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

Feb 4, 2024 – 08:30 AM EST

| | | |
|---|---|---|
| PDB ID | : | 1PYP |
| Title | : | X-RAY DIFFRACTION STUDY OF INORGANIC PYROPHOSPHATASE FROM BAKER,S YEAST AT THE 3 ANGSTROMS RESOLUTION (RUSSIAN) |
| Authors | : | Harutyunyan, E.H.; Terzyan, S.S.; Vainshtein, B.K. |
| Deposited on | : | 1983-02-03 |
| 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

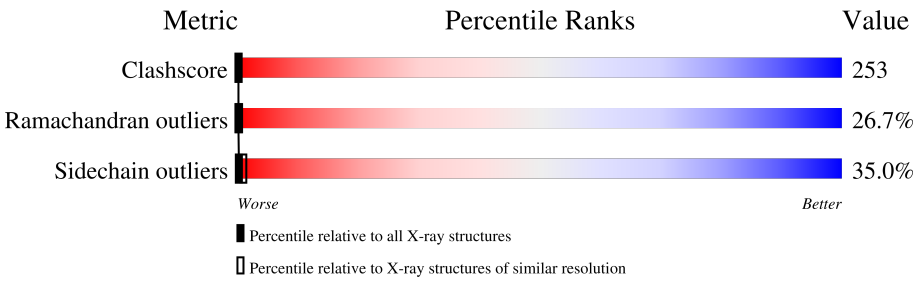
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 285 | 6% 38% 39% 16% • |
| 1 | B | 285 | 6% 38% 39% 16% • |

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4472 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 INORGANIC PYROPHOSPHATASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 281 | 2236 | 1435 | 369 | 429 | 3 | 0 | 0 | 1 |
| 1 | B | 281 | 2236 | 1435 | 369 | 429 | 3 | 0 | 0 | 1 |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 40 | ASP | ASN | conflict | UNP P00817 |
| A | 71 | ASN | ASP | conflict | UNP P00817 |
| A | ? | - | LYS | deletion | UNP P00817 |
| A | 116 | ASN | ASP | conflict | UNP P00817 |
| A | 122 | GLN | GLU | conflict | UNP P00817 |
| A | 135 | GLU | GLN | conflict | UNP P00817 |
| A | 185 | ASP | ASN | conflict | UNP P00817 |
| A | 223 | ASN | ASP | conflict | UNP P00817 |
| A | 265 | PRO | LEU | conflict | UNP P00817 |
| B | 40 | ASP | ASN | conflict | UNP P00817 |
| B | 71 | ASN | ASP | conflict | UNP P00817 |
| B | ? | - | LYS | deletion | UNP P00817 |
| B | 116 | ASN | ASP | conflict | UNP P00817 |
| B | 122 | GLN | GLU | conflict | UNP P00817 |
| B | 135 | GLU | GLN | conflict | UNP P00817 |
| B | 185 | ASP | ASN | conflict | UNP P00817 |
| B | 223 | ASN | ASP | conflict | UNP P00817 |
| B | 265 | PRO | LEU | conflict | UNP P00817 |

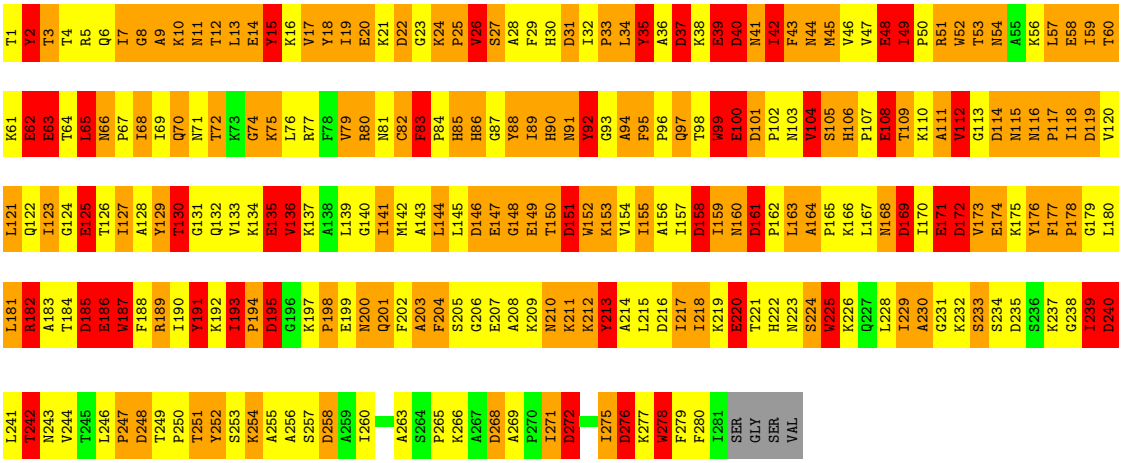
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

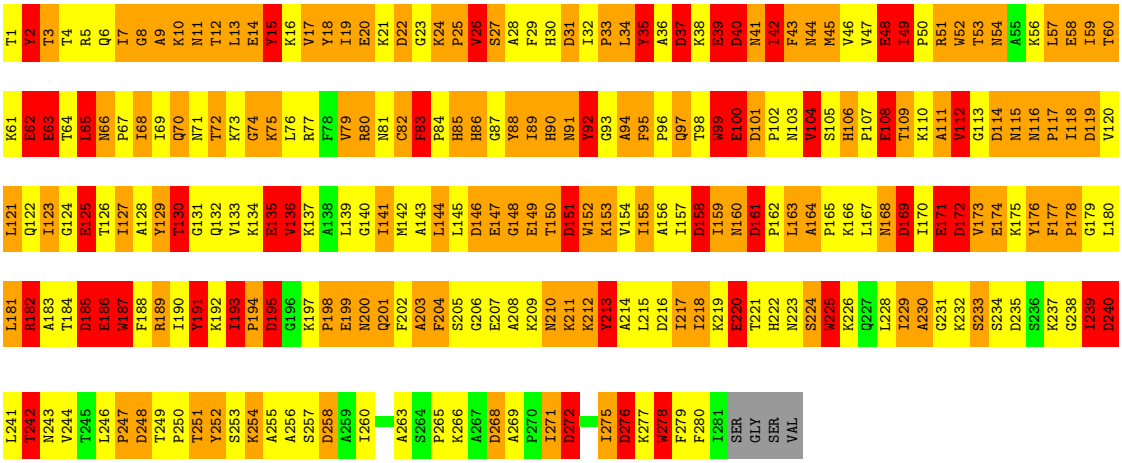
• Molecule 1: INORGANIC PYROPHOSPHATASE

Chain A: 6% 38% 39% 16%




• Molecule 1: INORGANIC PYROPHOSPHATASE

Chain B: 6% 38% 39% 16%



# 4 Data and refinement statistics (i)

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

| Property | Value | Source |
|---|---|---|
| Space group | P 1 1 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 52.23Å 70.29Å 95.47Å<br>90.00° 90.00° 99.59° | Depositor |
| Resolution (Å) | (Not available) – 3.00 | Depositor |
| % Data completeness<br>(in resolution range) | (Not available) ((Not available)-3.00) | Depositor |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| Refinement program | unknown | Depositor |
| R, $R_{free}$ | (Not available) , (Not available) | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 4472 | wwPDB-VP |
| Average B, all atoms ($Å^2$) | 0.0 | wwPDB-VP |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | 1.18 | 25/2295 (1.1%) | 1.40 | 72/3123 (2.3%) |
| 1 | B | 1.18 | 25/2295 (1.1%) | 1.40 | 72/3123 (2.3%) |
| All | All | 1.18 | 50/4590 (1.1%) | 1.40 | 144/6246 (2.3%) |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 225 | TRP | NE1-CE2 | -7.35 | 1.28 | 1.37 |
| 1 | A | 278 | TRP | NE1-CE2 | -7.34 | 1.28 | 1.37 |
| 1 | B | 278 | TRP | NE1-CE2 | -7.34 | 1.28 | 1.37 |
| 1 | A | 99 | TRP | NE1-CE2 | -7.34 | 1.28 | 1.37 |
| 1 | B | 99 | TRP | NE1-CE2 | -7.33 | 1.28 | 1.37 |
| 1 | B | 225 | TRP | NE1-CE2 | -7.31 | 1.28 | 1.37 |
| 1 | B | 187 | TRP | NE1-CE2 | -7.30 | 1.28 | 1.37 |
| 1 | A | 152 | TRP | NE1-CE2 | -7.29 | 1.28 | 1.37 |
| 1 | A | 187 | TRP | NE1-CE2 | -7.28 | 1.28 | 1.37 |
| 1 | B | 52 | TRP | NE1-CE2 | -7.28 | 1.28 | 1.37 |
| 1 | A | 52 | TRP | NE1-CE2 | -7.26 | 1.28 | 1.37 |
| 1 | B | 152 | TRP | NE1-CE2 | -7.26 | 1.28 | 1.37 |
| 1 | B | 220 | GLU | CD-OE1 | -5.29 | 1.19 | 1.25 |
| 1 | A | 220 | GLU | CD-OE1 | -5.27 | 1.19 | 1.25 |
| 1 | B | 62 | GLU | CD-OE1 | -5.25 | 1.19 | 1.25 |
| 1 | B | 48 | GLU | CD-OE1 | -5.22 | 1.20 | 1.25 |
| 1 | A | 174 | GLU | CD-OE1 | -5.22 | 1.20 | 1.25 |
| 1 | B | 20 | GLU | CD-OE1 | -5.22 | 1.20 | 1.25 |
| 1 | B | 125 | GLU | CD-OE1 | -5.22 | 1.20 | 1.25 |
| 1 | B | 186 | GLU | CD-OE1 | -5.22 | 1.20 | 1.25 |
| 1 | A | 62 | GLU | CD-OE1 | -5.22 | 1.20 | 1.25 |
| 1 | A | 20 | GLU | CD-OE1 | -5.21 | 1.20 | 1.25 |
| 1 | A | 186 | GLU | CD-OE1 | -5.21 | 1.20 | 1.25 |
| 1 | B | 199 | GLU | CD-OE1 | -5.21 | 1.20 | 1.25 |
| 1 | A | 48 | GLU | CD-OE1 | -5.21 | 1.20 | 1.25 |
| 1 | A | 199 | GLU | CD-OE1 | -5.21 | 1.20 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 174 | GLU | CD-OE1 | -5.21 | 1.20 | 1.25 |
| 1 | B | 147 | GLU | CD-OE1 | -5.20 | 1.20 | 1.25 |
| 1 | A | 149 | GLU | CD-OE1 | -5.20 | 1.20 | 1.25 |
| 1 | A | 125 | GLU | CD-OE1 | -5.20 | 1.20 | 1.25 |
| 1 | A | 207 | GLU | CD-OE1 | -5.20 | 1.20 | 1.25 |
| 1 | B | 149 | GLU | CD-OE1 | -5.19 | 1.20 | 1.25 |
| 1 | A | 100 | GLU | CD-OE1 | -5.19 | 1.20 | 1.25 |
| 1 | A | 147 | GLU | CD-OE1 | -5.19 | 1.20 | 1.25 |
| 1 | B | 63 | GLU | CD-OE1 | -5.19 | 1.20 | 1.25 |
| 1 | B | 14 | GLU | CD-OE1 | -5.18 | 1.20 | 1.25 |
| 1 | A | 39 | GLU | CD-OE1 | -5.17 | 1.20 | 1.25 |
| 1 | B | 100 | GLU | CD-OE1 | -5.17 | 1.20 | 1.25 |
| 1 | B | 108 | GLU | CD-OE1 | -5.17 | 1.20 | 1.25 |
| 1 | B | 135 | GLU | CD-OE1 | -5.17 | 1.20 | 1.25 |
| 1 | B | 39 | GLU | CD-OE1 | -5.17 | 1.20 | 1.25 |
| 1 | B | 207 | GLU | CD-OE1 | -5.17 | 1.20 | 1.25 |
| 1 | A | 63 | GLU | CD-OE1 | -5.16 | 1.20 | 1.25 |
| 1 | A | 108 | GLU | CD-OE1 | -5.16 | 1.20 | 1.25 |
| 1 | A | 14 | GLU | CD-OE1 | -5.16 | 1.20 | 1.25 |
| 1 | A | 58 | GLU | CD-OE1 | -5.16 | 1.20 | 1.25 |
| 1 | A | 135 | GLU | CD-OE1 | -5.15 | 1.20 | 1.25 |
| 1 | B | 171 | GLU | CD-OE1 | -5.13 | 1.20 | 1.25 |
| 1 | A | 171 | GLU | CD-OE1 | -5.13 | 1.20 | 1.25 |
| 1 | B | 58 | GLU | CD-OE1 | -5.11 | 1.20 | 1.25 |

