 1:A:140:PRO:O | 1:A:144:ARG:HD3 | 2.05 | 0.57 |
| 1:B:304:LEU:HB3 | 1:B:312:ILE:CD1 | 2.35 | 0.57 |
| 1:A:141:GLU:O | 1:A:144:ARG:HG2 | 2.05 | 0.57 |
| 1:A:232:ILE:O | 1:B:231:VAL:HG13 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:245:VAL:HG12 | 1:B:249:LEU:HD12 | 1.86 | 0.56 |
| 1:B:312:ILE:N | 1:B:312:ILE:HD12 | 2.20 | 0.56 |
| 1:A:124:LEU:HD21 | 1:A:295:ILE:HG12 | 1.87 | 0.56 |
| 1:A:181:GLU:OE1 | 1:A:181:GLU:HA | 2.05 | 0.56 |
| 1:B:180:LEU:O | 1:B:184:GLY:HA2 | 2.04 | 0.56 |
| 1:B:208:VAL:O | 1:B:208:VAL:HG12 | 2.05 | 0.56 |
| 1:A:232:ILE:HD13 | 1:B:234:ILE:HD13 | 1.88 | 0.56 |
| 1:A:374:GLU:HB3 | 1:A:377:ASP:CB | 2.31 | 0.56 |
| 1:B:423:HIS:O | 1:B:426:GLU:CD | 2.44 | 0.56 |
| 1:A:104:LEU:HD12 | 1:A:107:MSE:CE | 2.35 | 0.56 |
| 1:B:351:LEU:O | 1:B:354:LYS:HB2 | 2.06 | 0.56 |
| 1:B:202:LYS:HE2 | 1:B:203:TYR:CE2 | 2.41 | 0.56 |
| 1:B:80:LEU:CD1 | 1:B:107:MSE:HE3 | 2.34 | 0.56 |
| 1:B:258:GLU:OE1 | 1:B:260:TYR:OH | 2.22 | 0.56 |
| 1:A:373:PHE:HB2 | 1:A:402:GLY:O | 2.06 | 0.56 |
| 1:B:304:LEU:HB3 | 1:B:312:ILE:HD11 | 1.86 | 0.56 |
| 1:A:292:LEU:HD12 | 1:A:293:ALA:N | 2.21 | 0.56 |
| 1:B:436:ASP:O | 1:B:439:LEU:HG | 2.05 | 0.56 |
| 1:B:426:GLU:CG | 1:B:427:ALA:N | 2.68 | 0.56 |
| 1:B:139:TYR:C | 1:B:141:GLU:H | 2.09 | 0.56 |
| 1:A:138:VAL:HG23 | 1:A:139:TYR:N | 2.21 | 0.56 |
| 1:A:401:GLY:C | 1:A:403:TYR:H | 2.08 | 0.56 |
| 1:A:326:ILE:HG23 | 1:A:328:HIS:HB2 | 1.88 | 0.56 |
| 1:B:205:ASP:HA | 1:B:208:VAL:CG2 | 2.35 | 0.55 |
| 1:B:200:ARG:HB3 | 1:B:270:LEU:HD13 | 1.88 | 0.55 |
| 1:B:400:ALA:H | 1:B:404:LEU:HA | 1.69 | 0.55 |
| 1:A:427:ALA:C | 1:A:435:ARG:HH12 | 2.09 | 0.55 |
| 1:A:27:GLU:O | 1:A:27:GLU:HG2 | 2.06 | 0.55 |
| 1:A:291:ASN:HB3 | 1:A:391:ILE:HD12 | 1.88 | 0.55 |
| 1:B:207:LYS:O | 1:B:208:VAL:C | 2.44 | 0.55 |
| 1:B:139:TYR:O | 1:B:141:GLU:N | 2.40 | 0.55 |
| 1:B:319:ASP:HB2 | 1:B:379:ILE:CG2 | 2.37 | 0.55 |
| 1:A:26:ASN:ND2 | 1:A:30:ARG:HD2 | 2.22 | 0.55 |
| 1:A:316:ALA:HA | 1:B:440:LYS:CD | 2.36 | 0.55 |
| 1:B:426:GLU:CD | 1:B:427:ALA:N | 2.59 | 0.55 |
| 1:B:347:PHE:HB3 | 1:B:352:LEU:HD11 | 1.89 | 0.55 |
| 1:A:26:ASN:HB3 | 1:A:30:ARG:HG2 | 1.89 | 0.55 |
| 1:B:293:ALA:HB3 | 1:B:395:ILE:HD11 | 1.88 | 0.55 |
| 1:A:57:SER:O | 1:A:64:ILE:HG22 | 2.06 | 0.55 |
| 1:A:368:LEU:N | 1:A:368:LEU:HD23 | 2.22 | 0.55 |
| 1:B:429:ILE:HD12 | 1:B:438:ALA:HB2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:161:LEU:O | 1:B:164:GLU:HB3 | 2.06 | 0.54 |
| 1:B:381:MSE:HE3 | 1:B:383:GLN:HE21 | 1.72 | 0.54 |
| 1:B:347:PHE:HB2 | 1:B:352:LEU:HD11 | 1.88 | 0.54 |
| 1:A:126:ASP:O | 3:A:454:GOL:H31 | 2.07 | 0.54 |
| 1:B:191:LEU:O | 1:B:192:THR:C | 2.46 | 0.54 |
| 1:B:201:LYS:HA | 1:B:205:ASP:OD2 | 2.07 | 0.54 |
| 1:B:389:GLU:O | 1:B:393:PRO:HD2 | 2.07 | 0.54 |
| 1:A:135:ARG:HG2 | 1:B:90:TYR:CE2 | 2.42 | 0.54 |
| 1:A:430:ASN:CG | 1:A:431:ALA:N | 2.60 | 0.54 |
| 1:A:374:GLU:HG3 | 1:A:375:GLN:OE1 | 2.07 | 0.54 |
| 1:A:27:GLU:C | 1:A:29:ILE:H | 2.10 | 0.54 |
| 1:B:21:GLU:O | 1:B:24:ARG:HB2 | 2.06 | 0.54 |
| 1:B:343:PRO:HG2 | 1:B:346:SER:HB3 | 1.89 | 0.54 |
| 1:A:102:GLU:HG3 | 3:A:454:GOL:H2 | 1.88 | 0.54 |
| 1:B:206:THR:HB | 1:B:207:LYS:NZ | 2.23 | 0.54 |
| 1:B:137:PRO:HG2 | 1:B:279:TYR:CE2 | 2.41 | 0.54 |
| 1:A:133:LEU:HB3 | 1:A:342:PRO:HB3 | 1.89 | 0.54 |
| 1:B:172:HIS:NE2 | 1:B:176:VAL:HG12 | 2.22 | 0.54 |
| 1:A:325:LEU:HG | 1:A:326:ILE:H | 1.73 | 0.54 |
| 1:A:44:LYS:HG3 | 1:A:397:HIS:CE1 | 2.38 | 0.54 |
| 1:A:397:HIS:HD2 | 1:A:397:HIS:O | 1.90 | 0.54 |
| 1:A:133:LEU:CD1 | 1:A:347:PHE:CZ | 2.91 | 0.54 |
| 1:B:301:THR:O | 1:B:304:LEU:HB2 | 2.07 | 0.54 |
| 1:B:21:GLU:HA | 1:B:24:ARG:CG | 2.36 | 0.54 |
| 1:A:244:SER:N | 1:A:247:GLU:OE1 | 2.41 | 0.54 |
| 1:B:218:VAL:HG12 | 1:B:220:ILE:HG12 | 1.90 | 0.54 |
| 1:A:166:LEU:CD1 | 1:A:354:LYS:HD2 | 2.38 | 0.54 |
| 1:B:322:ILE:HG13 | 1:B:323:ARG:N | 2.22 | 0.54 |
| 1:A:302:LYS:CE | 1:A:306:ARG:HH22 | 2.21 | 0.54 |
| 1:A:197:GLU:O | 1:A:201:LYS:HG3 | 2.08 | 0.54 |
| 1:B:10:GLU:OE2 | 1:B:14:LYS:HE2 | 2.08 | 0.54 |
| 1:A:326:ILE:HG23 | 1:A:328:HIS:H | 1.72 | 0.53 |
| 1:A:200:ARG:HG3 | 1:A:201:LYS:N | 2.23 | 0.53 |