All (144) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 172 | ASP | CB-CG-OD1 | 7.35 | 124.92 | 118.30 |
| 1 | A | 172 | ASP | CB-CG-OD1 | 7.35 | 124.91 | 118.30 |
| 1 | B | 169 | ASP | CB-CG-OD1 | 7.34 | 124.91 | 118.30 |
| 1 | A | 158 | ASP | CB-CG-OD1 | 7.33 | 124.90 | 118.30 |
| 1 | B | 22 | ASP | CB-CG-OD1 | 7.32 | 124.89 | 118.30 |
| 1 | B | 101 | ASP | CB-CG-OD1 | 7.32 | 124.89 | 118.30 |
| 1 | B | 258 | ASP | CB-CG-OD1 | 7.32 | 124.89 | 118.30 |
| 1 | A | 272 | ASP | CB-CG-OD1 | 7.32 | 124.88 | 118.30 |
| 1 | A | 258 | ASP | CB-CG-OD1 | 7.31 | 124.88 | 118.30 |
| 1 | B | 235 | ASP | CB-CG-OD1 | 7.31 | 124.88 | 118.30 |
| 1 | B | 268 | ASP | CB-CG-OD1 | 7.31 | 124.88 | 118.30 |
| 1 | A | 169 | ASP | CB-CG-OD1 | 7.31 | 124.88 | 118.30 |
| 1 | B | 151 | ASP | CB-CG-OD1 | 7.31 | 124.88 | 118.30 |
| 1 | A | 151 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 146 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | A | 195 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | A | 235 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | A | 22 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | A | 276 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | B | 37 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | A | 40 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | A | 101 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | B | 195 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | B | 119 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | A | 37 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | A | 185 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | A | 216 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | A | 268 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | B | 216 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | B | 158 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | B | 272 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | B | 276 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | A | 248 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | A | 114 | ASP | CB-CG-OD1 | 7.28 | 124.85 | 118.30 |
| 1 | A | 161 | ASP | CB-CG-OD1 | 7.28 | 124.85 | 118.30 |
| 1 | B | 161 | ASP | CB-CG-OD1 | 7.28 | 124.85 | 118.30 |
| 1 | B | 40 | ASP | CB-CG-OD1 | 7.27 | 124.85 | 118.30 |
| 1 | B | 185 | ASP | CB-CG-OD1 | 7.27 | 124.84 | 118.30 |
| 1 | A | 146 | ASP | CB-CG-OD1 | 7.27 | 124.84 | 118.30 |
| 1 | B | 248 | ASP | CB-CG-OD1 | 7.26 | 124.84 | 118.30 |
| 1 | B | 240 | ASP | CB-CG-OD1 | 7.26 | 124.83 | 118.30 |
| 1 | B | 114 | ASP | CB-CG-OD1 | 7.25 | 124.83 | 118.30 |
| 1 | A | 240 | ASP | CB-CG-OD1 | 7.25 | 124.83 | 118.30 |
| 1 | A | 119 | ASP | CB-CG-OD1 | 7.25 | 124.82 | 118.30 |
| 1 | A | 31 | ASP | CB-CG-OD1 | 7.24 | 124.82 | 118.30 |
| 1 | B | 31 | ASP | CB-CG-OD1 | 7.23 | 124.80 | 118.30 |
| 1 | B | 62 | GLU | OE1-CD-OE2 | 5.86 | 130.34 | 123.30 |
| 1 | B | 207 | GLU | OE1-CD-OE2 | 5.84 | 130.31 | 123.30 |
| 1 | A | 207 | GLU | OE1-CD-OE2 | 5.82 | 130.29 | 123.30 |
| 1 | A | 20 | GLU | OE1-CD-OE2 | 5.82 | 130.28 | 123.30 |
| 1 | A | 62 | GLU | OE1-CD-OE2 | 5.82 | 130.28 | 123.30 |
| 1 | B | 135 | GLU | OE1-CD-OE2 | 5.81 | 130.27 | 123.30 |
| 1 | B | 186 | GLU | OE1-CD-OE2 | 5.80 | 130.27 | 123.30 |
| 1 | B | 63 | GLU | OE1-CD-OE2 | 5.80 | 130.26 | 123.30 |
| 1 | A | 186 | GLU | OE1-CD-OE2 | 5.80 | 130.26 | 123.30 |
| 1 | A | 220 | GLU | OE1-CD-OE2 | 5.80 | 130.26 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 58 | GLU | OE1-CD-OE2 | 5.80 | 130.26 | 123.30 |
| 1 | A | 135 | GLU | OE1-CD-OE2 | 5.80 | 130.26 | 123.30 |
| 1 | B | 149 | GLU | OE1-CD-OE2 | 5.80 | 130.26 | 123.30 |
| 1 | B | 20 | GLU | OE1-CD-OE2 | 5.79 | 130.25 | 123.30 |
| 1 | B | 220 | GLU | OE1-CD-OE2 | 5.79 | 130.25 | 123.30 |
| 1 | B | 14 | GLU | OE1-CD-OE2 | 5.79 | 130.25 | 123.30 |
| 1 | A | 14 | GLU | OE1-CD-OE2 | 5.78 | 130.24 | 123.30 |
| 1 | B | 147 | GLU | OE1-CD-OE2 | 5.78 | 130.24 | 123.30 |
| 1 | A | 63 | GLU | OE1-CD-OE2 | 5.77 | 130.23 | 123.30 |
| 1 | A | 147 | GLU | OE1-CD-OE2 | 5.77 | 130.23 | 123.30 |
| 1 | A | 149 | GLU | OE1-CD-OE2 | 5.77 | 130.22 | 123.30 |
| 1 | A | 48 | GLU | OE1-CD-OE2 | 5.77 | 130.22 | 123.30 |
| 1 | A | 171 | GLU | OE1-CD-OE2 | 5.77 | 130.22 | 123.30 |
| 1 | A | 174 | GLU | OE1-CD-OE2 | 5.77 | 130.22 | 123.30 |
| 1 | B | 48 | GLU | OE1-CD-OE2 | 5.76 | 130.22 | 123.30 |
| 1 | A | 125 | GLU | OE1-CD-OE2 | 5.76 | 130.21 | 123.30 |
| 1 | B | 58 | GLU | OE1-CD-OE2 | 5.76 | 130.21 | 123.30 |
| 1 | B | 39 | GLU | OE1-CD-OE2 | 5.76 | 130.21 | 123.30 |
| 1 | A | 39 | GLU | OE1-CD-OE2 | 5.76 | 130.21 | 123.30 |
| 1 | A | 100 | GLU | OE1-CD-OE2 | 5.76 | 130.21 | 123.30 |
| 1 | B | 174 | GLU | OE1-CD-OE2 | 5.76 | 130.21 | 123.30 |
| 1 | A | 199 | GLU | OE1-CD-OE2 | 5.74 | 130.18 | 123.30 |
| 1 | A | 108 | GLU | OE1-CD-OE2 | 5.74 | 130.18 | 123.30 |
| 1 | B | 199 | GLU | OE1-CD-OE2 | 5.74 | 130.18 | 123.30 |
| 1 | B | 100 | GLU | OE1-CD-OE2 | 5.73 | 130.18 | 123.30 |
| 1 | B | 108 | GLU | OE1-CD-OE2 | 5.73 | 130.17 | 123.30 |
| 1 | B | 125 | GLU | OE1-CD-OE2 | 5.72 | 130.16 | 123.30 |
| 1 | B | 171 | GLU | OE1-CD-OE2 | 5.71 | 130.15 | 123.30 |
| 1 | B | 62 | GLU | CG-CD-OE2 | -5.20 | 107.91 | 118.30 |
| 1 | B | 220 | GLU | CG-CD-OE2 | -5.17 | 107.95 | 118.30 |
| 1 | B | 39 | GLU | CG-CD-OE2 | -5.17 | 107.95 | 118.30 |
| 1 | A | 20 | GLU | CG-CD-OE2 | -5.17 | 107.96 | 118.30 |
| 1 | B | 35 | TYR | CB-CG-CD1 | -5.17 | 117.90 | 121.00 |
| 1 | B | 174 | GLU | CG-CD-OE2 | -5.17 | 107.96 | 118.30 |
| 1 | A | 186 | GLU | CG-CD-OE2 | -5.17 | 107.96 | 118.30 |
| 1 | A | 62 | GLU | CG-CD-OE2 | -5.17 | 107.96 | 118.30 |
| 1 | A | 220 | GLU | CG-CD-OE2 | -5.17 | 107.96 | 118.30 |
| 1 | B | 135 | GLU | CG-CD-OE2 | -5.17 | 107.97 | 118.30 |
| 1 | B | 147 | GLU | CG-CD-OE2 | -5.16 | 107.97 | 118.30 |
| 1 | B | 20 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | A | 39 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | A | 171 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 174 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | B | 14 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | B | 48 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | B | 63 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | B | 125 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | B | 186 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | A | 58 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | A | 63 | GLU | CG-CD-OE2 | -5.16 | 107.98 | 118.30 |
| 1 | A | 207 | GLU | CG-CD-OE2 | -5.16 | 107.99 | 118.30 |
| 1 | A | 48 | GLU | CG-CD-OE2 | -5.16 | 107.99 | 118.30 |
| 1 | A | 147 | GLU | CG-CD-OE2 | -5.16 | 107.99 | 118.30 |
| 1 | B | 171 | GLU | CG-CD-OE2 | -5.16 | 107.99 | 118.30 |
| 1 | A | 125 | GLU | CG-CD-OE2 | -5.15 | 108.00 | 118.30 |
| 1 | A | 135 | GLU | CG-CD-OE2 | -5.15 | 108.00 | 118.30 |
| 1 | B | 108 | GLU | CG-CD-OE2 | -5.15 | 108.00 | 118.30 |
| 1 | A | 14 | GLU | CG-CD-OE2 | -5.15 | 108.01 | 118.30 |
| 1 | B | 207 | GLU | CG-CD-OE2 | -5.15 | 108.01 | 118.30 |
| 1 | B | 58 | GLU | CG-CD-OE2 | -5.14 | 108.01 | 118.30 |
| 1 | A | 199 | GLU | CG-CD-OE2 | -5.14 | 108.02 | 118.30 |
| 1 | B | 199 | GLU | CG-CD-OE2 | -5.14 | 108.03 | 118.30 |
| 1 | B | 2 | TYR | CB-CG-CD1 | -5.13 | 117.92 | 121.00 |
| 1 | A | 108 | GLU | CG-CD-OE2 | -5.13 | 108.04 | 118.30 |
| 1 | A | 100 | GLU | CG-CD-OE2 | -5.13 | 108.04 | 118.30 |
| 1 | A | 149 | GLU | CG-CD-OE2 | -5.13 | 108.04 | 118.30 |
| 1 | B | 149 | GLU | CG-CD-OE2 | -5.12 | 108.05 | 118.30 |
| 1 | A | 191 | TYR | CB-CG-CD1 | -5.12 | 117.93 | 121.00 |
| 1 | B | 191 | TYR | CB-CG-CD1 | -5.12 | 117.93 | 121.00 |
| 1 | A | 92 | TYR | CB-CG-CD1 | -5.11 | 117.93 | 121.00 |
| 1 | B | 92 | TYR | CB-CG-CD1 | -5.11 | 117.94 | 121.00 |
| 1 | B | 100 | GLU | CG-CD-OE2 | -5.11 | 108.08 | 118.30 |
| 1 | A | 35 | TYR | CB-CG-CD1 | -5.11 | 117.94 | 121.00 |
| 1 | A | 213 | TYR | CB-CG-CD1 | -5.10 | 117.94 | 121.00 |
| 1 | A | 252 | TYR | CB-CG-CD1 | -5.10 | 117.94 | 121.00 |
| 1 | B | 88 | TYR | CB-CG-CD1 | -5.10 | 117.94 | 121.00 |
| 1 | A | 18 | TYR | CB-CG-CD1 | -5.09 | 117.94 | 121.00 |
| 1 | A | 2 | TYR | CB-CG-CD1 | -5.09 | 117.94 | 121.00 |
| 1 | B | 213 | TYR | CB-CG-CD1 | -5.09 | 117.95 | 121.00 |
| 1 | B | 129 | TYR | CB-CG-CD1 | -5.06 | 117.97 | 121.00 |
| 1 | B | 176 | TYR | CB-CG-CD1 | -5.05 | 117.97 | 121.00 |
| 1 | A | 176 | TYR | CB-CG-CD1 | -5.05 | 117.97 | 121.00 |
| 1 | B | 18 | TYR | CB-CG-CD1 | -5.05 | 117.97 | 121.00 |
| 1 | A | 88 | TYR | CB-CG-CD1 | -5.04 | 117.98 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 252 | TYR | CB-CG-CD1 | -5.03 | 117.98 | 121.00 |
| 1 | A | 129 | TYR | CB-CG-CD1 | -5.02 | 117.99 | 121.00 |
| 1 | B | 15 | TYR | CB-CG-CD1 | -5.02 | 117.99 | 121.00 |
| 1 | A | 15 | TYR | CB-CG-CD1 | -5.01 | 117.99 | 121.00 |

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 | A | 2236 | 0 | 2198 | 1132 | 10 |
| 1 | B | 2236 | 0 | 2198 | 1138 | 13 |
| All | All | 4472 | 0 | 4396 | 2241 | 13 |

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 253.