| 1:B:172:HIS:CB | 1:B:191:LEU:HD21 | 2.38 | 0.53 |
| 1:A:230:ARG:HG3 | 1:B:234:ILE:HG13 | 1.89 | 0.53 |
| 1:A:378:VAL:CG1 | 1:B:440:LYS:HE3 | 2.36 | 0.53 |
| 1:A:70:LEU:HD11 | 1:A:72:VAL:HG12 | 1.91 | 0.53 |
| 1:A:130:THR:OG1 | 1:A:299:PHE:HZ | 1.92 | 0.53 |
| 1:A:197:GLU:CG | 1:A:201:LYS:HE3 | 2.39 | 0.53 |
| 1:A:119:GLU:HG2 | 1:A:120:LYS:HG3 | 1.90 | 0.53 |
| 1:A:392:LEU:N | 1:A:393:PRO:HD2 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:95:GLN:HA | 1:B:98:ARG:HG2 | 1.91 | 0.53 |
| 1:B:350:PHE:CD1 | 1:B:351:LEU:HD12 | 2.44 | 0.53 |
| 1:A:313:VAL:CG1 | 1:A:313:VAL:O | 2.57 | 0.53 |
| 1:A:200:ARG:CG | 1:A:201:LYS:N | 2.71 | 0.53 |
| 1:A:136:PRO:HB2 | 1:A:138:VAL:CG1 | 2.39 | 0.53 |
| 1:A:133:LEU:HD11 | 1:A:347:PHE:HZ | 1.71 | 0.53 |
| 1:A:124:LEU:CD1 | 1:A:395:ILE:HD11 | 2.39 | 0.53 |
| 1:B:166:LEU:HD12 | 1:B:169:LEU:HD12 | 1.89 | 0.53 |
| 1:B:418:TYR:CD2 | 1:B:419:LYS:HG2 | 2.44 | 0.53 |
| 1:B:171:ASP:HA | 1:B:174:ARG:NH1 | 2.24 | 0.53 |
| 1:B:29:ILE:C | 1:B:30:ARG:HG2 | 2.29 | 0.53 |
| 1:B:362:ILE:HG13 | 1:B:363:ASP:H | 1.72 | 0.53 |
| 1:B:381:MSE:CE | 1:B:383:GLN:HE21 | 2.22 | 0.53 |
| 1:A:132:SER:O | 1:A:136:PRO:HB3 | 2.09 | 0.53 |
| 1:B:220:ILE:O | 1:B:256:LYS:HA | 2.09 | 0.53 |
| 1:B:175:LYS:NZ | 1:B:186:TYR:OH | 2.42 | 0.52 |
| 1:B:247:GLU:O | 1:B:250:GLN:HB3 | 2.08 | 0.52 |
| 1:B:305:ALA:N | 1:B:312:ILE:HD11 | 2.24 | 0.52 |
| 1:A:343:PRO:HG3 | 1:A:345:TRP:CZ2 | 2.44 | 0.52 |
| 1:B:104:LEU:HD22 | 1:B:107:MSE:HE1 | 1.92 | 0.52 |
| 1:B:169:LEU:HD13 | 1:B:281:TYR:CG | 2.44 | 0.52 |
| 1:B:357:ASN:HA | 1:B:360:LYS:CE | 2.36 | 0.52 |
| 1:B:175:LYS:O | 1:B:179:HIS:ND1 | 2.43 | 0.52 |
| 1:A:44:LYS:HA | 1:A:397:HIS:CE1 | 2.43 | 0.52 |
| 1:A:26:ASN:CB | 1:A:30:ARG:HG2 | 2.39 | 0.52 |
| 1:A:200:ARG:HD3 | 1:A:267:TYR:CZ | 2.44 | 0.52 |
| 1:B:80:LEU:HD13 | 1:B:107:MSE:HE3 | 1.92 | 0.52 |
| 1:A:432:LEU:CD2 | 1:B:13:THR:HG21 | 2.39 | 0.52 |
| 1:A:23:VAL:O | 1:A:25:GLU:O | 2.27 | 0.52 |
| 1:B:304:LEU:C | 1:B:312:ILE:HD11 | 2.30 | 0.52 |
| 1:B:114:ARG:NH1 | 1:B:170:ARG:HH12 | 2.04 | 0.52 |
| 1:B:400:ALA:HB2 | 1:B:405:ARG:HB3 | 1.92 | 0.52 |
| 1:A:429:ILE:HD13 | 1:A:434:ASN:O | 2.10 | 0.52 |
| 1:B:106:ASN:HB2 | 1:B:282:SER:CB | 2.39 | 0.52 |
| 1:A:279:TYR:CE2 | 1:A:283:ILE:HD11 | 2.44 | 0.52 |
| 1:A:300:TYR:CE1 | 1:A:303:THR:HB | 2.45 | 0.52 |
| 1:A:197:GLU:O | 1:A:200:ARG:HG2 | 2.10 | 0.52 |
| 1:A:72:VAL:HG21 | 1:A:409:LEU:HB3 | 1.91 | 0.52 |
| 1:B:79:ARG:O | 1:B:185:ASN:HB2 | 2.10 | 0.52 |
| 1:B:392:LEU:HB3 | 1:B:393:PRO:HD3 | 1.92 | 0.52 |
| 1:B:423:HIS:O | 1:B:426:GLU:OE1 | 2.27 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:26:ASN:CB | 1:A:30:ARG:CG | 2.88 | 0.52 |
| 1:A:81:SER:O | 1:A:189:PRO:CD | 2.58 | 0.52 |
| 1:B:283:ILE:HG22 | 1:B:287:LEU:CD1 | 2.39 | 0.52 |
| 1:A:428:LEU:O | 1:A:430:ASN:OD1 | 2.27 | 0.51 |
| 1:A:27:GLU:H | 1:A:27:GLU:CD | 2.13 | 0.51 |
| 1:B:138:VAL:HG12 | 1:B:142:ASP:OD2 | 2.11 | 0.51 |
| 1:B:26:ASN:C | 1:B:28:GLN:N | 2.62 | 0.51 |
| 1:B:378:VAL:HG12 | 1:B:379:ILE:N | 2.26 | 0.51 |
| 1:A:281:TYR:HA | 1:A:355:PHE:CE1 | 2.45 | 0.51 |
| 1:A:352:LEU:HD21 | 1:A:362:ILE:CD1 | 2.40 | 0.51 |
| 1:B:205:ASP:C | 1:B:207:LYS:N | 2.62 | 0.51 |
| 1:A:29:ILE:HD11 | 1:A:33:ILE:CG1 | 2.39 | 0.51 |
| 1:A:29:ILE:HA | 1:A:32:ILE:CG2 | 2.41 | 0.51 |
| 1:B:176:VAL:CG2 | 1:B:177:GLU:N | 2.74 | 0.51 |
| 1:B:89:ASN:OD1 | 1:B:92:THR:N | 2.44 | 0.51 |
| 1:A:87:LYS:HZ1 | 1:B:19:GLU:CD | 2.14 | 0.51 |
| 1:B:31:ASN:HD22 | 1:B:35:SER:HB2 | 1.76 | 0.51 |
| 1:A:321:VAL:CG1 | 1:A:325:LEU:HD21 | 2.33 | 0.51 |
| 1:B:271:HIS:O | 1:B:275:SER:HB2 | 2.10 | 0.51 |
| 1:B:335:GLU:C | 1:B:336:ILE:HD12 | 2.31 | 0.51 |
| 1:A:300:TYR:CE1 | 1:A:304:LEU:CB | 2.93 | 0.51 |
| 1:B:26:ASN:C | 1:B:28:GLN:H | 2.12 | 0.51 |
| 1:B:195:VAL:CG1 | 1:B:199:LEU:HD22 | 2.41 | 0.50 |
| 1:A:144:ARG:NH1 | 1:B:229:PRO:HG2 | 2.22 | 0.50 |
| 1:B:225:LEU:HD13 | 1:B:227:TYR:HB2 | 1.94 | 0.50 |
| 1:B:271:HIS:HA | 1:B:274:LEU:CD1 | 2.41 | 0.50 |
| 1:B:137:PRO:HG2 | 1:B:279:TYR:OH | 2.11 | 0.50 |
| 1:A:135:ARG:HG2 | 1:B:90:TYR:CD2 | 2.46 | 0.50 |
| 1:B:219:LYS:O | 1:B:220:ILE:HG12 | 2.11 | 0.50 |
| 1:B:285:LYS:O | 1:B:288:GLU:HB2 | 2.12 | 0.50 |
| 1:B:231:VAL:CG1 | 1:B:232:ILE:N | 2.75 | 0.50 |
| 1:B:72:VAL:HG21 | 1:B:409:LEU:CB | 2.42 | 0.50 |
| 1:B:114:ARG:NH1 | 1:B:170:ARG:NH1 | 2.54 | 0.50 |
| 1:A:104:LEU:HD12 | 1:A:107:MSE:HE1 | 1.92 | 0.50 |
| 1:B:256:LYS:O | 1:B:257:VAL:HG13 | 2.12 | 0.50 |
| 1:B:357:ASN:O | 1:B:360:LYS:HG2 | 2.11 | 0.50 |
| 1:A:94:ASP:OD2 | 1:A:98:ARG:HD2 | 2.12 | 0.50 |
| 1:A:54:ARG:CB | 1:A:101:MSE:HE3 | 2.20 | 0.50 |
| 1:B:359:GLU:O | 1:B:362:ILE:HG12 | 2.12 | 0.50 |
| 1:B:191:LEU:O | 1:B:193:ASP:N | 2.45 | 0.50 |
| 1:B:352:LEU:HD12 | 1:B:352:LEU:N | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:308:LEU:C | 1:A:310:VAL:H | 2.14 | 0.50 |
| 1:A:100:GLN:HA | 1:A:103:THR:CG2 | 2.42 | 0.50 |
| 1:B:106:ASN:HA | 1:B:286:LEU:HD22 | 1.92 | 0.50 |
| 1:B:82:TYR:OH | 1:B:193:ASP:OD2 | 2.28 | 0.49 |
| 1:B:404:LEU:N | 1:B:404:LEU:HD12 | 2.27 | 0.49 |
| 1:B:47:ILE:HB | 1:B:398:HIS:CD2 | 2.47 | 0.49 |
| 1:B:284:ASP:OD1 | 1:B:357:ASN:CB | 2.51 | 0.49 |
| 1:B:204:ILE:HG22 | 1:B:208:VAL:CG2 | 2.42 | 0.49 |
| 1:A:302:LYS:HG2 | 1:A:306:ARG:NH1 | 2.27 | 0.49 |
| 1:B:228:SER:O | 1:B:229:PRO:C | 2.48 | 0.49 |
| 1:B:259:LEU:HB3 | 1:B:261:LEU:HD21 | 1.94 | 0.49 |
| 1:B:418:TYR:CE2 | 1:B:419:LYS:HG2 | 2.47 | 0.49 |
| 1:A:390:LYS:HB3 | 1:A:390:LYS:HZ3 | 1.78 | 0.49 |
| 1:A:10:GLU:O | 1:A:11:ARG:C | 2.49 | 0.49 |
| 1:B:175:LYS:O | 1:B:178:GLU:HB2 | 2.12 | 0.49 |
| 1:B:182:LYS:CG | 1:B:183:ASN:H | 2.24 | 0.49 |
| 1:B:102:GLU:HB3 | 1:B:279:TYR:HE1 | 1.77 | 0.49 |
| 1:B:360:LYS:O | 1:B:364:LYS:HB3 | 2.12 | 0.49 |
| 1:A:392:LEU:O | 1:A:396:LEU:HG | 2.12 | 0.49 |
| 1:A:333:TYR:HB2 | 1:A:371:VAL:HG22 | 1.94 | 0.49 |
| 1:B:305:ALA:HA | 1:B:310:VAL:O | 2.12 | 0.49 |
| 1:A:285:LYS:HE2 | 1:A:285:LYS:HA | 1.94 | 0.49 |
| 1:B:172:HIS:HD2 | 1:B:175:LYS:HE3 | 1.78 | 0.49 |
| 1:A:43:GLU:HG2 | 1:A:120:LYS:HZ2 | 1.76 | 0.49 |
| 1:A:299:PHE:CE2 | 1:A:300:TYR:CE2 | 3.00 | 0.49 |
| 1:A:136:PRO:HG2 | 1:A:138:VAL:CG2 | 2.43 | 0.49 |
| 1:B:110:TYR:HE2 | 1:B:114:ARG:CZ | 2.25 | 0.49 |
| 1:B:369:ALA:CB | 1:B:388:ILE:HG12 | 2.42 | 0.49 |
| 1:A:419:LYS:O | 1:A:422:ARG:HG2 | 2.13 | 0.49 |
| 1:B:13:THR:O | 1:B:17:LEU:HG | 2.13 | 0.49 |
| 1:B:65:TYR:CZ | 1:B:84:ASN:HB3 | 2.48 | 0.49 |
| 1:B:368:LEU:HD13 | 1:B:381:MSE:HE1 | 1.93 | 0.49 |
| 1:A:316:ALA:HB3 | 1:B:60:SER:OG | 2.12 | 0.49 |
| 1:A:23:VAL:HG12 | 1:A:321:VAL:HG21 | 1.95 | 0.49 |
| 1:A:322:ILE:HG23 | 1:A:326:ILE:CG2 | 2.42 | 0.49 |
| 1:A:428:LEU:HD12 | 1:A:429:ILE:H | 1.78 | 0.49 |
| 1:A:430:ASN:HB3 | 1:A:435:ARG:NE | 2.28 | 0.49 |
| 1:A:209:ILE:HG22 | 1:A:210:ALA:N | 2.28 | 0.49 |
| 1:B:325:LEU:CG | 1:B:326:ILE:N | 2.74 | 0.48 |
| 1:B:31:ASN:ND2 | 1:B:35:SER:HB2 | 2.28 | 0.48 |
| 1:B:267:TYR:C | 1:B:267:TYR:CD2 | 2.85 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:134:VAL:CG2 | 1:B:135:ARG:N | 2.76 | 0.48 |
| 1:B:103:THR:HG21 | 1:B:278:GLU:HG2 | 1.94 | 0.48 |
| 1:B:26:ASN:O | 1:B:28:GLN:N | 2.46 | 0.48 |
| 1:B:434:ASN:OD1 | 1:B:434:ASN:C | 2.52 | 0.48 |
| 1:B:124:LEU:HD13 | 1:B:395:ILE:CD1 | 2.43 | 0.48 |
| 1:B:114:ARG:HH22 | 1:B:170:ARG:HH12 | 1.59 | 0.48 |
| 1:A:305:ALA:HA | 1:A:312:ILE:H | 1.78 | 0.48 |
| 1:B:141:GLU:O | 1:B:144:ARG:HB3 | 2.13 | 0.48 |
| 1:A:370:TYR:HB3 | 1:A:379:ILE:HG21 | 1.95 | 0.48 |
| 1:A:329:GLU:HG2 | 1:A:329:GLU:O | 2.13 | 0.48 |
| 1:B:199:LEU:HD12 | 1:B:203:TYR:CD2 | 2.49 | 0.48 |
| 1:B:219:LYS:HA | 1:B:257:VAL:O | 2.13 | 0.48 |
| 1:A:343:PRO:HG2 | 1:A:346:SER:HB3 | 1.95 | 0.48 |
| 1:A:27:GLU:O | 1:A:29:ILE:N | 2.46 | 0.48 |
| 1:B:145:SER:HB3 | 1:B:269:ALA:HA | 1.96 | 0.48 |
| 1:B:37:LYS:HD2 | 1:B:333:TYR:CZ | 2.49 | 0.48 |
| 1:A:324:THR:HG22 | 1:A:325:LEU:N | 2.28 | 0.48 |
| 1:A:397:HIS:CD2 | 1:A:397:HIS:O | 2.67 | 0.48 |
| 1:A:358:ILE:O | 1:A:362:ILE:HG13 | 2.14 | 0.48 |
| 1:A:241:ARG:HD2 | 1:B:246:ASP:OD1 | 2.13 | 0.48 |
| 1:A:82:TYR:OH | 1:A:193:ASP:OD1 | 2.29 | 0.48 |
| 1:B:197:GLU:O | 1:B:201:LYS:HG2 | 2.14 | 0.48 |
| 1:B:381:MSE:HE3 | 1:B:383:GLN:HG2 | 1.95 | 0.48 |
| 1:A:29:ILE:CA | 1:A:32:ILE:HG22 | 2.44 | 0.48 |
| 1:B:223:LYS:N | 4:B:457:HOH:O | 2.46 | 0.48 |