All (2241) 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:1:THR:HG21 | 1:B:19:ILE:CD1 | 1.22 | 1.68 |
| 1:B:19:ILE:CD1 | 1:B:26:VAL:HG11 | 1.27 | 1.64 |
| 1:A:1:THR:HG21 | 1:A:19:ILE:CD1 | 1.22 | 1.62 |
| 1:B:9:ALA:CB | 1:B:15:TYR:HB2 | 1.19 | 1.61 |
| 1:B:42:ILE:HD12 | 1:B:159:ILE:CD1 | 1.29 | 1.60 |
| 1:A:190:ILE:HA | 1:A:193:ILE:CG1 | 1.25 | 1.60 |
| 1:A:9:ALA:CB | 1:A:15:TYR:HB2 | 1.19 | 1.59 |
| 1:B:190:ILE:HA | 1:B:193:ILE:CG1 | 1.25 | 1.59 |
| 1:A:19:ILE:CD1 | 1:A:26:VAL:HG11 | 1.27 | 1.58 |
| 1:A:105:SER:CB | 1:A:112:VAL:HA | 1.33 | 1.56 |
| 1:A:42:ILE:HD12 | 1:A:159:ILE:CD1 | 1.29 | 1.56 |
| 1:B:1:THR:CG2 | 1:B:19:ILE:HD11 | 1.09 | 1.55 |
| 1:B:123:ILE:HD11 | 1:B:177:PHE:CE2 | 1.05 | 1.55 |
| 1:B:9:ALA:HB3 | 1:B:15:TYR:CB | 1.33 | 1.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:98:THR:HG23 | 1:B:221:THR:C | 1.22 | 1.54 |
| 1:A:123:ILE:HD11 | 1:A:177:PHE:CE2 | 1.05 | 1.54 |
| 1:A:1:THR:CG2 | 1:A:19:ILE:HD11 | 1.09 | 1.53 |
| 1:B:105:SER:CB | 1:B:112:VAL:HA | 1.33 | 1.53 |
| 1:A:95:PHE:CE2 | 1:A:218:ILE:HD11 | 1.45 | 1.52 |
| 1:B:222:HIS:NE2 | 1:B:226:LYS:CE | 1.72 | 1.52 |
| 1:A:5:ARG:NH1 | 1:A:260:ILE:CG2 | 1.72 | 1.51 |
| 1:A:222:HIS:NE2 | 1:A:226:LYS:CE | 1.72 | 1.50 |
| 1:B:95:PHE:CE2 | 1:B:218:ILE:HD11 | 1.45 | 1.50 |
| 1:A:98:THR:HG23 | 1:A:221:THR:C | 1.22 | 1.50 |
| 1:A:9:ALA:HB3 | 1:A:15:TYR:CB | 1.33 | 1.49 |
| 1:A:19:ILE:HD13 | 1:A:26:VAL:CG1 | 1.43 | 1.49 |
| 1:B:5:ARG:NH1 | 1:B:260:ILE:CG2 | 1.72 | 1.48 |
| 1:B:19:ILE:HD13 | 1:B:26:VAL:CG1 | 1.43 | 1.48 |
| 1:A:5:ARG:HH12 | 1:A:260:ILE:CG2 | 1.24 | 1.46 |
| 1:B:98:THR:CG2 | 1:B:221:THR:OG1 | 1.63 | 1.46 |
| 1:A:123:ILE:CD1 | 1:A:177:PHE:CE2 | 1.99 | 1.45 |
| 1:A:98:THR:CG2 | 1:A:221:THR:OG1 | 1.63 | 1.44 |
| 1:A:1:THR:CG2 | 1:A:19:ILE:CD1 | 1.81 | 1.44 |
| 1:A:139:LEU:HB2 | 1:A:155:ILE:CG2 | 1.47 | 1.44 |
| 1:B:139:LEU:HB2 | 1:B:155:ILE:CG2 | 1.47 | 1.44 |
| 1:B:123:ILE:CD1 | 1:B:177:PHE:CE2 | 1.99 | 1.42 |
| 1:B:49:ILE:CD1 | 1:B:92:TYR:CD1 | 2.03 | 1.42 |
| 1:B:5:ARG:HH12 | 1:B:260:ILE:CG2 | 1.24 | 1.42 |
| 1:A:123:ILE:CD1 | 1:A:177:PHE:CD2 | 2.03 | 1.40 |
| 1:B:123:ILE:CD1 | 1:B:177:PHE:CD2 | 2.03 | 1.40 |
| 1:A:49:ILE:CD1 | 1:A:92:TYR:CD1 | 2.03 | 1.40 |
| 1:B:123:ILE:HD11 | 1:B:177:PHE:CD2 | 1.55 | 1.39 |
| 1:A:7:ILE:CG2 | 1:A:16:LYS:H | 1.37 | 1.38 |
| 1:A:80:ARG:HD2 | 1:A:279:PHE:CE1 | 1.59 | 1.37 |
| 1:B:80:ARG:HD2 | 1:B:279:PHE:CE1 | 1.59 | 1.37 |
| 1:A:123:ILE:HD11 | 1:A:177:PHE:CD2 | 1.55 | 1.37 |
| 1:B:1:THR:CG2 | 1:B:19:ILE:CD1 | 1.81 | 1.36 |
| 1:B:23:GLY:O | 1:B:24:LYS:CG | 1.73 | 1.36 |
| 1:A:174:GLU:O | 1:A:178:PRO:CB | 1.74 | 1.35 |
| 1:B:5:ARG:NH1 | 1:B:260:ILE:HG21 | 1.02 | 1.35 |
| 1:B:83:PHE:CD1 | 1:B:280:PHE:CE2 | 2.15 | 1.35 |
| 1:A:105:SER:HB3 | 1:A:112:VAL:CA | 1.58 | 1.34 |
| 1:B:7:ILE:CG2 | 1:B:16:LYS:H | 1.37 | 1.34 |
| 1:A:83:PHE:CD1 | 1:A:280:PHE:CE2 | 2.15 | 1.34 |
| 1:A:23:GLY:O | 1:A:24:LYS:CG | 1.73 | 1.33 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:105:SER:HB3 | 1:B:112:VAL:CA | 1.58 | 1.33 |
| 1:A:5:ARG:NH1 | 1:A:260:ILE:HG21 | 1.02 | 1.33 |
| 1:A:277:LYS:CE | 1:B:125:GLU:OE2 | 1.77 | 1.32 |
| 1:B:49:ILE:HD11 | 1:B:92:TYR:CD1 | 1.64 | 1.32 |
| 1:A:74:GLY:O | 1:A:75:LYS:CG | 1.77 | 1.32 |
| 1:B:112:VAL:O | 1:B:150:THR:CB | 1.77 | 1.32 |
| 1:B:59:ILE:HG22 | 1:B:67:PRO:N | 1.43 | 1.32 |
| 1:B:98:THR:HG21 | 1:B:221:THR:CB | 1.60 | 1.32 |
| 1:A:59:ILE:HG22 | 1:A:67:PRO:N | 1.43 | 1.31 |
| 1:B:74:GLY:O | 1:B:75:LYS:CG | 1.77 | 1.31 |
| 1:A:142:MET:CE | 1:A:202:PHE:CZ | 2.14 | 1.31 |
| 1:B:142:MET:CE | 1:B:202:PHE:CZ | 2.14 | 1.31 |
| 1:B:174:GLU:O | 1:B:178:PRO:CB | 1.74 | 1.31 |
| 1:A:52:TRP:N | 1:A:88:TYR:O | 1.64 | 1.30 |
| 1:A:98:THR:HG21 | 1:A:221:THR:CB | 1.60 | 1.30 |
| 1:A:125:GLU:OE2 | 1:B:277:LYS:CE | 1.77 | 1.30 |
| 1:A:112:VAL:O | 1:A:150:THR:CB | 1.77 | 1.29 |
| 1:B:52:TRP:N | 1:B:88:TYR:O | 1.64 | 1.29 |
| 1:A:57:LEU:CA | 1:A:68:ILE:O | 1.80 | 1.28 |
| 1:B:42:ILE:CG1 | 1:B:43:PHE:H | 1.43 | 1.28 |
| 1:B:112:VAL:O | 1:B:150:THR:HB | 1.11 | 1.28 |
| 1:A:53:THR:O | 1:A:88:TYR:HB2 | 1.30 | 1.28 |
| 1:A:82:CYS:SG | 1:A:190:ILE:HG13 | 1.73 | 1.28 |
| 1:B:82:CYS:SG | 1:B:190:ILE:HG13 | 1.73 | 1.28 |
| 1:A:27:SER:CA | 1:A:64:THR:HG23 | 1.62 | 1.28 |
| 1:B:53:THR:O | 1:B:88:TYR:HB2 | 1.30 | 1.28 |
| 1:A:42:ILE:CG1 | 1:A:43:PHE:H | 1.44 | 1.28 |
| 1:A:190:ILE:CA | 1:A:193:ILE:CG1 | 2.12 | 1.27 |
| 1:B:27:SER:CA | 1:B:64:THR:HG23 | 1.62 | 1.27 |
| 1:B:83:PHE:CE1 | 1:B:280:PHE:CE2 | 2.22 | 1.27 |
| 1:A:58:GLU:HG3 | 1:A:70:GLN:NE2 | 1.48 | 1.27 |
| 1:A:49:ILE:HD11 | 1:A:92:TYR:CD1 | 1.64 | 1.27 |
| 1:B:57:LEU:CA | 1:B:68:ILE:O | 1.80 | 1.26 |
| 1:A:112:VAL:O | 1:A:150:THR:HB | 1.11 | 1.26 |
| 1:A:83:PHE:CE1 | 1:A:280:PHE:CE2 | 2.22 | 1.26 |
| 1:B:58:GLU:HG3 | 1:B:70:GLN:NE2 | 1.48 | 1.26 |
| 1:B:142:MET:O | 1:B:153:LYS:N | 1.68 | 1.25 |
| 1:B:190:ILE:CA | 1:B:193:ILE:CG1 | 2.12 | 1.25 |
| 1:A:98:THR:HG23 | 1:A:221:THR:O | 1.14 | 1.25 |
| 1:B:7:ILE:CG2 | 1:B:7:ILE:O | 1.83 | 1.24 |
| 1:B:32:ILE:O | 1:B:97:GLN:HG3 | 1.38 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:49:ILE:HD12 | 1:A:92:TYR:CG | 1.73 | 1.24 |
| 1:A:142:MET:O | 1:A:153:LYS:N | 1.68 | 1.24 |
| 1:A:164:ALA:HB3 | 1:A:165:PRO:CD | 1.68 | 1.23 |
| 1:B:98:THR:HG23 | 1:B:221:THR:O | 1.14 | 1.23 |
| 1:B:218:ILE:O | 1:B:221:THR:HG22 | 1.05 | 1.23 |
| 1:A:27:SER:HA | 1:A:64:THR:CG2 | 1.68 | 1.23 |
| 1:B:192:LYS:HB3 | 1:B:197:LYS:CB | 1.67 | 1.23 |
| 1:A:42:ILE:CG2 | 1:A:137:LYS:HG2 | 1.69 | 1.22 |
| 1:A:9:ALA:CB | 1:A:15:TYR:CB | 1.99 | 1.22 |
| 1:B:27:SER:HA | 1:B:64:THR:CG2 | 1.68 | 1.22 |
| 1:A:192:LYS:HB3 | 1:A:197:LYS:CB | 1.67 | 1.22 |
| 1:B:164:ALA:HB3 | 1:B:165:PRO:CD | 1.68 | 1.22 |
| 1:A:163:LEU:CD2 | 1:A:176:TYR:HD2 | 1.53 | 1.22 |
| 1:B:49:ILE:HD12 | 1:B:92:TYR:CG | 1.73 | 1.21 |
| 1:A:32:ILE:O | 1:A:97:GLN:HG3 | 1.38 | 1.21 |
| 1:B:42:ILE:CG2 | 1:B:137:LYS:HG2 | 1.69 | 1.21 |
| 1:A:100:GLU:O | 1:A:114:ASP:O | 1.58 | 1.21 |
| 1:A:7:ILE:CG2 | 1:A:7:ILE:O | 1.83 | 1.21 |
| 1:A:218:ILE:O | 1:A:221:THR:HG22 | 1.05 | 1.21 |
| 1:B:9:ALA:CB | 1:B:15:TYR:CB | 1.99 | 1.20 |
| 1:B:222:HIS:NE2 | 1:B:226:LYS:HE3 | 1.37 | 1.20 |
| 1:A:38:LYS:CG | 1:A:41:ASN:HB2 | 1.73 | 1.19 |
| 1:B:163:LEU:CD2 | 1:B:176:TYR:HD2 | 1.53 | 1.19 |
| 1:A:193:ILE:HB | 1:A:194:PRO:HD3 | 1.19 | 1.19 |
| 1:B:142:MET:HE3 | 1:B:202:PHE:CE1 | 1.77 | 1.19 |
| 1:A:222:HIS:NE2 | 1:A:226:LYS:HE3 | 1.37 | 1.19 |
| 1:B:49:ILE:HD12 | 1:B:92:TYR:CD1 | 1.73 | 1.19 |
| 1:A:218:ILE:O | 1:A:221:THR:CG2 | 1.91 | 1.18 |
| 1:B:27:SER:CB | 1:B:64:THR:HG23 | 1.73 | 1.18 |
| 1:B:218:ILE:O | 1:B:221:THR:CG2 | 1.91 | 1.18 |
| 1:B:190:ILE:HA | 1:B:193:ILE:CD1 | 1.75 | 1.17 |
| 1:A:27:SER:CB | 1:A:64:THR:HG23 | 1.73 | 1.17 |
| 1:B:98:THR:CG2 | 1:B:221:THR:C | 2.12 | 1.17 |
| 1:B:100:GLU:O | 1:B:114:ASP:O | 1.58 | 1.17 |
| 1:A:5:ARG:NH2 | 1:A:25:PRO:HB3 | 1.59 | 1.17 |
| 1:A:51:ARG:HG2 | 1:A:89:ILE:HA | 1.26 | 1.17 |
| 1:B:9:ALA:HB1 | 1:B:15:TYR:HB2 | 1.21 | 1.17 |
| 1:A:7:ILE:HG21 | 1:A:16:LYS:H | 1.02 | 1.17 |
| 1:B:10:LYS:HG3 | 1:B:268:ASP:OD2 | 1.44 | 1.17 |
| 1:A:10:LYS:HG3 | 1:A:268:ASP:OD2 | 1.44 | 1.17 |
| 1:A:98:THR:CG2 | 1:A:221:THR:C | 2.12 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:38:LYS:CG | 1:B:41:ASN:HB2 | 1.73 | 1.17 |
| 1:B:142:MET:HE3 | 1:B:202:PHE:CZ | 1.77 | 1.17 |
| 1:A:49:ILE:HD12 | 1:A:92:TYR:CD1 | 1.73 | 1.16 |
| 1:A:163:LEU:HD21 | 1:A:176:TYR:HD2 | 1.07 | 1.16 |
| 1:A:190:ILE:HA | 1:A:193:ILE:CD1 | 1.75 | 1.16 |
| 1:A:42:ILE:HG13 | 1:A:136:VAL:O | 1.00 | 1.16 |
| 1:A:42:ILE:HG12 | 1:A:43:PHE:N | 1.14 | 1.16 |
| 1:B:74:GLY:O | 1:B:75:LYS:HG3 | 1.00 | 1.16 |
| 1:A:74:GLY:O | 1:A:75:LYS:HG3 | 1.00 | 1.15 |
| 1:A:164:ALA:HB3 | 1:A:165:PRO:HD3 | 1.26 | 1.15 |
| 1:A:7:ILE:HB | 1:A:16:LYS:O | 1.47 | 1.15 |
| 1:B:5:ARG:NH2 | 1:B:25:PRO:HB3 | 1.59 | 1.15 |
| 1:B:110:LYS:O | 1:B:112:VAL:N | 1.80 | 1.15 |
| 1:A:110:LYS:O | 1:A:112:VAL:N | 1.80 | 1.15 |
| 1:B:193:ILE:HB | 1:B:194:PRO:HD3 | 1.19 | 1.15 |
| 1:A:83:PHE:CD1 | 1:A:280:PHE:CD2 | 2.35 | 1.14 |
| 1:B:34:LEU:O | 1:B:43:PHE:HB3 | 1.46 | 1.14 |
| 1:B:97:GLN:OE1 | 1:B:222:HIS:CE1 | 2.00 | 1.14 |
| 1:B:174:GLU:O | 1:B:178:PRO:HB3 | 0.96 | 1.14 |
| 1:A:27:SER:HA | 1:A:64:THR:HG23 | 1.14 | 1.14 |
| 1:A:34:LEU:O | 1:A:43:PHE:HB3 | 1.46 | 1.14 |
| 1:A:97:GLN:OE1 | 1:A:222:HIS:CE1 | 2.00 | 1.14 |
| 1:B:42:ILE:HG13 | 1:B:136:VAL:O | 1.00 | 1.14 |
| 1:B:190:ILE:CA | 1:B:193:ILE:HG13 | 1.76 | 1.14 |
| 1:A:5:ARG:HB3 | 1:A:263:ALA:HB2 | 1.20 | 1.14 |
| 1:B:26:VAL:CG2 | 1:B:27:SER:H | 1.57 | 1.14 |
| 1:A:26:VAL:CG2 | 1:A:27:SER:H | 1.57 | 1.14 |
| 1:A:127:ILE:HG22 | 1:A:128:ALA:N | 1.49 | 1.14 |
| 1:B:83:PHE:CD1 | 1:B:280:PHE:CD2 | 2.35 | 1.14 |
| 1:B:163:LEU:HD21 | 1:B:176:TYR:HD2 | 1.07 | 1.14 |
| 1:A:42:ILE:CG1 | 1:A:136:VAL:O | 1.95 | 1.13 |
| 1:A:69:ILE:O | 1:A:70:GLN:O | 1.65 | 1.13 |
| 1:A:142:MET:CB | 1:A:153:LYS:HB2 | 1.78 | 1.13 |