| 1:A:47:ILE:HG13 | 1:A:122:ALA:HB3 | 1.96 | 0.48 |
| 1:A:245:VAL:CG2 | 1:B:241:ARG:HA | 2.44 | 0.48 |
| 1:A:374:GLU:HB2 | 1:A:402:GLY:HA3 | 1.92 | 0.48 |
| 1:B:348:PRO:O | 1:B:352:LEU:HD13 | 2.14 | 0.48 |
| 1:B:354:LYS:N | 1:B:354:LYS:HD2 | 2.28 | 0.48 |
| 1:A:87:LYS:HZ1 | 1:B:19:GLU:HG3 | 1.71 | 0.47 |
| 1:A:138:VAL:HG23 | 1:A:139:TYR:H | 1.79 | 0.47 |
| 1:A:328:HIS:CE1 | 1:A:330:LYS:HE3 | 2.49 | 0.47 |
| 1:B:415:LYS:O | 1:B:416:ILE:C | 2.51 | 0.47 |
| 1:B:204:ILE:O | 1:B:207:LYS:HB2 | 2.14 | 0.47 |
| 1:B:381:MSE:HE3 | 1:B:383:GLN:CG | 2.44 | 0.47 |
| 1:B:248:LEU:C | 1:B:248:LEU:HD12 | 2.34 | 0.47 |
| 1:B:72:VAL:HG21 | 1:B:409:LEU:HB3 | 1.97 | 0.47 |
| 1:A:8:SER:HA | 1:A:11:ARG:HD3 | 1.97 | 0.47 |
| 1:A:204:ILE:HD13 | 1:A:270:LEU:HD22 | 1.96 | 0.47 |
| 1:B:373:PHE:CD2 | 1:B:399:LYS:HE3 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:378:VAL:HG13 | 1:B:440:LYS:HZ2 | 1.79 | 0.47 |
| 1:B:164:GLU:OE2 | 1:B:203:TYR:OH | 2.21 | 0.47 |
| 1:B:179:HIS:HA | 1:B:182:LYS:HD3 | 1.96 | 0.47 |
| 1:B:243:LYS:CB | 1:B:247:GLU:OE2 | 2.62 | 0.47 |
| 1:B:232:ILE:HD11 | 1:B:236:VAL:HG21 | 1.96 | 0.47 |
| 1:B:90:TYR:CD1 | 1:B:91:GLY:N | 2.78 | 0.47 |
| 1:B:45:SER:OG | 1:B:398:HIS:CD2 | 2.68 | 0.47 |
| 1:B:149:MSE:CE | 1:B:266:ILE:O | 2.63 | 0.47 |
| 1:A:320:ALA:CA | 1:B:434:ASN:HD21 | 2.28 | 0.47 |
| 1:A:80:LEU:HD13 | 1:A:108:LEU:HD13 | 1.96 | 0.47 |
| 1:A:124:LEU:HD21 | 1:A:295:ILE:CG1 | 2.44 | 0.47 |
| 1:A:292:LEU:HB3 | 1:A:385:THR:CG2 | 2.45 | 0.47 |
| 1:B:135:ARG:HG2 | 1:B:136:PRO:HD2 | 1.96 | 0.47 |
| 1:B:247:GLU:HG2 | 1:B:248:LEU:N | 2.29 | 0.47 |
| 1:B:400:ALA:HB2 | 1:B:405:ARG:N | 2.30 | 0.47 |
| 1:A:133:LEU:N | 1:A:133:LEU:HD13 | 2.29 | 0.47 |
| 1:A:29:ILE:O | 1:A:30:ARG:C | 2.53 | 0.47 |
| 1:A:31:ASN:OD1 | 1:A:32:ILE:N | 2.46 | 0.47 |
| 1:A:21:GLU:HA | 1:A:24:ARG:HB3 | 1.97 | 0.47 |
| 1:B:64:ILE:HG21 | 1:B:422:ARG:NH2 | 2.30 | 0.47 |
| 1:A:386:THR:HG21 | 1:A:390:LYS:NZ | 2.30 | 0.47 |
| 1:A:33:ILE:O | 1:A:36:TRP:CB | 2.64 | 0.47 |
| 1:B:128:THR:HG23 | 1:B:296:ALA:CB | 2.45 | 0.47 |
| 1:A:63:VAL:O | 1:A:85:ALA:HA | 2.15 | 0.47 |
| 1:A:23:VAL:O | 1:A:24:ARG:C | 2.52 | 0.46 |
| 1:B:273:THR:O | 1:B:277:ILE:HG13 | 2.14 | 0.46 |
| 1:B:345:TRP:CE3 | 1:B:346:SER:HA | 2.50 | 0.46 |
| 1:B:98:ARG:O | 1:B:101:MSE:HB3 | 2.15 | 0.46 |
| 1:A:67:LEU:HD22 | 1:A:101:MSE:CE | 2.46 | 0.46 |
| 1:A:43:GLU:O | 1:A:397:HIS:HB2 | 2.16 | 0.46 |
| 1:A:386:THR:HB | 4:A:465:HOH:O | 2.15 | 0.46 |
| 1:A:222:ARG:NH1 | 1:A:255:GLU:OE2 | 2.49 | 0.46 |
| 1:A:141:GLU:O | 1:A:144:ARG:CG | 2.63 | 0.46 |
| 1:A:221:PRO:O | 1:A:230:ARG:NH2 | 2.48 | 0.46 |
| 1:A:92:THR:O | 1:A:96:ILE:HG12 | 2.15 | 0.46 |
| 1:B:195:VAL:HG12 | 1:B:199:LEU:HD22 | 1.98 | 0.46 |
| 1:B:130:THR:O | 1:B:134:VAL:HG13 | 2.16 | 0.46 |
| 1:B:389:GLU:O | 1:B:393:PRO:CD | 2.63 | 0.46 |
| 1:A:57:SER:HB3 | 1:A:64:ILE:HG23 | 1.96 | 0.46 |
| 1:A:323:ARG:NH2 | 1:A:376:GLY:O | 2.48 | 0.46 |
| 1:B:343:PRO:HG2 | 1:B:346:SER:CB | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:249:LEU:O | 1:A:252:LEU:HB2 | 2.16 | 0.46 |
| 1:A:136:PRO:O | 1:A:138:VAL:N | 2.49 | 0.46 |
| 1:B:114:ARG:NH2 | 1:B:170:ARG:HH22 | 2.14 | 0.46 |
| 1:B:191:LEU:C | 1:B:193:ASP:N | 2.65 | 0.46 |
| 1:A:281:TYR:HA | 1:A:355:PHE:HE1 | 1.80 | 0.46 |
| 1:A:49:ALA:HA | 1:A:124:LEU:O | 2.15 | 0.46 |
| 1:B:164:GLU:CD | 1:B:202:LYS:HZ1 | 2.19 | 0.46 |
| 1:A:130:THR:HG1 | 1:A:299:PHE:HZ | 1.53 | 0.46 |
| 1:A:234:ILE:HA | 1:A:234:ILE:HD12 | 1.65 | 0.46 |
| 1:A:89:ASN:CG | 1:A:92:THR:HG23 | 2.37 | 0.46 |
| 1:B:405:ARG:HA | 1:B:408:GLN:NE2 | 2.31 | 0.46 |
| 1:A:133:LEU:CD1 | 1:A:133:LEU:N | 2.79 | 0.46 |
| 1:B:333:TYR:HE1 | 1:B:335:GLU:HB2 | 1.81 | 0.46 |
| 1:B:98:ARG:NH2 | 1:B:137:PRO:CB | 2.59 | 0.46 |
| 1:B:47:ILE:HB | 1:B:398:HIS:NE2 | 2.31 | 0.45 |
| 1:B:187:ASP:C | 1:B:189:PRO:HD3 | 2.36 | 0.45 |
| 1:B:230:ARG:HG3 | 1:B:231:VAL:N | 2.26 | 0.45 |
| 1:A:21:GLU:HB3 | 1:A:24:ARG:CZ | 2.47 | 0.45 |
| 1:B:48:TYR:HA | 1:B:73:GLY:HA3 | 1.98 | 0.45 |
| 1:B:172:HIS:CD2 | 1:B:175:LYS:HE3 | 2.51 | 0.45 |
| 1:A:300:TYR:HE1 | 1:A:304:LEU:CB | 2.29 | 0.45 |
| 1:A:217:LYS:HD2 | 1:A:260:TYR:HE1 | 1.81 | 0.45 |