| 1:A:193:ILE:HB | 1:A:194:PRO:CD | 1.76 | 1.13 |
| 1:A:139:LEU:CB | 1:A:155:ILE:HG21 | 1.78 | 1.13 |
| 1:B:193:ILE:HB | 1:B:194:PRO:CD | 1.76 | 1.13 |
| 1:A:42:ILE:CG1 | 1:A:43:PHE:N | 2.04 | 1.13 |
| 1:A:42:ILE:CD1 | 1:A:159:ILE:CD1 | 2.25 | 1.13 |
| 1:B:4:THR:HB | 1:B:19:ILE:HA | 1.29 | 1.13 |
| 1:A:190:ILE:CA | 1:A:193:ILE:HG13 | 1.76 | 1.13 |
| 1:B:7:ILE:O | 1:B:8:GLY:O | 1.65 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:42:ILE:CG1 | 1:B:136:VAL:O | 1.95 | 1.13 |
| 1:A:7:ILE:O | 1:A:8:GLY:O | 1.65 | 1.13 |
| 1:B:139:LEU:CB | 1:B:155:ILE:HG21 | 1.78 | 1.12 |
| 1:B:142:MET:CE | 1:B:202:PHE:CE1 | 2.32 | 1.12 |
| 1:A:135:GLU:O | 1:A:136:VAL:HB | 1.49 | 1.12 |
| 1:A:142:MET:HE3 | 1:A:202:PHE:CZ | 1.80 | 1.12 |
| 1:A:142:MET:CE | 1:A:202:PHE:CE1 | 2.32 | 1.12 |
| 1:B:42:ILE:CD1 | 1:B:159:ILE:CD1 | 2.25 | 1.12 |
| 1:A:174:GLU:O | 1:A:178:PRO:HB3 | 0.96 | 1.12 |
| 1:B:95:PHE:CE2 | 1:B:218:ILE:CD1 | 2.33 | 1.12 |
| 1:A:225:TRP:CZ3 | 1:A:226:LYS:HG2 | 1.85 | 1.11 |
| 1:B:51:ARG:HG2 | 1:B:89:ILE:HA | 1.26 | 1.11 |
| 1:A:7:ILE:O | 1:A:7:ILE:HG22 | 1.30 | 1.11 |
| 1:B:142:MET:CB | 1:B:153:LYS:HB2 | 1.78 | 1.11 |
| 1:A:95:PHE:CE2 | 1:A:218:ILE:CD1 | 2.33 | 1.11 |
| 1:B:5:ARG:HB3 | 1:B:263:ALA:HB2 | 1.20 | 1.11 |
| 1:B:42:ILE:CG1 | 1:B:43:PHE:N | 2.04 | 1.11 |
| 1:B:222:HIS:NE2 | 1:B:226:LYS:HE2 | 1.46 | 1.11 |
| 1:A:4:THR:HB | 1:A:19:ILE:HA | 1.28 | 1.11 |
| 1:A:26:VAL:O | 1:A:64:THR:HG21 | 1.51 | 1.11 |
| 1:A:42:ILE:CD1 | 1:A:159:ILE:HD11 | 1.81 | 1.11 |
| 1:A:190:ILE:HA | 1:A:193:ILE:HG13 | 1.11 | 1.11 |
| 1:A:200:ASN:O | 1:A:201:GLN:HG3 | 1.49 | 1.11 |
| 1:B:275:ILE:O | 1:B:277:LYS:N | 1.84 | 1.11 |
| 1:A:97:GLN:OE1 | 1:A:222:HIS:HE1 | 1.30 | 1.10 |
| 1:B:42:ILE:CD1 | 1:B:159:ILE:HD11 | 1.81 | 1.10 |
| 1:A:68:ILE:HG22 | 1:A:69:ILE:H | 1.14 | 1.10 |
| 1:A:275:ILE:O | 1:A:277:LYS:N | 1.84 | 1.10 |
| 1:B:57:LEU:HA | 1:B:68:ILE:O | 0.94 | 1.10 |
| 1:B:127:ILE:CG2 | 1:B:128:ALA:H | 1.63 | 1.10 |
| 1:B:144:LEU:CD2 | 1:B:153:LYS:HD3 | 1.81 | 1.10 |
| 1:A:127:ILE:CG2 | 1:A:128:ALA:H | 1.64 | 1.10 |
| 1:B:7:ILE:HB | 1:B:16:LYS:O | 1.47 | 1.10 |
| 1:B:68:ILE:HG22 | 1:B:69:ILE:H | 1.14 | 1.10 |
| 1:B:200:ASN:O | 1:B:201:GLN:HG3 | 1.49 | 1.10 |
| 1:A:9:ALA:HB1 | 1:A:15:TYR:HB2 | 1.21 | 1.10 |
| 1:A:13:LEU:HD23 | 1:A:76:LEU:HD11 | 1.26 | 1.10 |
| 1:A:57:LEU:HA | 1:A:68:ILE:O | 0.94 | 1.10 |
| 1:A:222:HIS:NE2 | 1:A:226:LYS:HE2 | 1.46 | 1.10 |
| 1:B:103:ASN:O | 1:B:104:VAL:HB | 1.37 | 1.10 |
| 1:A:103:ASN:O | 1:A:104:VAL:HB | 1.37 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:26:VAL:O | 1:B:64:THR:HG21 | 1.51 | 1.09 |
| 1:B:38:LYS:HG2 | 1:B:41:ASN:HB2 | 1.33 | 1.09 |
| 1:A:19:ILE:CD1 | 1:A:26:VAL:CG1 | 2.12 | 1.09 |
| 1:B:69:ILE:O | 1:B:70:GLN:O | 1.65 | 1.09 |
| 1:B:191:TYR:CE2 | 1:B:192:LYS:CG | 2.36 | 1.09 |
| 1:A:142:MET:HE3 | 1:A:202:PHE:CE1 | 1.85 | 1.09 |
| 1:B:7:ILE:HG21 | 1:B:16:LYS:H | 1.02 | 1.09 |
| 1:B:97:GLN:OE1 | 1:B:222:HIS:HE1 | 1.30 | 1.09 |
| 1:B:225:TRP:CZ3 | 1:B:226:LYS:HG2 | 1.85 | 1.09 |
| 1:B:127:ILE:HG22 | 1:B:128:ALA:N | 1.49 | 1.09 |
| 1:B:190:ILE:HA | 1:B:193:ILE:HG13 | 1.11 | 1.09 |
| 1:A:42:ILE:HD12 | 1:A:159:ILE:HD12 | 1.13 | 1.09 |
| 1:A:45:MET:HE1 | 1:A:120:VAL:HG12 | 1.31 | 1.09 |
| 1:B:26:VAL:HG22 | 1:B:27:SER:N | 1.62 | 1.09 |
| 1:B:96:PRO:O | 1:B:97:GLN:HB2 | 1.52 | 1.09 |
| 1:A:144:LEU:CD2 | 1:A:153:LYS:HD3 | 1.81 | 1.08 |
| 1:B:13:LEU:HD23 | 1:B:76:LEU:HD11 | 1.26 | 1.08 |
| 1:B:13:LEU:HD23 | 1:B:76:LEU:CD1 | 1.82 | 1.08 |
| 1:B:42:ILE:HG12 | 1:B:43:PHE:N | 1.14 | 1.08 |
| 1:B:49:ILE:HD11 | 1:B:92:TYR:HD1 | 0.94 | 1.08 |
| 1:B:98:THR:CG2 | 1:B:221:THR:O | 2.01 | 1.08 |
| 1:A:4:THR:CB | 1:A:19:ILE:HA | 1.83 | 1.08 |
| 1:A:13:LEU:HD23 | 1:A:76:LEU:CD1 | 1.82 | 1.08 |
| 1:A:51:ARG:HB3 | 1:A:51:ARG:HH11 | 1.03 | 1.08 |
| 1:A:191:TYR:CE2 | 1:A:192:LYS:CG | 2.36 | 1.08 |
| 1:A:98:THR:CG2 | 1:A:221:THR:O | 2.01 | 1.08 |
| 1:A:163:LEU:CD2 | 1:A:176:TYR:CD2 | 2.36 | 1.08 |
| 1:B:164:ALA:HB3 | 1:B:165:PRO:HD3 | 1.26 | 1.08 |
| 1:A:49:ILE:HD11 | 1:A:92:TYR:HD1 | 0.95 | 1.08 |
| 1:B:51:ARG:HB3 | 1:B:51:ARG:HH11 | 1.03 | 1.08 |
| 1:B:163:LEU:CD2 | 1:B:176:TYR:CD2 | 2.36 | 1.08 |
| 1:B:191:TYR:CE2 | 1:B:192:LYS:HG2 | 1.88 | 1.08 |
| 1:B:4:THR:CB | 1:B:19:ILE:HA | 1.83 | 1.07 |
| 1:B:19:ILE:CD1 | 1:B:26:VAL:CG1 | 2.12 | 1.07 |
| 1:B:29:PHE:CZ | 1:B:99:TRP:HD1 | 1.73 | 1.07 |
| 1:B:42:ILE:HD12 | 1:B:159:ILE:HD12 | 1.14 | 1.07 |
| 1:A:91:ASN:O | 1:A:92:TYR:HB2 | 1.51 | 1.07 |
| 1:B:12:THR:O | 1:B:13:LEU:HG | 1.55 | 1.07 |
| 1:A:96:PRO:O | 1:A:97:GLN:HB2 | 1.53 | 1.07 |
| 1:B:135:GLU:O | 1:B:136:VAL:HB | 1.49 | 1.07 |
| 1:B:91:ASN:O | 1:B:92:TYR:HB2 | 1.51 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:26:VAL:HG22 | 1:A:27:SER:N | 1.62 | 1.06 |
| 1:A:191:TYR:CE2 | 1:A:192:LYS:HG2 | 1.88 | 1.06 |
| 1:B:1:THR:N | 1:B:133:VAL:HG11 | 1.70 | 1.06 |
| 1:A:9:ALA:O | 1:A:10:LYS:HB2 | 1.50 | 1.06 |
| 1:B:7:ILE:O | 1:B:7:ILE:HG22 | 1.30 | 1.06 |
| 1:B:190:ILE:HA | 1:B:193:ILE:HG12 | 1.35 | 1.06 |
| 1:A:12:THR:O | 1:A:13:LEU:HG | 1.55 | 1.06 |
| 1:A:190:ILE:HA | 1:A:193:ILE:HG12 | 1.35 | 1.06 |
| 1:A:125:GLU:OE2 | 1:B:277:LYS:HE3 | 1.50 | 1.06 |
| 1:B:42:ILE:HG21 | 1:B:137:LYS:HG2 | 1.07 | 1.06 |
| 1:A:1:THR:N | 1:A:133:VAL:HG11 | 1.70 | 1.05 |
| 1:A:136:VAL:HA | 1:A:159:ILE:HG13 | 1.36 | 1.05 |
| 1:B:144:LEU:HD21 | 1:B:153:LYS:HD3 | 1.07 | 1.05 |
| 1:A:38:LYS:HG2 | 1:A:41:ASN:HB2 | 1.33 | 1.05 |
| 1:A:51:ARG:HH11 | 1:A:51:ARG:CB | 1.70 | 1.05 |
| 1:A:192:LYS:HD3 | 1:A:197:LYS:HD3 | 1.37 | 1.05 |
| 1:B:27:SER:HB2 | 1:B:64:THR:HG23 | 1.35 | 1.05 |
| 1:A:34:LEU:O | 1:A:43:PHE:CB | 2.04 | 1.05 |
| 1:B:27:SER:HA | 1:B:64:THR:HG23 | 1.15 | 1.05 |
| 1:B:51:ARG:HH11 | 1:B:51:ARG:CB | 1.70 | 1.05 |
| 1:A:29:PHE:CZ | 1:A:99:TRP:HD1 | 1.73 | 1.05 |
| 1:A:65:LEU:O | 1:A:66:ASN:ND2 | 1.90 | 1.05 |
| 1:A:277:LYS:HE3 | 1:B:125:GLU:OE2 | 1.50 | 1.04 |
| 1:B:9:ALA:O | 1:B:10:LYS:HB2 | 1.50 | 1.04 |
| 1:B:45:MET:HE1 | 1:B:120:VAL:HG12 | 1.39 | 1.04 |
| 1:B:65:LEU:O | 1:B:66:ASN:ND2 | 1.90 | 1.04 |
| 1:B:51:ARG:HG3 | 1:B:90:HIS:H | 1.21 | 1.04 |
| 1:A:83:PHE:HD1 | 1:A:280:PHE:CD2 | 1.74 | 1.04 |
| 1:B:34:LEU:O | 1:B:43:PHE:CB | 2.04 | 1.04 |
| 1:B:155:ILE:HG22 | 1:B:155:ILE:O | 1.56 | 1.04 |
| 1:A:144:LEU:HD21 | 1:A:153:LYS:HD3 | 1.07 | 1.04 |
| 1:B:136:VAL:HA | 1:B:159:ILE:HG13 | 1.36 | 1.04 |
| 1:A:49:ILE:O | 1:A:91:ASN:O | 1.77 | 1.03 |
| 1:A:1:THR:O | 1:A:2:TYR:HB2 | 1.56 | 1.03 |
| 1:A:26:VAL:HG22 | 1:A:27:SER:H | 0.88 | 1.03 |
| 1:A:56:LYS:NZ | 1:A:70:GLN:OE1 | 1.91 | 1.03 |
| 1:A:95:PHE:CD2 | 1:A:218:ILE:HD11 | 1.93 | 1.03 |
| 1:A:191:TYR:CD2 | 1:A:192:LYS:HG3 | 1.94 | 1.03 |
| 1:A:192:LYS:HB3 | 1:A:197:LYS:HB2 | 1.05 | 1.03 |
| 1:B:56:LYS:NZ | 1:B:70:GLN:OE1 | 1.91 | 1.03 |
| 1:B:129:TYR:HB2 | 1:B:132:GLN:OE1 | 1.13 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:192:LYS:HB3 | 1:B:197:LYS:HB2 | 1.05 | 1.03 |
| 1:A:42:ILE:HG21 | 1:A:137:LYS:HG2 | 1.07 | 1.03 |
| 1:B:1:THR:O | 1:B:2:TYR:HB2 | 1.56 | 1.03 |
| 1:B:123:ILE:CG1 | 1:B:123:ILE:O | 2.07 | 1.03 |
| 1:B:192:LYS:HD3 | 1:B:197:LYS:HD3 | 1.37 | 1.02 |
| 1:A:27:SER:HB2 | 1:A:64:THR:HG23 | 1.35 | 1.02 |
| 1:B:222:HIS:CD2 | 1:B:226:LYS:HE3 | 1.93 | 1.02 |
| 1:A:222:HIS:CD2 | 1:A:226:LYS:HE3 | 1.93 | 1.02 |
| 1:A:13:LEU:CD2 | 1:A:76:LEU:CD1 | 2.37 | 1.02 |
| 1:A:50:PRO:HB3 | 1:A:128:ALA:HB3 | 1.39 | 1.02 |
| 1:B:7:ILE:CG2 | 1:B:16:LYS:N | 2.22 | 1.02 |
| 1:B:42:ILE:HD12 | 1:B:159:ILE:HD11 | 1.03 | 1.02 |
| 1:B:80:ARG:HG3 | 1:B:194:PRO:HB2 | 1.42 | 1.02 |
| 1:B:95:PHE:CD2 | 1:B:218:ILE:HD11 | 1.93 | 1.02 |
| 1:A:48:GLU:O | 1:A:49:ILE:HG12 | 1.59 | 1.01 |
| 1:A:51:ARG:HG3 | 1:A:90:HIS:H | 1.21 | 1.01 |
| 1:A:80:ARG:HG3 | 1:A:194:PRO:HB2 | 1.42 | 1.01 |
| 1:A:136:VAL:CG1 | 1:A:156:ALA:HB1 | 1.90 | 1.01 |
| 1:A:204:PHE:O | 1:A:206:GLY:N | 1.93 | 1.01 |
| 1:B:142:MET:HB3 | 1:B:153:LYS:HB2 | 1.42 | 1.01 |
| 1:A:42:ILE:HD12 | 1:A:159:ILE:HD11 | 1.03 | 1.01 |
| 1:B:13:LEU:CD2 | 1:B:76:LEU:CD1 | 2.37 | 1.01 |
| 1:B:49:ILE:O | 1:B:91:ASN:O | 1.76 | 1.01 |
| 1:B:50:PRO:HB3 | 1:B:128:ALA:HB3 | 1.39 | 1.01 |
| 1:B:57:LEU:HD13 | 1:B:57:LEU:N | 1.74 | 1.01 |
| 1:B:137:LYS:HG3 | 1:B:159:ILE:HG12 | 1.40 | 1.01 |
| 1:A:125:GLU:OE2 | 1:B:277:LYS:HE2 | 1.58 | 1.01 |
| 1:A:137:LYS:HG3 | 1:A:159:ILE:HG12 | 1.40 | 1.01 |
| 1:A:155:ILE:HG22 | 1:A:155:ILE:O | 1.56 | 1.01 |
| 1:A:200:ASN:O | 1:A:201:GLN:CG | 2.08 | 1.01 |
| 1:B:26:VAL:HG22 | 1:B:27:SER:H | 0.88 | 1.01 |
| 1:B:48:GLU:O | 1:B:49:ILE:HG12 | 1.59 | 1.01 |
| 1:B:191:TYR:CD2 | 1:B:192:LYS:HG3 | 1.94 | 1.01 |
| 1:B:244:VAL:HA | 1:B:252:TYR:CD1 | 1.96 | 1.01 |
| 1:B:23:GLY:O | 1:B:24:LYS:HG3 | 0.83 | 1.01 |
| 1:A:7:ILE:CG2 | 1:A:16:LYS:N | 2.22 | 1.00 |
| 1:A:71:ASN:O | 1:A:72:THR:OG1 | 1.79 | 1.00 |
| 1:A:244:VAL:HA | 1:A:252:TYR:CD1 | 1.96 | 1.00 |
| 1:A:62:GLU:O | 1:A:63:GLU:HB2 | 1.60 | 1.00 |