| 1:A:37:LYS:CG | 1:A:38:PRO:HD2 | 2.42 | 0.45 |
| 1:A:126:ASP:OD1 | 1:A:126:ASP:C | 2.55 | 0.45 |
| 1:A:115:LYS:HZ3 | 1:A:181:GLU:CA | 2.30 | 0.45 |
| 1:A:302:LYS:HE3 | 1:A:306:ARG:HH22 | 1.80 | 0.45 |
| 1:A:431:ALA:O | 1:A:432:LEU:HD12 | 2.17 | 0.45 |
| 1:A:320:ALA:HA | 1:B:434:ASN:HD21 | 1.80 | 0.45 |
| 1:B:364:LYS:HG2 | 1:B:365:GLY:O | 2.16 | 0.45 |
| 1:A:27:GLU:OE2 | 1:A:29:ILE:HG22 | 2.16 | 0.45 |
| 1:B:422:ARG:C | 1:B:422:ARG:CD | 2.85 | 0.45 |
| 1:B:313:VAL:CG1 | 1:B:317:LEU:HB3 | 2.46 | 0.45 |
| 1:A:9:ILE:O | 1:A:13:THR:OG1 | 2.34 | 0.45 |
| 1:B:196:VAL:HG12 | 1:B:274:LEU:HD21 | 1.99 | 0.45 |
| 1:B:82:TYR:CE2 | 1:B:193:ASP:OD2 | 2.70 | 0.45 |
| 1:B:136:PRO:HB3 | 1:B:142:ASP:OD2 | 2.17 | 0.45 |
| 1:B:407:LEU:HD23 | 1:B:408:GLN:HG3 | 1.97 | 0.45 |
| 1:B:172:HIS:O | 1:B:175:LYS:HG2 | 2.17 | 0.45 |
| 1:B:192:THR:O | 1:B:196:VAL:HG13 | 2.17 | 0.45 |
| 1:B:28:GLN:NE2 | 1:B:30:ARG:HB3 | 2.32 | 0.45 |
| 1:B:218:VAL:HB | 1:B:259:LEU:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:346:SER:O | 1:A:347:PHE:HD1 | 1.98 | 0.45 |
| 1:B:350:PHE:HD2 | 1:B:350:PHE:H | 1.60 | 0.45 |
| 1:A:67:LEU:HA | 1:A:101:MSE:HE1 | 1.98 | 0.45 |
| 1:A:307:THR:HG23 | 1:A:309:GLY:N | 2.26 | 0.45 |
| 1:A:104:LEU:HA | 1:A:107:MSE:HE3 | 1.99 | 0.45 |
| 1:A:222:ARG:HD3 | 1:A:255:GLU:OE2 | 2.17 | 0.45 |
| 1:B:172:HIS:NE2 | 1:B:176:VAL:CG1 | 2.80 | 0.45 |
| 1:A:67:LEU:HD22 | 1:A:101:MSE:HE2 | 1.98 | 0.45 |
| 1:A:87:LYS:HZ1 | 1:B:19:GLU:CG | 2.26 | 0.45 |
| 1:A:139:TYR:O | 1:A:140:PRO:C | 2.55 | 0.44 |
| 1:B:217:LYS:HG2 | 1:B:260:TYR:CD1 | 2.48 | 0.44 |
| 1:A:48:TYR:CD1 | 1:A:112:ALA:HB1 | 2.52 | 0.44 |
| 1:B:130:THR:HG23 | 1:B:383:GLN:NE2 | 2.33 | 0.44 |
| 1:B:388:ILE:HG22 | 1:B:389:GLU:N | 2.31 | 0.44 |
| 1:B:240:SER:O | 1:B:243:LYS:HB2 | 2.18 | 0.44 |
| 1:B:408:GLN:O | 1:B:412:HIS:HB2 | 2.17 | 0.44 |
| 1:A:21:GLU:CG | 1:A:24:ARG:HD3 | 2.47 | 0.44 |
| 1:B:295:ILE:HD11 | 1:B:382:LEU:HD13 | 2.00 | 0.44 |
| 1:B:138:VAL:HG11 | 1:B:272:MSE:SE | 2.67 | 0.44 |
| 1:A:230:ARG:O | 1:B:233:PRO:HA | 2.16 | 0.44 |
| 1:A:430:ASN:C | 1:A:432:LEU:N | 2.71 | 0.44 |
| 1:A:102:GLU:HG3 | 3:A:454:GOL:C2 | 2.47 | 0.44 |
| 1:A:146:LEU:HD22 | 1:A:273:THR:HG23 | 2.00 | 0.44 |
| 1:B:205:ASP:C | 1:B:207:LYS:H | 2.20 | 0.44 |
| 1:A:299:PHE:C | 1:A:299:PHE:CD2 | 2.91 | 0.44 |
| 1:A:300:TYR:CD1 | 1:A:300:TYR:C | 2.91 | 0.44 |
| 1:B:407:LEU:HD23 | 1:B:408:GLN:CA | 2.48 | 0.44 |
| 1:B:134:VAL:HG23 | 1:B:135:ARG:N | 2.32 | 0.44 |
| 1:B:103:THR:OG1 | 1:B:279:TYR:HA | 2.18 | 0.44 |
| 1:B:89:ASN:OD1 | 1:B:92:THR:CB | 2.61 | 0.44 |
| 1:A:422:ARG:CG | 1:A:423:HIS:N | 2.81 | 0.44 |
| 1:A:428:LEU:CD1 | 1:A:429:ILE:N | 2.79 | 0.44 |
| 1:A:320:ALA:HB1 | 1:B:434:ASN:HD21 | 1.83 | 0.44 |
| 1:B:420:GLU:HG3 | 1:B:423:HIS:NE2 | 2.32 | 0.44 |
| 1:A:356:ARG:O | 1:A:360:LYS:HG3 | 2.17 | 0.44 |
| 1:B:179:HIS:HA | 1:B:182:LYS:CD | 2.48 | 0.44 |
| 1:B:206:THR:C | 1:B:207:LYS:HD2 | 2.38 | 0.44 |
| 1:B:318:LEU:HD23 | 1:B:370:TYR:CD1 | 2.53 | 0.44 |
| 1:A:299:PHE:HD2 | 1:A:299:PHE:C | 2.21 | 0.44 |
| 1:A:299:PHE:HE2 | 1:A:300:TYR:CE2 | 2.35 | 0.44 |
| 1:B:319:ASP:O | 1:B:322:ILE:HG12 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:320:ALA:CB | 1:B:434:ASN:HD21 | 2.30 | 0.44 |
| 1:A:392:LEU:O | 1:A:395:ILE:HG22 | 2.17 | 0.44 |
| 1:A:51:ASP:C | 1:A:414:VAL:HG21 | 2.38 | 0.44 |
| 1:B:180:LEU:HD23 | 1:B:180:LEU:HA | 1.51 | 0.43 |
| 1:B:191:LEU:O | 1:B:194:ASN:N | 2.51 | 0.43 |
| 1:B:333:TYR:CE1 | 1:B:388:ILE:HG21 | 2.53 | 0.43 |
| 1:B:373:PHE:CE1 | 1:B:399:LYS:HE3 | 2.53 | 0.43 |
| 1:A:27:GLU:C | 1:A:29:ILE:N | 2.71 | 0.43 |
| 1:A:263:LYS:HE3 | 1:A:263:LYS:HB2 | 1.74 | 0.43 |
| 1:B:89:ASN:ND2 | 1:B:92:THR:HB | 2.33 | 0.43 |
| 1:B:188:SER:N | 1:B:189:PRO:HD3 | 2.33 | 0.43 |
| 1:B:199:LEU:HD12 | 1:B:203:TYR:CE2 | 2.53 | 0.43 |
| 1:A:313:VAL:HG12 | 1:A:313:VAL:O | 2.18 | 0.43 |
| 1:A:313:VAL:CG1 | 1:A:318:LEU:HB2 | 2.46 | 0.43 |
| 1:A:8:SER:OG | 1:B:83:ALA:HB3 | 2.18 | 0.43 |
| 1:A:153:ILE:HD11 | 1:A:158:PHE:HA | 2.00 | 0.43 |
| 1:B:28:GLN:HG3 | 1:B:29:ILE:N | 2.32 | 0.43 |
| 1:A:26:ASN:HD22 | 1:A:30:ARG:NE | 2.16 | 0.43 |
| 1:A:386:THR:CG2 | 1:A:390:LYS:HB2 | 2.48 | 0.43 |
| 1:B:223:LYS:HA | 1:B:223:LYS:HD3 | 1.63 | 0.43 |
| 1:B:276:TYR:O | 1:B:279:TYR:HB3 | 2.18 | 0.43 |
| 1:A:27:GLU:OE2 | 1:A:29:ILE:CG2 | 2.66 | 0.43 |
| 1:B:116:LEU:HA | 1:B:116:LEU:HD12 | 1.88 | 0.43 |
| 1:B:136:PRO:CB | 1:B:142:ASP:OD2 | 2.67 | 0.43 |
| 1:B:130:THR:HG23 | 1:B:383:GLN:HE22 | 1.83 | 0.43 |
| 1:B:191:LEU:H | 1:B:191:LEU:HD13 | 1.82 | 0.43 |
| 1:B:101:MSE:CE | 1:B:101:MSE:HA | 2.47 | 0.43 |
| 1:B:138:VAL:HG22 | 1:B:138:VAL:O | 2.18 | 0.43 |
| 1:A:232:ILE:C | 1:B:231:VAL:HG13 | 2.39 | 0.43 |
| 1:A:316:ALA:HB2 | 1:B:440:LYS:HD3 | 2.01 | 0.43 |
| 1:B:116:LEU:HB3 | 1:B:121:ARG:HD3 | 2.00 | 0.43 |
| 1:A:21:GLU:OE1 | 1:A:24:ARG:NH1 | 2.50 | 0.43 |
| 1:A:386:THR:CG2 | 1:A:387:ASN:N | 2.82 | 0.43 |
| 1:B:370:TYR:CB | 1:B:379:ILE:HD11 | 2.40 | 0.43 |
| 1:A:243:LYS:HE2 | 1:A:243:LYS:HB3 | 1.81 | 0.43 |
| 1:B:284:ASP:OD2 | 1:B:355:PHE:HA | 2.19 | 0.43 |
| 1:B:360:LYS:O | 1:B:363:ASP:HB2 | 2.19 | 0.43 |
| 1:A:80:LEU:HD23 | 1:A:107:MSE:HE3 | 2.01 | 0.43 |
| 1:B:304:LEU:HD13 | 1:B:304:LEU:HA | 1.87 | 0.43 |
| 1:A:33:ILE:HA | 1:A:33:ILE:HD13 | 1.77 | 0.43 |
| 1:B:280:LEU:HD23 | 1:B:283:ILE:HD12 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:343:PRO:CG | 1:B:346:SER:HB3 | 2.49 | 0.43 |
| 1:B:14:LYS:O | 1:B:18:ASP:OD2 | 2.36 | 0.43 |
| 1:B:39:LEU:HG | 1:B:332:GLY:HA2 | 2.01 | 0.43 |
| 1:A:247:GLU:O | 1:A:251:GLU:HG3 | 2.19 | 0.42 |
| 1:A:425:LEU:O | 1:A:428:LEU:HD21 | 2.19 | 0.42 |
| 1:B:260:TYR:C | 1:B:261:LEU:HD23 | 2.39 | 0.42 |
| 1:A:79:ARG:HB3 | 1:A:185:ASN:CB | 2.48 | 0.42 |
| 1:A:130:THR:HG23 | 1:A:383:GLN:HE22 | 1.83 | 0.42 |
| 1:B:106:ASN:HB3 | 1:B:282:SER:O | 2.19 | 0.42 |
| 1:A:170:ARG:O | 1:A:174:ARG:HG3 | 2.18 | 0.42 |
| 1:A:369:ALA:HB2 | 1:A:388:ILE:HG13 | 1.99 | 0.42 |
| 1:A:26:ASN:HD22 | 1:A:30:ARG:HD2 | 1.83 | 0.42 |
| 1:A:319:ASP:C | 1:A:319:ASP:OD1 | 2.58 | 0.42 |
| 1:B:206:THR:HB | 1:B:207:LYS:HZ3 | 1.83 | 0.42 |
| 1:B:96:ILE:HD11 | 1:B:272:MSE:CE | 2.37 | 0.42 |
| 1:A:89:ASN:CB | 1:A:92:THR:HG23 | 2.49 | 0.42 |
| 1:B:202:LYS:O | 1:B:207:LYS:NZ | 2.53 | 0.42 |
| 1:B:368:LEU:HD22 | 1:B:383:GLN:HG2 | 2.02 | 0.42 |
| 1:B:373:PHE:CE2 | 1:B:399:LYS:CE | 2.98 | 0.42 |
| 1:A:64:ILE:O | 1:A:64:ILE:HG23 | 2.20 | 0.42 |
| 1:A:279:TYR:CZ | 1:A:283:ILE:HD11 | 2.54 | 0.42 |
| 1:A:60:SER:OG | 1:A:61:GLY:N | 2.52 | 0.42 |
| 1:B:179:HIS:CA | 1:B:182:LYS:HG2 | 2.44 | 0.42 |
| 1:B:95:GLN:CB | 1:B:138:VAL:HG23 | 2.47 | 0.42 |
| 1:B:218:VAL:N | 1:B:259:LEU:O | 2.52 | 0.42 |
| 1:B:284:ASP:OD2 | 1:B:355:PHE:HB3 | 2.20 | 0.42 |
| 1:B:318:LEU:O | 1:B:321:VAL:HB | 2.20 | 0.42 |
| 1:A:136:PRO:HG2 | 1:A:138:VAL:HG21 | 2.01 | 0.42 |
| 1:B:256:LYS:O | 1:B:257:VAL:CG1 | 2.68 | 0.42 |
| 1:A:316:ALA:HA | 1:B:440:LYS:HD2 | 2.01 | 0.42 |
| 1:B:287:LEU:CD1 | 1:B:358:ILE:HD13 | 2.50 | 0.42 |
| 1:A:125:MSE:HE1 | 1:A:286:LEU:HD11 | 2.01 | 0.42 |
| 1:B:171:ASP:HA | 1:B:174:ARG:HH11 | 1.83 | 0.42 |
| 1:B:65:TYR:CE1 | 1:B:100:GLN:OE1 | 2.73 | 0.42 |
| 1:A:89:ASN:N | 1:A:93:SER:HB3 | 2.34 | 0.42 |
| 1:A:342:PRO:HG2 | 1:A:362:ILE:HG12 | 2.01 | 0.42 |
| 1:B:369:ALA:HB2 | 1:B:388:ILE:HG12 | 2.02 | 0.42 |
| 1:A:374:GLU:HA | 1:A:374:GLU:OE1 | 2.19 | 0.42 |
| 1:B:439:LEU:HD12 | 1:B:440:LYS:H | 1.84 | 0.42 |
| 1:A:29:ILE:O | 1:A:29:ILE:HD12 | 2.19 | 0.42 |
| 1:A:386:THR:HG21 | 1:A:390:LYS:HZ3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:167:GLU:HG3 | 1:A:168:LYS:N | 2.35 | 0.42 |
| 1:B:405:ARG:O | 1:B:406:PRO:C | 2.56 | 0.42 |
| 1:B:350:PHE:CD2 | 1:B:350:PHE:N | 2.76 | 0.42 |
| 1:B:129:LEU:HD23 | 1:B:129:LEU:HA | 1.70 | 0.41 |
| 1:B:27:GLU:O | 1:B:28:GLN:C | 2.56 | 0.41 |
| 1:B:433:ARG:CG | 1:B:434:ASN:N | 2.79 | 0.41 |
| 1:A:236:VAL:HG12 | 1:A:248:LEU:HD11 | 2.02 | 0.41 |
| 1:B:84:ASN:ND2 | 1:B:193:ASP:OD2 | 2.54 | 0.41 |
| 1:B:334:LEU:HD12 | 1:B:334:LEU:C | 2.41 | 0.41 |
| 1:A:236:VAL:CG1 | 1:A:248:LEU:HD11 | 2.50 | 0.41 |
| 1:A:367:HIS:CE1 | 4:A:461:HOH:O | 2.72 | 0.41 |
| 1:B:56:VAL:HG13 | 1:B:63:VAL:HG13 | 2.02 | 0.41 |
| 1:B:364:LYS:HG2 | 1:B:365:GLY:N | 2.35 | 0.41 |
| 1:B:64:ILE:HG13 | 1:B:422:ARG:HH22 | 1.86 | 0.41 |