| 1:A:139:LEU:CB | 1:A:155:ILE:CG2 | 2.37 | 1.00 |
| 1:B:136:VAL:CG1 | 1:B:156:ALA:HB1 | 1.90 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:23:GLY:O | 1:A:24:LYS:HG3 | 0.83 | 1.00 |
| 1:A:123:ILE:O | 1:A:123:ILE:CG1 | 2.07 | 1.00 |
| 1:B:83:PHE:HD1 | 1:B:280:PHE:CD2 | 1.74 | 1.00 |
| 1:A:84:PRO:O | 1:A:85:HIS:CG | 2.15 | 1.00 |
| 1:A:109:THR:HG23 | 1:A:150:THR:OG1 | 1.61 | 1.00 |
| 1:B:9:ALA:CB | 1:B:15:TYR:CA | 2.39 | 1.00 |
| 1:B:109:THR:HG23 | 1:B:150:THR:OG1 | 1.61 | 1.00 |
| 1:A:129:TYR:HB2 | 1:A:132:GLN:OE1 | 1.13 | 1.00 |
| 1:B:84:PRO:O | 1:B:85:HIS:CG | 2.15 | 1.00 |
| 1:B:139:LEU:CB | 1:B:155:ILE:CG2 | 2.37 | 1.00 |
| 1:B:158:ASP:O | 1:B:161:ASP:N | 1.95 | 1.00 |
| 1:B:200:ASN:O | 1:B:201:GLN:CG | 2.08 | 1.00 |
| 1:A:277:LYS:HE2 | 1:B:125:GLU:OE2 | 1.58 | 0.99 |
| 1:A:129:TYR:CB | 1:A:132:GLN:OE1 | 2.10 | 0.99 |
| 1:A:142:MET:HB3 | 1:A:153:LYS:HB2 | 1.42 | 0.99 |
| 1:A:172:ASP:O | 1:A:174:GLU:N | 1.95 | 0.99 |
| 1:B:90:HIS:O | 1:B:91:ASN:HB2 | 1.60 | 0.99 |
| 1:B:204:PHE:O | 1:B:206:GLY:N | 1.93 | 0.99 |
| 1:A:17:VAL:HG21 | 1:A:67:PRO:HG2 | 1.43 | 0.99 |
| 1:B:129:TYR:CB | 1:B:132:GLN:OE1 | 2.10 | 0.99 |
| 1:B:5:ARG:HH11 | 1:B:260:ILE:HG21 | 1.17 | 0.99 |
| 1:A:9:ALA:CB | 1:A:15:TYR:CA | 2.39 | 0.99 |
| 1:A:90:HIS:O | 1:A:91:ASN:HB2 | 1.60 | 0.99 |
| 1:B:68:ILE:HG22 | 1:B:69:ILE:N | 1.75 | 0.99 |
| 1:B:115:ASN:O | 1:B:116:ASN:O | 1.81 | 0.99 |
| 1:A:158:ASP:O | 1:A:161:ASP:N | 1.95 | 0.99 |
| 1:A:163:LEU:HD23 | 1:A:176:TYR:CD2 | 1.98 | 0.99 |
| 1:A:80:ARG:CD | 1:A:279:PHE:CE1 | 2.46 | 0.99 |
| 1:B:62:GLU:O | 1:B:63:GLU:HB2 | 1.60 | 0.99 |
| 1:B:110:LYS:C | 1:B:112:VAL:H | 1.66 | 0.99 |
| 1:A:29:PHE:HZ | 1:A:99:TRP:CD1 | 1.81 | 0.98 |
| 1:B:71:ASN:O | 1:B:72:THR:OG1 | 1.79 | 0.98 |
| 1:A:69:ILE:HG21 | 1:A:76:LEU:HB3 | 1.45 | 0.98 |
| 1:B:29:PHE:HZ | 1:B:99:TRP:CD1 | 1.81 | 0.98 |
| 1:B:172:ASP:O | 1:B:174:GLU:N | 1.95 | 0.98 |
| 1:A:57:LEU:HD13 | 1:A:57:LEU:N | 1.74 | 0.98 |
| 1:B:98:THR:HG23 | 1:B:221:THR:CA | 1.93 | 0.98 |
| 1:A:115:ASN:O | 1:A:116:ASN:O | 1.81 | 0.98 |
| 1:B:17:VAL:HG21 | 1:B:67:PRO:HG2 | 1.43 | 0.98 |
| 1:B:42:ILE:HG21 | 1:B:137:LYS:CG | 1.94 | 0.98 |
| 1:B:105:SER:HB2 | 1:B:109:THR:HG22 | 1.44 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:98:THR:HG23 | 1:A:221:THR:CA | 1.93 | 0.97 |
| 1:A:105:SER:HB2 | 1:A:109:THR:HG22 | 1.44 | 0.97 |
| 1:A:146:ASP:HB2 | 1:A:192:LYS:HZ1 | 1.27 | 0.97 |
| 1:A:42:ILE:HG21 | 1:A:137:LYS:CG | 1.94 | 0.97 |
| 1:B:80:ARG:CD | 1:B:279:PHE:CE1 | 2.46 | 0.97 |
| 1:B:69:ILE:HG21 | 1:B:76:LEU:HB3 | 1.45 | 0.97 |
| 1:A:1:THR:OG1 | 1:A:32:ILE:CD1 | 2.13 | 0.97 |
| 1:A:36:ALA:O | 1:A:37:ASP:HB2 | 1.64 | 0.97 |
| 1:A:244:VAL:HA | 1:A:252:TYR:HD1 | 1.27 | 0.97 |
| 1:A:7:ILE:HG21 | 1:A:16:LYS:N | 1.80 | 0.97 |
| 1:B:127:ILE:HG22 | 1:B:128:ALA:H | 1.08 | 0.97 |
| 1:A:122:GLN:NE2 | 1:A:124:GLY:HA3 | 1.79 | 0.96 |
| 1:B:123:ILE:HD12 | 1:B:177:PHE:CD2 | 1.94 | 0.96 |
| 1:B:163:LEU:HD21 | 1:B:176:TYR:CD2 | 1.99 | 0.96 |
| 1:A:13:LEU:HD21 | 1:A:76:LEU:HD13 | 1.46 | 0.96 |
| 1:A:123:ILE:HD12 | 1:A:177:PHE:CD2 | 1.94 | 0.96 |
| 1:A:53:THR:H | 1:A:88:TYR:H | 1.09 | 0.96 |
| 1:A:105:SER:HB2 | 1:A:112:VAL:HA | 1.44 | 0.96 |
| 1:A:158:ASP:CG | 1:A:160:ASN:HD21 | 1.68 | 0.96 |
| 1:B:105:SER:HB2 | 1:B:112:VAL:HA | 1.44 | 0.96 |
| 1:B:244:VAL:HA | 1:B:252:TYR:HD1 | 1.27 | 0.96 |
| 1:A:277:LYS:CG | 1:B:125:GLU:OE2 | 2.13 | 0.96 |
| 1:A:139:LEU:HB2 | 1:A:155:ILE:HG22 | 1.48 | 0.96 |
| 1:B:134:LYS:HE3 | 1:B:158:ASP:OD1 | 1.65 | 0.96 |
| 1:B:163:LEU:HD23 | 1:B:176:TYR:CD2 | 1.98 | 0.96 |
| 1:A:5:ARG:HH12 | 1:A:260:ILE:CB | 1.79 | 0.96 |
| 1:A:59:ILE:HG22 | 1:A:66:ASN:C | 1.85 | 0.96 |
| 1:A:68:ILE:HG22 | 1:A:69:ILE:N | 1.75 | 0.96 |
| 1:A:142:MET:HE2 | 1:A:202:PHE:CZ | 1.97 | 0.96 |
| 1:A:209:LYS:HG3 | 1:A:213:TYR:CD2 | 2.00 | 0.96 |
| 1:B:51:ARG:CB | 1:B:51:ARG:NH1 | 2.28 | 0.96 |
| 1:B:209:LYS:HG3 | 1:B:213:TYR:CD2 | 2.00 | 0.96 |
| 1:A:125:GLU:OE2 | 1:B:277:LYS:CG | 2.13 | 0.96 |
| 1:B:67:PRO:O | 1:B:68:ILE:HG12 | 1.65 | 0.96 |
| 1:B:32:ILE:O | 1:B:97:GLN:CG | 2.14 | 0.96 |
| 1:B:142:MET:HE2 | 1:B:202:PHE:CZ | 2.01 | 0.96 |
| 1:A:98:THR:CG2 | 1:A:221:THR:CA | 2.44 | 0.95 |
| 1:A:80:ARG:HH11 | 1:A:279:PHE:HE1 | 1.14 | 0.95 |
| 1:B:83:PHE:CE1 | 1:B:280:PHE:HE2 | 1.81 | 0.95 |
| 1:B:122:GLN:NE2 | 1:B:124:GLY:HA3 | 1.79 | 0.95 |
| 1:B:158:ASP:CG | 1:B:160:ASN:HD21 | 1.68 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:59:ILE:HG22 | 1:B:66:ASN:C | 1.85 | 0.95 |
| 1:B:98:THR:CG2 | 1:B:221:THR:CA | 2.44 | 0.95 |
| 1:A:51:ARG:CB | 1:A:51:ARG:NH1 | 2.28 | 0.95 |
| 1:B:192:LYS:CB | 1:B:197:LYS:HB2 | 1.96 | 0.95 |
| 1:B:80:ARG:HH11 | 1:B:279:PHE:HE1 | 1.14 | 0.95 |
| 1:A:9:ALA:HB3 | 1:A:15:TYR:CA | 1.96 | 0.95 |
| 1:A:163:LEU:HD21 | 1:A:176:TYR:CD2 | 1.99 | 0.95 |
| 1:B:1:THR:OG1 | 1:B:32:ILE:CD1 | 2.13 | 0.95 |
| 1:B:13:LEU:HD21 | 1:B:76:LEU:HD13 | 1.46 | 0.95 |
| 1:B:146:ASP:HB2 | 1:B:192:LYS:HZ1 | 1.27 | 0.95 |
| 1:A:1:THR:H1 | 1:A:133:VAL:HG11 | 1.28 | 0.95 |
| 1:A:8:GLY:HA3 | 1:A:266:LYS:HG3 | 1.49 | 0.95 |
| 1:B:5:ARG:HH12 | 1:B:260:ILE:CB | 1.79 | 0.94 |
| 1:A:98:THR:HG21 | 1:A:221:THR:OG1 | 0.77 | 0.94 |
| 1:A:134:LYS:HE3 | 1:A:158:ASP:OD1 | 1.65 | 0.94 |
| 1:A:192:LYS:CB | 1:A:197:LYS:HB2 | 1.97 | 0.94 |
| 1:B:139:LEU:HB2 | 1:B:155:ILE:HG22 | 1.48 | 0.94 |
| 1:B:1:THR:HG21 | 1:B:19:ILE:HD12 | 0.95 | 0.94 |
| 1:A:110:LYS:C | 1:A:112:VAL:H | 1.66 | 0.94 |
| 1:A:144:LEU:HG | 1:A:151:ASP:HB3 | 1.46 | 0.94 |
| 1:B:98:THR:HG21 | 1:B:221:THR:OG1 | 0.77 | 0.94 |
| 1:A:25:PRO:CG | 1:A:257:SER:HB3 | 1.98 | 0.94 |
| 1:A:67:PRO:O | 1:A:68:ILE:HG12 | 1.66 | 0.94 |
| 1:B:144:LEU:HG | 1:B:151:ASP:HB3 | 1.46 | 0.94 |
| 1:A:32:ILE:O | 1:A:97:GLN:CG | 2.14 | 0.94 |
| 1:B:30:HIS:NE2 | 1:B:241:LEU:HA | 1.83 | 0.94 |
| 1:B:271:ILE:HB | 1:B:275:ILE:HD11 | 1.50 | 0.94 |
| 1:B:25:PRO:CG | 1:B:257:SER:HB3 | 1.98 | 0.93 |
| 1:B:36:ALA:O | 1:B:37:ASP:HB2 | 1.64 | 0.93 |
| 1:B:136:VAL:CA | 1:B:159:ILE:HG13 | 1.96 | 0.93 |
| 1:B:225:TRP:HZ3 | 1:B:226:LYS:HG2 | 1.25 | 0.93 |
| 1:B:19:ILE:HD12 | 1:B:26:VAL:HG11 | 1.49 | 0.93 |
| 1:B:50:PRO:O | 1:B:53:THR:OG1 | 1.86 | 0.93 |
| 1:B:13:LEU:CD2 | 1:B:76:LEU:HD11 | 1.97 | 0.93 |
| 1:A:136:VAL:CA | 1:A:159:ILE:HG13 | 1.96 | 0.93 |
| 1:A:38:LYS:CB | 1:A:41:ASN:HB2 | 1.99 | 0.93 |
| 1:A:50:PRO:O | 1:A:53:THR:OG1 | 1.86 | 0.93 |
| 1:A:271:ILE:HB | 1:A:275:ILE:HD11 | 1.50 | 0.93 |
| 1:B:7:ILE:HG21 | 1:B:16:LYS:N | 1.80 | 0.93 |
| 1:B:9:ALA:HB3 | 1:B:15:TYR:CA | 1.96 | 0.93 |
| 1:A:13:LEU:CD2 | 1:A:76:LEU:HD11 | 1.97 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:179:GLY:O | 1:B:183:ALA:HB2 | 1.69 | 0.93 |
| 1:B:190:ILE:CA | 1:B:193:ILE:HG12 | 1.90 | 0.93 |
| 1:B:32:ILE:CG2 | 1:B:96:PRO:HG2 | 1.99 | 0.93 |
| 1:A:105:SER:CB | 1:A:112:VAL:CA | 2.29 | 0.93 |
| 1:A:5:ARG:HH11 | 1:A:260:ILE:HG21 | 1.17 | 0.92 |
| 1:A:30:HIS:NE2 | 1:A:241:LEU:HA | 1.83 | 0.92 |
| 1:A:142:MET:HE2 | 1:A:202:PHE:CE1 | 2.01 | 0.92 |
| 1:B:105:SER:CB | 1:B:112:VAL:CA | 2.29 | 0.92 |
| 1:B:188:PHE:O | 1:B:191:TYR:HB3 | 1.69 | 0.92 |
| 1:A:1:THR:HG21 | 1:A:19:ILE:HD12 | 0.95 | 0.92 |
| 1:A:38:LYS:O | 1:A:41:ASN:N | 2.02 | 0.92 |
| 1:B:38:LYS:O | 1:B:41:ASN:N | 2.02 | 0.92 |
| 1:B:164:ALA:CB | 1:B:165:PRO:CD | 2.47 | 0.92 |
| 1:A:13:LEU:CD2 | 1:A:76:LEU:HD13 | 1.97 | 0.92 |
| 1:A:188:PHE:O | 1:A:191:TYR:HB3 | 1.69 | 0.92 |
| 1:B:82:CYS:SG | 1:B:190:ILE:CG1 | 2.57 | 0.92 |
| 1:A:42:ILE:HB | 1:A:137:LYS:HA | 1.52 | 0.92 |
| 1:A:89:ILE:O | 1:A:90:HIS:HB2 | 1.69 | 0.92 |
| 1:A:142:MET:CE | 1:A:202:PHE:HZ | 1.81 | 0.92 |
| 1:B:8:GLY:HA3 | 1:B:266:LYS:HG3 | 1.49 | 0.92 |
| 1:B:13:LEU:CD2 | 1:B:76:LEU:HD13 | 1.97 | 0.92 |
| 1:B:139:LEU:HB2 | 1:B:155:ILE:HG21 | 0.93 | 0.92 |
| 1:A:46:VAL:O | 1:A:93:GLY:HA2 | 1.70 | 0.92 |
| 1:A:51:ARG:HB3 | 1:A:51:ARG:NH1 | 1.83 | 0.92 |
| 1:A:97:GLN:HB3 | 1:A:222:HIS:HD1 | 1.33 | 0.92 |
| 1:B:42:ILE:HB | 1:B:137:LYS:HA | 1.52 | 0.92 |
| 1:A:82:CYS:SG | 1:A:190:ILE:CG1 | 2.57 | 0.92 |
| 1:A:83:PHE:CE1 | 1:A:280:PHE:HE2 | 1.81 | 0.92 |
| 1:B:29:PHE:HZ | 1:B:99:TRP:HD1 | 1.09 | 0.92 |
| 1:A:32:ILE:CG2 | 1:A:96:PRO:HG2 | 1.99 | 0.92 |
| 1:A:225:TRP:HZ3 | 1:A:226:LYS:HG2 | 1.25 | 0.92 |
| 1:B:38:LYS:CB | 1:B:41:ASN:HB2 | 1.99 | 0.92 |
| 1:A:58:GLU:HG3 | 1:A:70:GLN:HE21 | 1.29 | 0.92 |
| 1:A:190:ILE:O | 1:A:194:PRO:HD2 | 1.70 | 0.92 |
| 1:A:29:PHE:HZ | 1:A:99:TRP:HD1 | 1.09 | 0.91 |
| 1:A:41:ASN:HD21 | 1:A:137:LYS:HE2 | 1.36 | 0.91 |
| 1:A:222:HIS:CD2 | 1:A:226:LYS:HG3 | 2.05 | 0.91 |
| 1:A:64:THR:C | 1:A:65:LEU:HD22 | 1.91 | 0.91 |
| 1:B:6:GLN:OE1 | 1:B:265:PRO:HB3 | 1.70 | 0.91 |
| 1:B:58:GLU:HG3 | 1:B:70:GLN:HE21 | 1.29 | 0.91 |
| 1:A:6:GLN:OE1 | 1:A:265:PRO:HB3 | 1.70 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:53:THR:H | 1:B:88:TYR:H | 1.09 | 0.91 |
| 1:B:241:LEU:O | 1:B:243:ASN:OD1 | 1.88 | 0.91 |
| 1:A:139:LEU:HB2 | 1:A:155:ILE:HG21 | 0.93 | 0.91 |
| 1:A:171:GLU:O | 1:A:172:ASP:O | 1.89 | 0.91 |
| 1:B:64:THR:C | 1:B:65:LEU:HD22 | 1.91 | 0.91 |
| 1:A:242:THR:HA | 1:A:251:THR:HB | 1.53 | 0.91 |
| 1:B:41:ASN:HD21 | 1:B:137:LYS:HE2 | 1.36 | 0.91 |
| 1:B:109:THR:HG23 | 1:B:150:THR:HG1 | 1.32 | 0.91 |
| 1:B:190:ILE:O | 1:B:194:PRO:HD2 | 1.70 | 0.91 |
| 1:A:6:GLN:OE1 | 1:A:265:PRO:CB | 2.19 | 0.91 |
| 1:A:80:ARG:HD2 | 1:A:279:PHE:CD1 | 2.05 | 0.91 |
| 1:B:222:HIS:CD2 | 1:B:226:LYS:HG3 | 2.05 | 0.91 |
| 1:B:242:THR:HA | 1:B:251:THR:HB | 1.53 | 0.91 |
| 1:A:179:GLY:O | 1:A:183:ALA:HB2 | 1.69 | 0.91 |
| 1:A:42:ILE:HG21 | 1:A:159:ILE:CD1 | 2.01 | 0.91 |
| 1:B:46:VAL:O | 1:B:93:GLY:HA2 | 1.69 | 0.91 |
| 1:A:59:ILE:HG22 | 1:A:67:PRO:CA | 2.00 | 0.91 |
| 1:B:123:ILE:HD11 | 1:B:177:PHE:HE2 | 1.09 | 0.91 |
| 1:A:19:ILE:HD12 | 1:A:26:VAL:HG11 | 1.49 | 0.90 |
| 1:A:42:ILE:CD1 | 1:A:159:ILE:HD12 | 1.96 | 0.90 |
| 1:A:164:ALA:CB | 1:A:165:PRO:CD | 2.47 | 0.90 |
| 1:B:97:GLN:HB3 | 1:B:222:HIS:HD1 | 1.33 | 0.90 |
| 1:B:51:ARG:HB3 | 1:B:51:ARG:NH1 | 1.82 | 0.90 |
| 1:B:136:VAL:HG11 | 1:B:156:ALA:HB1 | 1.53 | 0.90 |
| 1:B:6:GLN:OE1 | 1:B:265:PRO:CB | 2.19 | 0.90 |
| 1:B:80:ARG:HD2 | 1:B:279:PHE:CD1 | 2.05 | 0.90 |
| 1:A:123:ILE:HD11 | 1:A:177:PHE:HE2 | 1.09 | 0.90 |
| 1:A:190:ILE:CA | 1:A:193:ILE:HG12 | 1.90 | 0.90 |
| 1:B:42:ILE:HG21 | 1:B:159:ILE:CD1 | 2.01 | 0.90 |
| 1:A:146:ASP:OD1 | 1:A:147:GLU:CD | 2.10 | 0.90 |
| 1:A:241:LEU:O | 1:A:243:ASN:OD1 | 1.88 | 0.90 |
| 1:B:200:ASN:C | 1:B:201:GLN:HG3 | 1.91 | 0.90 |
| 1:B:25:PRO:HG2 | 1:B:257:SER:CB | 2.02 | 0.90 |
| 1:B:163:LEU:HD22 | 1:B:177:PHE:CZ | 2.07 | 0.90 |
| 1:B:59:ILE:HG22 | 1:B:67:PRO:CA | 2.01 | 0.90 |
| 1:A:56:LYS:C | 1:A:57:LEU:HD13 | 1.92 | 0.89 |
| 1:B:98:THR:CG2 | 1:B:221:THR:CB | 2.39 | 0.89 |
| 1:B:166:LYS:HD3 | 1:B:176:TYR:HE2 | 1.37 | 0.89 |
| 1:A:204:PHE:C | 1:A:206:GLY:H | 1.76 | 0.89 |
| 1:B:38:LYS:O | 1:B:40:ASP:N | 2.05 | 0.89 |
| 1:B:45:MET:HE2 | 1:B:120:VAL:HG11 | 1.53 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:56:LYS:C | 1:B:57:LEU:HD13 | 1.92 | 0.89 |
| 1:B:89:ILE:O | 1:B:90:HIS:HB2 | 1.69 | 0.89 |
| 1:B:171:GLU:O | 1:B:172:ASP:O | 1.89 | 0.89 |
| 1:A:222:HIS:CE1 | 1:A:226:LYS:HE2 | 2.07 | 0.89 |
| 1:B:1:THR:H1 | 1:B:133:VAL:HG11 | 1.26 | 0.89 |
| 1:B:191:TYR:CE2 | 1:B:192:LYS:HG3 | 2.06 | 0.89 |
| 1:A:25:PRO:HG2 | 1:A:257:SER:CB | 2.02 | 0.89 |
| 1:A:244:VAL:HB | 1:A:254:LYS:HA | 1.52 | 0.89 |
| 1:B:29:PHE:CZ | 1:B:99:TRP:CD1 | 2.59 | 0.89 |
| 1:A:105:SER:H | 1:A:112:VAL:HG12 | 1.38 | 0.89 |
| 1:A:29:PHE:CE1 | 1:A:225:TRP:HD1 | 1.91 | 0.89 |
| 1:A:38:LYS:O | 1:A:40:ASP:N | 2.05 | 0.89 |
| 1:A:166:LYS:HD3 | 1:A:176:TYR:HE2 | 1.37 | 0.89 |
| 1:B:244:VAL:HB | 1:B:254:LYS:HA | 1.52 | 0.89 |
| 1:B:42:ILE:CD1 | 1:B:159:ILE:HD12 | 1.95 | 0.89 |
| 1:B:59:ILE:CG2 | 1:B:67:PRO:N | 2.35 | 0.89 |
| 1:B:146:ASP:OD1 | 1:B:147:GLU:CD | 2.10 | 0.89 |
| 1:B:158:ASP:O | 1:B:160:ASN:N | 2.06 | 0.89 |
| 1:B:222:HIS:CE1 | 1:B:226:LYS:HE2 | 2.07 | 0.89 |
| 1:A:127:ILE:HG22 | 1:A:128:ALA:H | 1.08 | 0.89 |
| 1:A:136:VAL:HG11 | 1:A:156:ALA:HB1 | 1.53 | 0.89 |
| 1:A:271:ILE:HB | 1:A:275:ILE:CD1 | 2.02 | 0.89 |
| 1:A:144:LEU:HD21 | 1:A:153:LYS:CD | 2.02 | 0.88 |
| 1:A:163:LEU:HD22 | 1:A:177:PHE:CZ | 2.07 | 0.88 |
| 1:A:191:TYR:CE2 | 1:A:192:LYS:HG3 | 2.06 | 0.88 |
| 1:B:81:ASN:OD1 | 1:B:87:GLY:HA2 | 1.73 | 0.88 |
| 1:A:45:MET:HE1 | 1:A:120:VAL:CG1 | 2.03 | 0.88 |
| 1:B:238:GLY:O | 1:B:239:ILE:HG23 | 1.74 | 0.88 |
| 1:A:30:HIS:HE2 | 1:A:241:LEU:HA | 1.38 | 0.88 |
| 1:B:29:PHE:CE1 | 1:B:225:TRP:HD1 | 1.91 | 0.88 |
| 1:B:83:PHE:O | 1:B:278:TRP:NE1 | 2.06 | 0.88 |
| 1:B:193:ILE:CB | 1:B:194:PRO:CD | 2.52 | 0.88 |
| 1:B:204:PHE:C | 1:B:206:GLY:H | 1.76 | 0.88 |
| 1:A:81:ASN:OD1 | 1:A:87:GLY:HA2 | 1.73 | 0.88 |
| 1:A:193:ILE:CB | 1:A:194:PRO:CD | 2.52 | 0.88 |
| 1:B:71:ASN:O | 1:B:72:THR:CB | 2.22 | 0.88 |
| 1:B:80:ARG:CD | 1:B:279:PHE:CD1 | 2.57 | 0.88 |
| 1:B:271:ILE:HB | 1:B:275:ILE:CD1 | 2.02 | 0.88 |
| 1:A:230:ALA:HB3 | 1:A:233:SER:OG | 1.72 | 0.88 |
| 1:A:10:LYS:H | 1:A:15:TYR:HB2 | 1.33 | 0.88 |
| 1:B:10:LYS:H | 1:B:15:TYR:HB2 | 1.33 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:238:GLY:O | 1:A:239:ILE:HG23 | 1.74 | 0.88 |
| 1:B:95:PHE:HE2 | 1:B:218:ILE:CD1 | 1.77 | 0.88 |
| 1:A:51:ARG:CG | 1:A:90:HIS:H | 1.86 | 0.87 |
| 1:B:30:HIS:HE2 | 1:B:241:LEU:HA | 1.38 | 0.87 |
| 1:A:80:ARG:CD | 1:A:279:PHE:CD1 | 2.57 | 0.87 |
| 1:B:1:THR:OG1 | 1:B:32:ILE:HD11 | 1.74 | 0.87 |
| 1:B:54:ASN:O | 1:B:79:VAL:N | 2.07 | 0.87 |
| 1:B:51:ARG:CG | 1:B:90:HIS:H | 1.86 | 0.87 |
| 1:B:163:LEU:HD23 | 1:B:167:LEU:HD11 | 1.57 | 0.87 |
| 1:A:54:ASN:O | 1:A:79:VAL:N | 2.07 | 0.87 |
| 1:A:200:ASN:C | 1:A:201:GLN:HG3 | 1.91 | 0.87 |
| 1:B:29:PHE:HE1 | 1:B:98:THR:O | 1.57 | 0.87 |
| 1:B:51:ARG:HG2 | 1:B:89:ILE:CA | 2.04 | 0.87 |
| 1:B:230:ALA:HB3 | 1:B:233:SER:OG | 1.73 | 0.87 |
| 1:A:12:THR:O | 1:A:13:LEU:CG | 2.22 | 0.87 |
| 1:A:83:PHE:O | 1:A:278:TRP:NE1 | 2.06 | 0.87 |
| 1:A:163:LEU:HD23 | 1:A:167:LEU:HD11 | 1.57 | 0.87 |
| 1:B:12:THR:O | 1:B:13:LEU:CG | 2.22 | 0.87 |
| 1:B:105:SER:H | 1:B:112:VAL:HG12 | 1.38 | 0.87 |
| 1:A:59:ILE:CG2 | 1:A:67:PRO:N | 2.35 | 0.87 |
| 1:A:123:ILE:O | 1:A:123:ILE:HG12 | 1.74 | 0.87 |
| 1:B:42:ILE:HG21 | 1:B:159:ILE:HD11 | 1.57 | 0.87 |
| 1:A:158:ASP:O | 1:A:160:ASN:N | 2.06 | 0.87 |
| 1:B:182:ARG:HD3 | 1:B:185:ASP:OD2 | 1.74 | 0.87 |
| 1:B:32:ILE:HG21 | 1:B:96:PRO:HG2 | 1.56 | 0.87 |
| 1:A:51:ARG:HG2 | 1:A:89:ILE:CA | 2.04 | 0.87 |
| 1:A:147:GLU:OE1 | 1:A:192:LYS:NZ | 2.08 | 0.86 |
| 1:A:182:ARG:HD3 | 1:A:185:ASP:OD2 | 1.74 | 0.86 |
| 1:A:9:ALA:HB3 | 1:A:15:TYR:CG | 2.09 | 0.86 |
| 1:B:25:PRO:HG2 | 1:B:257:SER:HB3 | 1.56 | 0.86 |
| 1:A:10:LYS:O | 1:A:11:ASN:CG | 2.14 | 0.86 |
| 1:A:23:GLY:C | 1:A:24:LYS:HG3 | 1.96 | 0.86 |
| 1:B:9:ALA:HB3 | 1:B:15:TYR:CG | 2.09 | 0.86 |
| 1:B:1:THR:CG2 | 1:B:26:VAL:HG11 | 2.06 | 0.86 |
| 1:B:109:THR:HG22 | 1:B:109:THR:O | 1.75 | 0.86 |
| 1:A:1:THR:CG2 | 1:A:26:VAL:HG11 | 2.06 | 0.86 |
| 1:A:33:PRO:O | 1:A:34:LEU:HG | 1.75 | 0.86 |
| 1:A:25:PRO:HG2 | 1:A:257:SER:HB3 | 1.56 | 0.86 |
| 1:A:218:ILE:C | 1:A:221:THR:HG22 | 1.96 | 0.86 |
| 1:B:19:ILE:O | 1:B:26:VAL:CG1 | 2.24 | 0.86 |
| 1:A:32:ILE:HG21 | 1:A:96:PRO:HG2 | 1.56 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:71:ASN:O | 1:A:72:THR:CB | 2.22 | 0.86 |
| 1:A:109:THR:HG22 | 1:A:109:THR:O | 1.75 | 0.86 |
| 1:A:163:LEU:HA | 1:A:166:LYS:HD2 | 1.58 | 0.86 |
| 1:B:10:LYS:O | 1:B:11:ASN:CG | 2.14 | 0.86 |
| 1:A:1:THR:OG1 | 1:A:32:ILE:HD11 | 1.74 | 0.85 |
| 1:A:10:LYS:H | 1:A:15:TYR:CB | 1.88 | 0.85 |
| 1:A:95:PHE:HE2 | 1:A:218:ILE:CD1 | 1.77 | 0.85 |
| 1:A:192:LYS:HD3 | 1:A:197:LYS:CD | 2.06 | 0.85 |
| 1:B:33:PRO:O | 1:B:34:LEU:HG | 1.76 | 0.85 |
| 1:B:123:ILE:O | 1:B:123:ILE:HG12 | 1.74 | 0.85 |
| 1:B:147:GLU:OE1 | 1:B:192:LYS:NZ | 2.08 | 0.85 |
| 1:B:163:LEU:HA | 1:B:166:LYS:HD2 | 1.57 | 0.85 |
| 1:B:192:LYS:HD3 | 1:B:197:LYS:CD | 2.06 | 0.85 |
| 1:B:23:GLY:C | 1:B:24:LYS:HG3 | 1.96 | 0.85 |
| 1:B:17:VAL:CG2 | 1:B:67:PRO:HG2 | 2.07 | 0.85 |
| 1:A:17:VAL:CG2 | 1:A:67:PRO:HG2 | 2.07 | 0.85 |
| 1:A:45:MET:CE | 1:A:120:VAL:CG1 | 2.55 | 0.85 |
| 1:B:56:LYS:HZ3 | 1:B:70:GLN:HE22 | 1.23 | 0.85 |
| 1:B:49:ILE:HG13 | 1:B:92:TYR:HB3 | 1.58 | 0.85 |
| 1:B:7:ILE:O | 1:B:7:ILE:HG23 | 1.76 | 0.85 |
| 1:B:10:LYS:H | 1:B:15:TYR:CB | 1.88 | 0.85 |
| 1:A:29:PHE:HE1 | 1:A:98:THR:O | 1.57 | 0.85 |
| 1:B:5:ARG:NH1 | 1:B:260:ILE:HG22 | 1.88 | 0.85 |
| 1:B:142:MET:CE | 1:B:202:PHE:HZ | 1.80 | 0.84 |
| 1:A:19:ILE:O | 1:A:26:VAL:CG1 | 2.24 | 0.84 |
| 1:A:5:ARG:NH1 | 1:A:260:ILE:HG22 | 1.88 | 0.84 |
| 1:B:45:MET:CE | 1:B:120:VAL:CG1 | 2.55 | 0.84 |
| 1:B:5:ARG:HB3 | 1:B:263:ALA:CB | 2.05 | 0.84 |
| 1:B:225:TRP:CE3 | 1:B:226:LYS:HG2 | 2.13 | 0.84 |
| 1:A:7:ILE:O | 1:A:7:ILE:HG23 | 1.76 | 0.84 |
| 1:B:7:ILE:HG22 | 1:B:16:LYS:H | 1.42 | 0.84 |
| 1:B:19:ILE:HD13 | 1:B:26:VAL:HG11 | 0.84 | 0.84 |
| 1:A:57:LEU:HB3 | 1:A:68:ILE:N | 1.93 | 0.84 |
| 1:A:94:ALA:HA | 1:A:118:ILE:O | 1.77 | 0.84 |
| 1:B:144:LEU:HD21 | 1:B:153:LYS:CD | 2.02 | 0.84 |
| 1:A:48:GLU:OE2 | 1:A:93:GLY:O | 1.96 | 0.84 |
| 1:A:214:ALA:O | 1:A:217:ILE:HG22 | 1.77 | 0.84 |
| 1:B:1:THR:HG22 | 1:B:19:ILE:HD11 | 0.84 | 0.84 |
| 1:A:42:ILE:HG21 | 1:A:159:ILE:HD11 | 1.57 | 0.84 |
| 1:A:109:THR:HG23 | 1:A:150:THR:HG1 | 1.40 | 0.84 |
| 1:B:57:LEU:HB3 | 1:B:68:ILE:N | 1.93 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:94:ALA:HA | 1:B:118:ILE:O | 1.77 | 0.84 |
| 1:A:10:LYS:CG | 1:A:268:ASP:OD2 | 2.26 | 0.84 |
| 1:A:29:PHE:CE1 | 1:A:98:THR:O | 2.31 | 0.83 |
| 1:A:33:PRO:HA | 1:A:97:GLN:CD | 1.98 | 0.83 |
| 1:A:38:LYS:HB3 | 1:A:41:ASN:HB2 | 1.59 | 0.83 |
| 1:A:49:ILE:HG13 | 1:A:92:TYR:HB3 | 1.58 | 0.83 |
| 1:A:136:VAL:HG13 | 1:A:156:ALA:HB1 | 1.60 | 0.83 |
| 1:B:29:PHE:CE1 | 1:B:98:THR:O | 2.31 | 0.83 |
| 1:B:38:LYS:HB3 | 1:B:41:ASN:HB2 | 1.59 | 0.83 |
| 1:B:81:ASN:O | 1:B:82:CYS:O | 1.95 | 0.83 |
| 1:A:1:THR:HG22 | 1:A:19:ILE:HD11 | 0.84 | 0.83 |