| 1:A:89:ASN:HB3 | 1:A:92:THR:HG23 | 2.02 | 0.41 |
| 1:A:57:SER:HB3 | 1:A:64:ILE:CG2 | 2.51 | 0.41 |
| 1:B:293:ALA:CB | 1:B:395:ILE:HD11 | 2.50 | 0.41 |
| 1:B:196:VAL:HG23 | 1:B:197:GLU:N | 2.35 | 0.41 |
| 1:B:32:ILE:HD13 | 1:B:325:LEU:HD21 | 1.97 | 0.41 |
| 1:B:434:ASN:OD1 | 1:B:436:ASP:CG | 2.59 | 0.41 |
| 1:B:362:ILE:CG1 | 1:B:363:ASP:N | 2.79 | 0.41 |
| 1:A:173:TYR:CE1 | 1:A:285:LYS:HG3 | 2.56 | 0.41 |
| 1:B:295:ILE:CD1 | 1:B:382:LEU:HD13 | 2.51 | 0.41 |
| 1:A:250:GLN:O | 1:A:254:GLU:HB2 | 2.20 | 0.41 |
| 1:A:138:VAL:CG2 | 1:A:139:TYR:N | 2.83 | 0.41 |
| 1:A:129:LEU:HD13 | 1:A:294:TYR:CE2 | 2.55 | 0.41 |
| 1:B:396:LEU:HA | 1:B:396:LEU:HD23 | 1.76 | 0.41 |
| 1:A:198:LYS:HB2 | 1:A:198:LYS:HE3 | 1.86 | 0.41 |
| 1:B:166:LEU:HA | 1:B:166:LEU:HD12 | 1.83 | 0.41 |
| 1:B:135:ARG:CG | 1:B:136:PRO:HD2 | 2.51 | 0.41 |
| 1:B:95:GLN:HB3 | 1:B:138:VAL:HA | 2.03 | 0.41 |
| 1:B:371:VAL:O | 1:B:379:ILE:HA | 2.21 | 0.41 |
| 1:A:340:VAL:CG1 | 1:A:341:VAL:N | 2.54 | 0.41 |
| 1:A:395:ILE:HA | 1:A:395:ILE:HD13 | 1.68 | 0.41 |
| 1:A:27:GLU:N | 1:A:27:GLU:CD | 2.74 | 0.41 |
| 1:B:153:ILE:O | 1:B:157:ASP:HB2 | 2.19 | 0.41 |
| 1:B:176:VAL:HG12 | 1:B:186:TYR:HE2 | 1.86 | 0.41 |
| 1:B:139:TYR:C | 1:B:141:GLU:N | 2.73 | 0.41 |
| 1:B:336:ILE:HD13 | 1:B:368:LEU:O | 2.21 | 0.41 |
| 1:B:89:ASN:OD1 | 1:B:92:THR:CA | 2.69 | 0.41 |
| 1:A:352:LEU:HA | 1:A:352:LEU:HD12 | 1.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:70:LEU:HD12 | 1:B:78:LEU:O | 2.20 | 0.41 |
| 1:B:190:ILE:HG23 | 1:B:192:THR:OG1 | 2.21 | 0.41 |
| 1:B:149:MSE:HG3 | 1:B:273:THR:HG21 | 2.02 | 0.41 |
| 1:A:95:GLN:NE2 | 1:A:138:VAL:O | 2.53 | 0.41 |
| 1:B:47:ILE:HG21 | 1:B:406:PRO:HG2 | 2.03 | 0.41 |
| 1:A:59:LEU:HD13 | 1:A:64:ILE:HG22 | 2.02 | 0.41 |
| 1:A:43:GLU:HG2 | 1:A:120:LYS:HZ3 | 1.85 | 0.41 |
| 1:B:304:LEU:O | 1:B:310:VAL:HG13 | 2.21 | 0.41 |
| 1:A:6:LYS:O | 1:A:9:ILE:HG22 | 2.21 | 0.41 |
| 1:B:436:ASP:O | 1:B:437:PRO:C | 2.58 | 0.41 |
| 1:A:104:LEU:HA | 1:A:107:MSE:CE | 2.51 | 0.41 |
| 1:B:245:VAL:HG12 | 1:B:249:LEU:CD1 | 2.48 | 0.41 |
| 1:B:166:LEU:O | 1:B:169:LEU:HB2 | 2.21 | 0.40 |
| 1:B:169:LEU:O | 1:B:172:HIS:HB3 | 2.21 | 0.40 |
| 1:A:434:ASN:OD1 | 1:A:434:ASN:O | 2.40 | 0.40 |
| 1:B:164:GLU:OE2 | 1:B:202:LYS:CE | 2.70 | 0.40 |
| 1:B:373:PHE:CE2 | 1:B:374:GLU:CD | 2.95 | 0.40 |
| 1:B:356:ARG:HA | 1:B:359:GLU:HB3 | 2.04 | 0.40 |
| 1:A:79:ARG:O | 1:A:185:ASN:HA | 2.22 | 0.40 |
| 1:A:11:ARG:H | 1:A:11:ARG:CD | 2.34 | 0.40 |
| 1:A:26:ASN:HD22 | 1:A:30:ARG:CD | 2.34 | 0.40 |
| 1:A:171:ASP:O | 1:A:174:ARG:HB2 | 2.21 | 0.40 |
| 1:B:419:LYS:O | 1:B:422:ARG:HB3 | 2.21 | 0.40 |
| 1:A:67:LEU:HD13 | 1:A:101:MSE:HA | 2.03 | 0.40 |
| 1:A:130:THR:HG23 | 1:A:383:GLN:NE2 | 2.36 | 0.40 |
| 1:B:404:LEU:O | 1:B:407:LEU:HB3 | 2.22 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 418/471 (89%) | 370 (88%) | 46 (11%) | 2 (0%) | 34 76 |
| 1 | B | 411/471 (87%) | 345 (84%) | 62 (15%) | 4 (1%) | 19 63 |
| All | All | 829/942 (88%) | 715 (86%) | 108 (13%) | 6 (1%) | 26 71 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 29 | ILE |
| 1 | A | 310 | VAL |
| 1 | B | 27 | GLU |
| 1 | B | 312 | ILE |
| 1 | B | 230 | ARG |
| 1 | A | 375 | GLN |

### 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 | A | 378/410 (92%) | 325 (86%) | 53 (14%) | 4 19 |
| 1 | B | 380/410 (93%) | 318 (84%) | 62 (16%) | 3 13 |
| All | All | 758/820 (92%) | 643 (85%) | 115 (15%) | 3 16 |

All (115) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 7 | GLN |
| 1 | A | 13 | THR |
| 1 | A | 27 | GLU |
| 1 | A | 29 | ILE |
| 1 | A | 48 | TYR |
| 1 | A | 50 | VAL |
| 1 | A | 56 | VAL |
| 1 | A | 58 | ARG |
| 1 | A | 72 | VAL |
| 1 | A | 90 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 92 | THR |
| 1 | A | 95 | GLN |
| 1 | A | 102 | GLU |
| 1 | A | 103 | THR |
| 1 | A | 126 | ASP |
| 1 | A | 128 | THR |
| 1 | A | 133 | LEU |
| 1 | A | 142 | ASP |
| 1 | A | 144 | ARG |
| 1 | A | 155 | GLU |
| 1 | A | 160 | ASN |
| 1 | A | 188 | SER |
| 1 | A | 191 | LEU |
| 1 | A | 234 | ILE |
| 1 | A | 246 | ASP |
| 1 | A | 249 | LEU |