| 1:B:214:ALA:O | 1:B:217:ILE:HG22 | 1.77 | 0.83 |
| 1:B:218:ILE:C | 1:B:221:THR:HG22 | 1.96 | 0.83 |
| 1:B:247:PRO:HA | 1:B:252:TYR:CD2 | 2.13 | 0.83 |
| 1:A:19:ILE:HD13 | 1:A:26:VAL:HG11 | 0.84 | 0.83 |
| 1:A:56:LYS:HZ3 | 1:A:70:GLN:HE22 | 1.24 | 0.83 |
| 1:A:69:ILE:O | 1:A:69:ILE:HG22 | 1.78 | 0.83 |
| 1:B:26:VAL:O | 1:B:64:THR:CG2 | 2.26 | 0.83 |
| 1:A:129:TYR:O | 1:A:132:GLN:N | 2.11 | 0.83 |
| 1:B:48:GLU:OE2 | 1:B:93:GLY:O | 1.96 | 0.83 |
| 1:B:122:GLN:HA | 1:B:156:ALA:O | 1.79 | 0.83 |
| 1:A:1:THR:O | 1:A:2:TYR:CB | 2.27 | 0.83 |
| 1:B:200:ASN:O | 1:B:201:GLN:CB | 2.27 | 0.83 |
| 1:A:3:THR:O | 1:A:20:GLU:N | 2.11 | 0.83 |
| 1:A:5:ARG:HB3 | 1:A:263:ALA:CB | 2.05 | 0.83 |
| 1:B:109:THR:O | 1:B:109:THR:CG2 | 2.27 | 0.83 |
| 1:A:225:TRP:CE3 | 1:A:226:LYS:HG2 | 2.13 | 0.82 |
| 1:A:247:PRO:HA | 1:A:252:TYR:CD2 | 2.13 | 0.82 |
| 1:B:33:PRO:HA | 1:B:97:GLN:CD | 1.98 | 0.82 |
| 1:B:1:THR:O | 1:B:2:TYR:CB | 2.27 | 0.82 |
| 1:B:3:THR:O | 1:B:20:GLU:N | 2.11 | 0.82 |
| 1:B:7:ILE:HG22 | 1:B:15:TYR:HA | 1.59 | 0.82 |
| 1:B:53:THR:N | 1:B:88:TYR:H | 1.77 | 0.82 |
| 1:B:129:TYR:O | 1:B:132:GLN:N | 2.11 | 0.82 |
| 1:A:7:ILE:HG22 | 1:A:15:TYR:HA | 1.59 | 0.82 |
| 1:A:29:PHE:CZ | 1:A:99:TRP:CD1 | 2.59 | 0.82 |
| 1:A:81:ASN:OD1 | 1:A:87:GLY:CA | 2.27 | 0.82 |
| 1:A:130:THR:O | 1:A:130:THR:CG2 | 2.27 | 0.82 |
| 1:B:12:THR:HG23 | 1:B:269:ALA:HB2 | 1.61 | 0.82 |
| 1:B:130:THR:CG2 | 1:B:130:THR:O | 2.27 | 0.82 |
| 1:B:136:VAL:HG13 | 1:B:156:ALA:HB1 | 1.60 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:190:ILE:HA | 1:B:193:ILE:HD11 | 1.61 | 0.82 |
| 1:A:1:THR:OG1 | 1:A:32:ILE:HD12 | 1.78 | 0.82 |
| 1:A:57:LEU:N | 1:A:57:LEU:CD1 | 2.43 | 0.82 |
| 1:A:53:THR:N | 1:A:88:TYR:H | 1.76 | 0.82 |
| 1:A:81:ASN:O | 1:A:82:CYS:O | 1.95 | 0.82 |
| 1:B:1:THR:OG1 | 1:B:32:ILE:HD12 | 1.78 | 0.82 |
| 1:A:12:THR:HG23 | 1:A:269:ALA:HB2 | 1.61 | 0.82 |
| 1:B:96:PRO:O | 1:B:97:GLN:CB | 2.28 | 0.82 |
| 1:A:96:PRO:O | 1:A:97:GLN:CB | 2.28 | 0.82 |
| 1:A:122:GLN:HA | 1:A:156:ALA:O | 1.79 | 0.81 |
| 1:A:129:TYR:CD2 | 1:A:132:GLN:HG3 | 2.15 | 0.81 |
| 1:B:81:ASN:OD1 | 1:B:87:GLY:CA | 2.27 | 0.81 |
| 1:B:123:ILE:O | 1:B:123:ILE:HG13 | 1.79 | 0.81 |
| 1:A:25:PRO:CD | 1:A:257:SER:HB3 | 2.10 | 0.81 |
| 1:A:182:ARG:HH11 | 1:A:185:ASP:CB | 1.93 | 0.81 |
| 1:B:10:LYS:CG | 1:B:268:ASP:OD2 | 2.26 | 0.81 |
| 1:B:69:ILE:HG22 | 1:B:77:ARG:H | 1.45 | 0.81 |
| 1:B:157:ILE:CG2 | 1:B:158:ASP:N | 2.43 | 0.81 |
| 1:A:109:THR:O | 1:A:109:THR:CG2 | 2.27 | 0.81 |
| 1:B:69:ILE:O | 1:B:69:ILE:HG22 | 1.78 | 0.81 |
| 1:B:142:MET:HE2 | 1:B:202:PHE:CE1 | 2.09 | 0.81 |
| 1:A:74:GLY:C | 1:A:75:LYS:HG3 | 2.00 | 0.81 |
| 1:A:103:ASN:HA | 1:A:112:VAL:HG11 | 1.63 | 0.81 |
| 1:A:125:GLU:OE2 | 1:B:277:LYS:HG3 | 1.81 | 0.81 |
| 1:B:5:ARG:NH2 | 1:B:25:PRO:CB | 2.43 | 0.81 |
| 1:B:182:ARG:HH11 | 1:B:185:ASP:CB | 1.93 | 0.81 |
| 1:B:45:MET:CE | 1:B:120:VAL:HG12 | 2.11 | 0.81 |
| 1:B:57:LEU:N | 1:B:57:LEU:CD1 | 2.43 | 0.81 |
| 1:A:190:ILE:HA | 1:A:193:ILE:HD11 | 1.61 | 0.81 |
| 1:B:27:SER:CA | 1:B:64:THR:CG2 | 2.42 | 0.81 |
| 1:A:26:VAL:O | 1:A:64:THR:CG2 | 2.26 | 0.81 |
| 1:B:25:PRO:CD | 1:B:257:SER:HB3 | 2.10 | 0.81 |
| 1:A:4:THR:HG22 | 1:A:19:ILE:HG12 | 1.61 | 0.81 |
| 1:A:7:ILE:HG22 | 1:A:16:LYS:H | 1.42 | 0.81 |
| 1:A:31:ASP:O | 1:A:32:ILE:HD13 | 1.81 | 0.81 |
| 1:A:157:ILE:CG2 | 1:A:158:ASP:N | 2.43 | 0.81 |
| 1:B:190:ILE:C | 1:B:193:ILE:HG12 | 2.01 | 0.81 |
| 1:B:4:THR:HG22 | 1:B:19:ILE:HG12 | 1.61 | 0.80 |
| 1:B:67:PRO:C | 1:B:68:ILE:HG12 | 2.01 | 0.80 |
| 1:B:192:LYS:CB | 1:B:197:LYS:CB | 2.56 | 0.80 |
| 1:A:166:LYS:HD3 | 1:A:176:TYR:CE2 | 2.15 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:200:ASN:O | 1:A:201:GLN:CB | 2.27 | 0.80 |
| 1:B:74:GLY:C | 1:B:75:LYS:HG3 | 2.00 | 0.80 |
| 1:B:129:TYR:CD2 | 1:B:132:GLN:HG3 | 2.15 | 0.80 |
| 1:A:59:ILE:HA | 1:A:66:ASN:O | 1.81 | 0.80 |
| 1:B:49:ILE:HD12 | 1:B:92:TYR:CB | 2.11 | 0.80 |
| 1:B:59:ILE:HA | 1:B:66:ASN:O | 1.81 | 0.80 |
| 1:B:166:LYS:HD3 | 1:B:176:TYR:CE2 | 2.15 | 0.80 |
| 1:B:164:ALA:HB3 | 1:B:165:PRO:HD2 | 1.64 | 0.80 |
| 1:A:167:LEU:HD21 | 1:A:177:PHE:CE1 | 2.17 | 0.80 |
| 1:B:173:VAL:O | 1:B:177:PHE:N | 2.15 | 0.80 |
| 1:A:69:ILE:HG22 | 1:A:77:ARG:H | 1.45 | 0.80 |
| 1:A:173:VAL:O | 1:A:177:PHE:N | 2.15 | 0.80 |
| 1:B:25:PRO:HD2 | 1:B:257:SER:HB3 | 1.62 | 0.80 |
| 1:B:130:THR:O | 1:B:130:THR:HG22 | 1.82 | 0.80 |
| 1:A:19:ILE:HD11 | 1:A:26:VAL:HG11 | 1.60 | 0.80 |
| 1:A:164:ALA:HB3 | 1:A:165:PRO:HD2 | 1.64 | 0.80 |
| 1:B:26:VAL:CG2 | 1:B:27:SER:N | 2.30 | 0.80 |
| 1:B:103:ASN:HA | 1:B:112:VAL:HG11 | 1.63 | 0.80 |
| 1:B:182:ARG:HH11 | 1:B:185:ASP:HB3 | 1.46 | 0.80 |
| 1:A:8:GLY:HA2 | 1:A:266:LYS:H | 1.47 | 0.80 |
| 1:A:155:ILE:CG2 | 1:A:155:ILE:O | 2.31 | 0.80 |
| 1:A:182:ARG:NH1 | 1:A:185:ASP:HB3 | 1.97 | 0.80 |
| 1:A:190:ILE:C | 1:A:193:ILE:HG12 | 2.01 | 0.80 |
| 1:B:31:ASP:O | 1:B:32:ILE:HD13 | 1.81 | 0.80 |
| 1:A:25:PRO:HD2 | 1:A:257:SER:HB3 | 1.63 | 0.79 |
| 1:A:45:MET:HE2 | 1:A:120:VAL:HG11 | 1.62 | 0.79 |
| 1:A:51:ARG:NH1 | 1:A:51:ARG:HB2 | 1.98 | 0.79 |
| 1:A:249:THR:O | 1:A:251:THR:N | 2.14 | 0.79 |
| 1:A:5:ARG:NH2 | 1:A:25:PRO:CB | 2.43 | 0.79 |
| 1:A:49:ILE:HD12 | 1:A:92:TYR:CB | 2.11 | 0.79 |
| 1:A:93:GLY:O | 1:A:94:ALA:HB2 | 1.82 | 0.79 |
| 1:A:123:ILE:O | 1:A:123:ILE:HG13 | 1.79 | 0.79 |
| 1:A:130:THR:O | 1:A:130:THR:HG22 | 1.82 | 0.79 |
| 1:A:277:LYS:HG3 | 1:B:125:GLU:OE2 | 1.81 | 0.79 |
| 1:B:167:LEU:HD21 | 1:B:177:PHE:CE1 | 2.17 | 0.79 |
| 1:B:182:ARG:NH1 | 1:B:185:ASP:HB3 | 1.97 | 0.79 |
| 1:A:217:ILE:O | 1:A:220:GLU:OE1 | 2.01 | 0.79 |
| 1:B:27:SER:HB2 | 1:B:64:THR:CG2 | 2.13 | 0.79 |
| 1:B:56:LYS:HZ3 | 1:B:70:GLN:NE2 | 1.80 | 0.79 |
| 1:A:67:PRO:C | 1:A:68:ILE:HG12 | 2.01 | 0.79 |
| 1:A:152:TRP:O | 1:A:153:LYS:HD2 | 1.82 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:89:ILE:O | 1:A:90:HIS:CB | 2.29 | 0.79 |
| 1:B:8:GLY:HA2 | 1:B:266:LYS:H | 1.47 | 0.79 |
| 1:A:98:THR:CG2 | 1:A:221:THR:CB | 2.39 | 0.79 |
| 1:B:155:ILE:CG2 | 1:B:155:ILE:O | 2.30 | 0.79 |
| 1:B:191:TYR:HE2 | 1:B:192:LYS:CG | 1.95 | 0.79 |
| 1:B:217:ILE:O | 1:B:220:GLU:OE1 | 2.01 | 0.79 |
| 1:B:152:TRP:O | 1:B:153:LYS:HD2 | 1.82 | 0.78 |
| 1:B:166:LYS:CD | 1:B:176:TYR:HE2 | 1.96 | 0.78 |
| 1:A:164:ALA:CB | 1:A:165:PRO:HD3 | 2.09 | 0.78 |
| 1:B:225:TRP:CZ3 | 1:B:229:ILE:HD11 | 2.18 | 0.78 |
| 1:B:249:THR:O | 1:B:251:THR:N | 2.14 | 0.78 |
| 1:B:68:ILE:CG2 | 1:B:69:ILE:H | 1.95 | 0.78 |
| 1:A:83:PHE:C | 1:A:83:PHE:HD2 | 1.87 | 0.78 |
| 1:B:1:THR:HG23 | 1:B:26:VAL:HG21 | 1.65 | 0.78 |
| 1:B:9:ALA:HB3 | 1:B:15:TYR:HB2 | 0.81 | 0.78 |
| 1:A:166:LYS:CD | 1:A:176:TYR:HE2 | 1.96 | 0.78 |
| 1:A:174:GLU:O | 1:A:178:PRO:CG | 2.32 | 0.78 |
| 1:A:225:TRP:CZ3 | 1:A:229:ILE:HD11 | 2.18 | 0.78 |
| 1:B:51:ARG:NH1 | 1:B:51:ARG:HB2 | 1.98 | 0.78 |
| 1:B:89:ILE:O | 1:B:90:HIS:CB | 2.29 | 0.78 |
| 1:B:174:GLU:O | 1:B:178:PRO:CG | 2.32 | 0.78 |
| 1:A:83:PHE:C | 1:A:83:PHE:CD2 | 2.55 | 0.78 |
| 1:B:83:PHE:HD2 | 1:B:83:PHE:C | 1.87 | 0.78 |
| 1:B:102:PRO:O | 1:B:112:VAL:HB | 1.84 | 0.78 |
| 1:A:28:ALA:HB3 | 1:A:59:ILE:HD12 | 1.64 | 0.78 |
| 1:B:191:TYR:CD2 | 1:B:192:LYS:CG | 2.65 | 0.77 |
| 1:A:192:LYS:CB | 1:A:197:LYS:CB | 2.56 | 0.77 |
| 1:A:1:THR:HG23 | 1:A:26:VAL:HG21 | 1.65 | 0.77 |
| 1:A:7:ILE:HG21 | 1:A:14:GLU:O | 1.85 | 0.77 |
| 1:B:1:THR:HG22 | 1:B:19:ILE:CD1 | 1.75 | 0.77 |
| 1:B:142:MET:CB | 1:B:153:LYS:CB | 2.62 | 0.77 |
| 1:A:8:GLY:O | 1:A:9:ALA:HB2 | 1.84 | 0.77 |
| 1:A:45:MET:CE | 1:A:120:VAL:HG12 | 2.11 | 0.77 |
| 1:A:91:ASN:O | 1:A:92:TYR:CB | 2.32 | 0.77 |
| 1:A:146:ASP:HB2 | 1:A:192:LYS:NZ | 1.99 | 0.77 |
| 1:A:191:TYR:CD2 | 1:A:192:LYS:CG | 2.66 | 0.77 |
| 1:B:35:TYR:H | 1:B:35:TYR:HD2 | 1.32 | 0.77 |
| 1:B:161:ASP:OD1 | 1:B:162:PRO:HD2 | 1.84 | 0.77 |
| 1:A:191:TYR:HE2 | 1:A:192:LYS:CG | 1.95 | 0.77 |
| 1:B:83:PHE:C | 1:B:83:PHE:CD2 | 2.55 | 0.77 |
| 1:A:102:PRO:O | 1:A:112:VAL:HB | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:122:GLN:NE2 | 1:A:124:GLY:CA | 2.48 | 0.77 |
| 1:B:7:ILE:HG21 | 1:B:14:GLU:O | 1.85 | 0.77 |
| 1:B:54:ASN:HB3 | 1:B:79:VAL:O | 1.84 | 0.77 |
| 1:B:93:GLY:O | 1:B:94:ALA:HB2 | 1.82 | 0.77 |
| 1:B:244:VAL:HB | 1:B:254:LYS:CA | 2.15 | 0.77 |
| 1:A:161:ASP:OD1 | 1:A:162:PRO:HD2 | 1.84 | 0.77 |
| 1:B:122:GLN:NE2 | 1:B:124:GLY:CA | 2.48 | 0.77 |
| 1:B:246:LEU:C | 1:B:248:ASP:H | 1.88 | 0.77 |
| 1:A:56:LYS:HZ3 | 1:A:70:GLN:NE2 | 1.82 | 0.77 |
| 1:B:192:LYS:HB3 | 1:B:197:LYS:HB3 | 1.65 | 0.76 |
| 1:A:83:PHE:CD1 | 1:A:280:PHE:CZ | 2.74 | 0.76 |
| 1:B:48:GLU:C | 1:B:49:ILE:HG12 | 2.06 | 0.76 |
| 1:B:53:THR:H | 1:B:88:TYR:N | 1.83 | 0.76 |
| 1:A:94:ALA:O | 1:A:96:PRO:N | 2.18 | 0.76 |
| 1:B:83:PHE:CD1 | 1:B:280:PHE:CZ | 2.74 | 0.76 |
| 1:B:2:TYR:HB2 | 1:B:21:LYS:HA | 1.68 | 0.76 |
| 1:A:35:TYR:H | 1:A:35:TYR:HD2 | 1.32 | 0.76 |
| 1:A:27:SER:CA | 1:A:64:THR:CG2 | 2.42 | 0.76 |
| 1:B:28:ALA:HB3 | 1:B:59:ILE:HD12 | 1.64 | 0.76 |