| 1 | A | 258 | GLU |
| 1 | A | 266 | ILE |
| 1 | A | 280 | LEU |
| 1 | A | 282 | SER |
| 1 | A | 292 | LEU |
| 1 | A | 299 | PHE |
| 1 | A | 300 | TYR |
| 1 | A | 303 | THR |
| 1 | A | 318 | LEU |
| 1 | A | 321 | VAL |
| 1 | A | 324 | THR |
| 1 | A | 325 | LEU |
| 1 | A | 328 | HIS |
| 1 | A | 349 | ASP |
| 1 | A | 352 | LEU |
| 1 | A | 353 | SER |
| 1 | A | 363 | ASP |
| 1 | A | 368 | LEU |
| 1 | A | 381 | MSE |
| 1 | A | 385 | THR |
| 1 | A | 386 | THR |
| 1 | A | 395 | ILE |
| 1 | A | 414 | VAL |
| 1 | A | 423 | HIS |
| 1 | A | 424 | THR |
| 1 | A | 425 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 428 | LEU |
| 1 | B | 20 | LEU |
| 1 | B | 30 | ARG |
| 1 | B | 31 | ASN |
| 1 | B | 48 | TYR |
| 1 | B | 82 | TYR |
| 1 | B | 101 | MSE |
| 1 | B | 102 | GLU |
| 1 | B | 104 | LEU |
| 1 | B | 114 | ARG |
| 1 | B | 117 | GLU |
| 1 | B | 123 | ILE |
| 1 | B | 126 | ASP |
| 1 | B | 129 | LEU |
| 1 | B | 139 | TYR |
| 1 | B | 150 | ARG |
| 1 | B | 153 | ILE |
| 1 | B | 161 | LEU |
| 1 | B | 162 | LEU |
| 1 | B | 166 | LEU |
| 1 | B | 180 | LEU |
| 1 | B | 181 | GLU |
| 1 | B | 185 | ASN |
| 1 | B | 186 | TYR |
| 1 | B | 191 | LEU |
| 1 | B | 192 | THR |
| 1 | B | 199 | LEU |
| 1 | B | 216 | VAL |
| 1 | B | 225 | LEU |
| 1 | B | 236 | VAL |
| 1 | B | 247 | GLU |
| 1 | B | 248 | LEU |
| 1 | B | 249 | LEU |
| 1 | B | 274 | LEU |
| 1 | B | 275 | SER |
| 1 | B | 291 | ASN |
| 1 | B | 298 | SER |
| 1 | B | 301 | THR |
| 1 | B | 302 | LYS |
| 1 | B | 312 | ILE |
| 1 | B | 317 | LEU |
| 1 | B | 325 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 326 | ILE |
| 1 | B | 333 | TYR |
| 1 | B | 334 | LEU |
| 1 | B | 340 | VAL |
| 1 | B | 341 | VAL |
| 1 | B | 350 | PHE |
| 1 | B | 366 | ILE |
| 1 | B | 371 | VAL |
| 1 | B | 374 | GLU |
| 1 | B | 377 | ASP |
| 1 | B | 379 | ILE |
| 1 | B | 385 | THR |
| 1 | B | 407 | LEU |
| 1 | B | 414 | VAL |
| 1 | B | 415 | LYS |
| 1 | B | 418 | TYR |
| 1 | B | 422 | ARG |
| 1 | B | 424 | THR |
| 1 | B | 426 | GLU |
| 1 | B | 428 | LEU |
| 1 | B | 432 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 7 | GLN |
| 1 | A | 26 | ASN |
| 1 | A | 95 | GLN |
| 1 | A | 271 | HIS |
| 1 | A | 397 | HIS |
| 1 | B | 28 | GLN |
| 1 | B | 172 | HIS |
| 1 | B | 185 | ASN |
| 1 | B | 398 | HIS |
| 1 | B | 408 | GLN |
| 1 | B | 411 | HIS |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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 | $\#\|Z\| > 2$ |
| 3 | GOL | A | 454 | - | 5,5,5 | 0.32 | 0 | 5,5,5 | 0.33 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | GOL | A | 454 | - | - | 0/4/4/4 | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 454 | GOL | 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 | A | 417/471 (88%) | -0.16 | 10 (2%) 62 45 | 52, 103, 201, 270 | 0 |
| 1 | B | 414/471 (87%) | -0.11 | 9 (2%) 65 49 | 72, 130, 200, 374 | 0 |
| All | All | 831/942 (88%) | -0.13 | 19 (2%) 64 47 | 52, 118, 201, 374 | 0 |

All (19) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 34 | ASN | 6.5 |
| 1 | A | 301 | THR | 6.1 |
| 1 | B | 35 | SER | 4.9 |
| 1 | A | 338 | HIS | 3.1 |
| 1 | B | 318 | LEU | 3.0 |
| 1 | A | 402 | GLY | 3.0 |
| 1 | A | 30 | ARG | 2.9 |
| 1 | B | 325 | LEU | 2.8 |
| 1 | B | 322 | ILE | 2.7 |
| 1 | B | 300 | TYR | 2.6 |
| 1 | A | 26 | ASN | 2.6 |
| 1 | A | 66 | PHE | 2.3 |
| 1 | A | 344 | LYS | 2.3 |
| 1 | B | 370 | TYR | 2.3 |
| 1 | B | 437 | PRO | 2.3 |
| 1 | A | 403 | TYR | 2.1 |
| 1 | A | 326 | ILE | 2.1 |
| 1 | B | 266 | ILE | 2.0 |
| 1 | A | 426 | GLU | 2.0 |

## 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 (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ 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 | GOL | A | 454 | 6/6 | 0.80 | 0.86 | 13.80 | 95,114,126,129 | 0 |
| 2 | MN | A | 453 | 1/1 | 0.90 | 0.10 | - | 131,131,131,131 | 0 |
| 2 | MN | B | 453 | 1/1 | 0.29 | 0.26 | - | 235,235,235,235 | 0 |
| 2 | MN | B | 452 | 1/1 | 0.94 | 0.20 | - | 103,103,103,103 | 0 |
| 2 | MN | A | 452 | 1/1 | 0.99 | 0.28 | - | 93,93,93,93 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.