| 1:B:114:ASP:HB3 | 1:B:149:GLU:OE1 | 1.85 | 0.76 |
| 1:B:193:ILE:N | 1:B:197:LYS:O | 2.19 | 0.76 |
| 1:A:68:ILE:CG2 | 1:A:69:ILE:H | 1.95 | 0.76 |
| 1:A:83:PHE:HA | 1:A:278:TRP:CD1 | 2.20 | 0.76 |
| 1:A:95:PHE:CD2 | 1:A:218:ILE:CD1 | 2.65 | 0.76 |
| 1:A:193:ILE:N | 1:A:197:LYS:O | 2.19 | 0.76 |
| 1:B:83:PHE:HA | 1:B:278:TRP:CD1 | 2.20 | 0.76 |
| 1:B:122:GLN:CB | 1:B:156:ALA:O | 2.34 | 0.76 |
| 1:A:48:GLU:C | 1:A:49:ILE:HG12 | 2.06 | 0.76 |
| 1:A:54:ASN:HB3 | 1:A:79:VAL:O | 1.84 | 0.76 |
| 1:A:97:GLN:O | 1:A:225:TRP:CD2 | 2.39 | 0.76 |
| 1:A:114:ASP:HB3 | 1:A:149:GLU:OE1 | 1.85 | 0.76 |
| 1:B:44:ASN:N | 1:B:44:ASN:OD1 | 2.18 | 0.76 |
| 1:B:118:ILE:HD12 | 1:B:221:THR:OG1 | 1.86 | 0.76 |
| 1:B:146:ASP:HB2 | 1:B:192:LYS:NZ | 1.99 | 0.76 |
| 1:A:182:ARG:HH11 | 1:A:185:ASP:HB3 | 1.46 | 0.76 |
| 1:B:19:ILE:HD11 | 1:B:26:VAL:HG11 | 1.60 | 0.76 |
| 1:B:94:ALA:O | 1:B:96:PRO:N | 2.18 | 0.76 |
| 1:B:98:THR:HA | 1:B:225:TRP:HB3 | 1.68 | 0.75 |
| 1:B:147:GLU:CD | 1:B:192:LYS:HZ3 | 1.89 | 0.75 |
| 1:A:1:THR:HG22 | 1:A:19:ILE:CD1 | 1.75 | 0.75 |
| 1:B:80:ARG:HD2 | 1:B:279:PHE:HE1 | 1.47 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1:THR:CB | 1:A:19:ILE:HD11 | 2.12 | 0.75 |
| 1:A:53:THR:H | 1:A:88:TYR:N | 1.83 | 0.75 |
| 1:A:142:MET:CB | 1:A:153:LYS:CB | 2.62 | 0.75 |
| 1:B:32:ILE:HG21 | 1:B:96:PRO:CG | 2.17 | 0.75 |
| 1:A:9:ALA:HB3 | 1:A:15:TYR:HB2 | 0.81 | 0.75 |
| 1:A:44:ASN:OD1 | 1:A:44:ASN:N | 2.18 | 0.75 |
| 1:B:24:LYS:HB3 | 1:B:25:PRO:HD2 | 1.68 | 0.75 |
| 1:A:244:VAL:HB | 1:A:254:LYS:CA | 2.15 | 0.75 |
| 1:A:32:ILE:HG21 | 1:A:96:PRO:CG | 2.17 | 0.75 |
| 1:B:8:GLY:O | 1:B:9:ALA:HB2 | 1.84 | 0.75 |
| 1:B:137:LYS:HG3 | 1:B:159:ILE:CG1 | 2.16 | 0.75 |
| 1:A:139:LEU:HD12 | 1:A:155:ILE:CG2 | 2.17 | 0.75 |
| 1:A:192:LYS:HB3 | 1:A:197:LYS:HB3 | 1.65 | 0.75 |
| 1:B:1:THR:HG21 | 1:B:26:VAL:HG11 | 1.67 | 0.75 |
| 1:B:97:GLN:O | 1:B:225:TRP:CD2 | 2.39 | 0.75 |
| 1:B:19:ILE:O | 1:B:26:VAL:HG13 | 1.86 | 0.75 |
| 1:A:277:LYS:CD | 1:B:125:GLU:OE2 | 2.35 | 0.74 |
| 1:B:6:GLN:HG2 | 1:B:15:TYR:HE1 | 1.51 | 0.74 |
| 1:B:38:LYS:HB3 | 1:B:41:ASN:CB | 2.17 | 0.74 |
| 1:B:142:MET:HB3 | 1:B:153:LYS:CB | 2.17 | 0.74 |
| 1:A:137:LYS:HG3 | 1:A:159:ILE:CG1 | 2.16 | 0.74 |
| 1:A:36:ALA:O | 1:A:37:ASP:CB | 2.34 | 0.74 |
| 1:A:98:THR:HA | 1:A:225:TRP:HB3 | 1.68 | 0.74 |
| 1:A:122:GLN:CB | 1:A:156:ALA:O | 2.34 | 0.74 |
| 1:B:101:ASP:OD1 | 1:B:102:PRO:HD2 | 1.87 | 0.74 |
| 1:A:27:SER:HB2 | 1:A:64:THR:CG2 | 2.13 | 0.74 |
| 1:A:45:MET:CE | 1:A:120:VAL:HG11 | 2.17 | 0.74 |
| 1:B:164:ALA:CB | 1:B:165:PRO:HD3 | 2.09 | 0.74 |
| 1:B:1:THR:O | 1:B:21:LYS:HA | 1.87 | 0.74 |
| 1:B:80:ARG:HG3 | 1:B:194:PRO:CB | 2.18 | 0.74 |
| 1:A:28:ALA:O | 1:A:65:LEU:HD23 | 1.87 | 0.74 |
| 1:A:38:LYS:HB3 | 1:A:41:ASN:CB | 2.17 | 0.74 |
| 1:A:177:PHE:N | 1:A:177:PHE:CD1 | 2.56 | 0.74 |
| 1:B:28:ALA:O | 1:B:65:LEU:HD23 | 1.87 | 0.74 |
| 1:A:24:LYS:HB3 | 1:A:25:PRO:HD2 | 1.68 | 0.74 |
| 1:B:84:PRO:O | 1:B:85:HIS:CB | 2.35 | 0.74 |
| 1:B:95:PHE:CD2 | 1:B:218:ILE:CD1 | 2.65 | 0.74 |
| 1:A:5:ARG:HH22 | 1:A:25:PRO:HB3 | 1.52 | 0.74 |
| 1:A:6:GLN:HG2 | 1:A:15:TYR:HE1 | 1.51 | 0.74 |
| 1:A:157:ILE:HG22 | 1:A:158:ASP:N | 2.02 | 0.74 |
| 1:A:69:ILE:HB | 1:A:76:LEU:HD12 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:125:GLU:OE2 | 1:B:277:LYS:CD | 2.35 | 0.73 |
| 1:B:176:TYR:HB3 | 1:B:177:PHE:CE1 | 2.23 | 0.73 |
| 1:A:1:THR:O | 1:A:21:LYS:HA | 1.88 | 0.73 |
| 1:A:118:ILE:HD12 | 1:A:221:THR:OG1 | 1.86 | 0.73 |
| 1:A:95:PHE:HE2 | 1:A:218:ILE:HD11 | 0.92 | 0.73 |
| 1:A:97:GLN:HB3 | 1:A:222:HIS:ND1 | 2.04 | 0.73 |
| 1:A:101:ASP:OD1 | 1:A:102:PRO:HD2 | 1.87 | 0.73 |
| 1:A:147:GLU:CD | 1:A:192:LYS:HZ3 | 1.91 | 0.73 |
| 1:B:57:LEU:CB | 1:B:68:ILE:O | 2.35 | 0.73 |
| 1:B:146:ASP:CB | 1:B:192:LYS:HZ1 | 2.01 | 0.73 |
| 1:A:2:TYR:HB2 | 1:A:21:LYS:HA | 1.68 | 0.73 |
| 1:A:80:ARG:HG3 | 1:A:194:PRO:CB | 2.18 | 0.73 |
| 1:A:144:LEU:HD23 | 1:A:144:LEU:N | 2.03 | 0.73 |
| 1:B:38:LYS:HG2 | 1:B:41:ASN:CB | 2.17 | 0.73 |
| 1:A:19:ILE:O | 1:A:26:VAL:HG13 | 1.86 | 0.73 |
| 1:B:84:PRO:C | 1:B:85:HIS:CG | 2.61 | 0.73 |
| 1:B:93:GLY:O | 1:B:94:ALA:CB | 2.37 | 0.73 |
| 1:B:45:MET:CE | 1:B:120:VAL:HG11 | 2.17 | 0.73 |
| 1:B:139:LEU:HD12 | 1:B:155:ILE:CG2 | 2.17 | 0.73 |
| 1:A:57:LEU:CB | 1:A:68:ILE:O | 2.35 | 0.73 |
| 1:A:84:PRO:O | 1:A:85:HIS:CB | 2.35 | 0.73 |
| 1:A:176:TYR:HB3 | 1:A:177:PHE:CE1 | 2.23 | 0.73 |
| 1:B:244:VAL:CB | 1:B:254:LYS:HA | 2.18 | 0.73 |
| 1:B:91:ASN:O | 1:B:92:TYR:CB | 2.32 | 0.73 |
| 1:A:47:VAL:HG21 | 1:A:129:TYR:H | 1.53 | 0.72 |
| 1:A:93:GLY:O | 1:A:94:ALA:CB | 2.37 | 0.72 |
| 1:B:144:LEU:N | 1:B:144:LEU:HD23 | 2.03 | 0.72 |
| 1:B:157:ILE:HG22 | 1:B:158:ASP:N | 2.02 | 0.72 |
| 1:A:10:LYS:N | 1:A:15:TYR:HB2 | 2.04 | 0.72 |
| 1:A:60:THR:HA | 1:A:65:LEU:HD12 | 1.71 | 0.72 |
| 1:B:177:PHE:N | 1:B:177:PHE:CD1 | 2.56 | 0.72 |
| 1:B:69:ILE:HB | 1:B:76:LEU:HD12 | 1.69 | 0.72 |
| 1:A:38:LYS:HG2 | 1:A:41:ASN:CB | 2.16 | 0.72 |
| 1:A:1:THR:HG21 | 1:A:26:VAL:HG11 | 1.67 | 0.72 |
| 1:A:84:PRO:C | 1:A:85:HIS:CG | 2.61 | 0.72 |
| 1:B:1:THR:HB | 1:B:133:VAL:HG21 | 1.71 | 0.72 |
| 1:A:129:TYR:CD2 | 1:A:132:GLN:CG | 2.72 | 0.72 |
| 1:A:246:LEU:C | 1:A:248:ASP:H | 1.89 | 0.72 |
| 1:B:1:THR:CB | 1:B:19:ILE:HD11 | 2.12 | 0.72 |
| 1:B:47:VAL:HG21 | 1:B:129:TYR:H | 1.53 | 0.72 |
| 1:A:1:THR:HB | 1:A:133:VAL:HG21 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:4:THR:HB | 1:A:19:ILE:CA | 2.13 | 0.72 |
| 1:A:82:CYS:HG | 1:A:190:ILE:HG13 | 1.52 | 0.72 |
| 1:A:105:SER:HB3 | 1:A:112:VAL:HA | 0.72 | 0.72 |
| 1:B:129:TYR:O | 1:B:130:THR:C | 2.28 | 0.72 |
| 1:A:191:TYR:HD2 | 1:A:192:LYS:HG3 | 1.55 | 0.72 |
| 1:A:253:SER:C | 1:A:255:ALA:H | 1.92 | 0.72 |
| 1:B:4:THR:HB | 1:B:19:ILE:CA | 2.13 | 0.72 |
| 1:B:19:ILE:O | 1:B:26:VAL:HG12 | 1.90 | 0.72 |
| 1:B:51:ARG:C | 1:B:88:TYR:O | 2.28 | 0.72 |
| 1:A:69:ILE:O | 1:A:70:GLN:C | 2.28 | 0.71 |
| 1:B:60:THR:HA | 1:B:65:LEU:HD12 | 1.71 | 0.71 |
| 1:B:253:SER:C | 1:B:255:ALA:H | 1.92 | 0.71 |
| 1:B:97:GLN:HB3 | 1:B:222:HIS:ND1 | 2.04 | 0.71 |
| 1:A:25:PRO:CG | 1:A:257:SER:CB | 2.65 | 0.71 |
| 1:A:49:ILE:CD1 | 1:A:92:TYR:CG | 2.50 | 0.71 |
| 1:A:41:ASN:ND2 | 1:A:137:LYS:HE2 | 2.05 | 0.71 |
| 1:B:29:PHE:H | 1:B:96:PRO:HB2 | 1.56 | 0.71 |
| 1:A:272:ASP:O | 1:A:275:ILE:HG13 | 1.91 | 0.71 |
| 1:B:5:ARG:HH22 | 1:B:25:PRO:HB3 | 1.52 | 0.71 |
| 1:A:56:LYS:C | 1:A:57:LEU:CD1 | 2.59 | 0.71 |
| 1:A:142:MET:HB3 | 1:A:153:LYS:CB | 2.17 | 0.71 |
| 1:B:69:ILE:O | 1:B:70:GLN:C | 2.28 | 0.71 |
| 1:A:158:ASP:CB | 1:A:160:ASN:HD21 | 2.04 | 0.71 |
| 1:A:244:VAL:CB | 1:A:254:LYS:HA | 2.18 | 0.71 |
| 1:B:129:TYR:CD2 | 1:B:132:GLN:CG | 2.72 | 0.71 |
| 1:A:29:PHE:CE1 | 1:A:225:TRP:CD1 | 2.78 | 0.71 |
| 1:A:105:SER:HB3 | 1:A:112:VAL:CG1 | 2.21 | 0.71 |
| 1:A:51:ARG:C | 1:A:88:TYR:O | 2.28 | 0.71 |
| 1:B:4:THR:HG22 | 1:B:19:ILE:CG1 | 2.21 | 0.71 |
| 1:B:232:LYS:O | 1:B:233:SER:C | 2.29 | 0.71 |
| 1:A:1:THR:H3 | 1:A:133:VAL:HG11 | 1.54 | 0.71 |
| 1:A:11:ASN:O | 1:A:12:THR:C | 2.29 | 0.71 |
| 1:B:7:ILE:O | 1:B:8:GLY:C | 2.29 | 0.71 |
| 1:B:27:SER:HA | 1:B:64:THR:HG22 | 1.71 | 0.71 |
| 1:A:105:SER:HB3 | 1:A:112:VAL:CB | 2.21 | 0.70 |
| 1:B:56:LYS:C | 1:B:57:LEU:CD1 | 2.59 | 0.70 |
| 1:B:158:ASP:CB | 1:B:160:ASN:HD21 | 2.04 | 0.70 |
| 1:A:28:ALA:CB | 1:A:59:ILE:HD12 | 2.21 | 0.70 |
| 1:A:129:TYR:O | 1:A:130:THR:C | 2.28 | 0.70 |
| 1:B:41:ASN:ND2 | 1:B:137:LYS:HE2 | 2.05 | 0.70 |
| 1:B:42:ILE:CG2 | 1:B:159:ILE:HD11 | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:158:ASP:HB3 | 1:B:161:ASP:HB3 | 1.74 | 0.70 |
| 1:B:191:TYR:HD2 | 1:B:192:LYS:HG3 | 1.55 | 0.70 |
| 1:A:146:ASP:CB | 1:A:192:LYS:HZ1 | 2.02 | 0.70 |
| 1:A:174:GLU:C | 1:A:178:PRO:HB3 | 2.05 | 0.70 |
| 1:B:25:PRO:CG | 1:B:257:SER:CB | 2.65 | 0.70 |
| 1:B:49:ILE:CD1 | 1:B:92:TYR:CB | 2.69 | 0.70 |
| 1:B:249:THR:C | 1:B:251:THR:H | 1.94 | 0.70 |
| 1:A:192:LYS:NZ | 1:A:200:ASN:HD21 | 1.90 | 0.70 |
| 1:B:36:ALA:O | 1:B:37:ASP:CB | 2.34 | 0.70 |
| 1:B:242:THR:O | 1:B:243:ASN:OD1 | 2.09 | 0.70 |
| 1:A:49:ILE:CD1 | 1:A:92:TYR:CB | 2.69 | 0.70 |
| 1:A:122:GLN:CA | 1:A:156:ALA:O | 2.40 | 0.70 |
| 1:A:7:ILE:O | 1:A:8:GLY:C | 2.29 | 0.70 |
| 1:A:29:PHE:H | 1:A:96:PRO:HB2 | 1.56 | 0.70 |
| 1:A:42:ILE:CG2 | 1:A:159:ILE:HD11 | 2.21 | 0.70 |
| 1:A:45:MET:SD | 1:A:93:GLY:HA3 | 2.31 | 0.70 |
| 1:A:158:ASP:HB3 | 1:A:161:ASP:HB3 | 1.74 | 0.70 |
| 1:B:122:GLN:CA | 1:B:156:ALA:O | 2.40 | 0.70 |
| 1:A:81:ASN:O | 1:A:82:CYS:C | 2.30 | 0.70 |
| 1:A:28:ALA:O | 1:A:29:PHE:HB3 | 1.91 | 0.70 |
| 1:A:242:THR:O | 1:A:243:ASN:OD1 | 2.09 | 0.70 |
| 1:B:45:MET:SD | 1:B:93:GLY:HA3 | 2.31 | 0.70 |
| 1:A:4:THR:HG22 | 1:A:19:ILE:CG1 | 2.21 | 0.69 |
| 1:A:112:VAL:O | 1:A:150:THR:OG1 | 2.10 | 0.69 |
| 1:B:28:ALA:CB | 1:B:59:ILE:HD12 | 2.21 | 0.69 |
| 1:B:94:ALA:O | 1:B:96:PRO:HD3 | 1.92 | 0.69 |
| 1:A:47:VAL:HG22 | 1:A:131:GLY:H | 1.57 | 0.69 |
| 1:A:232:LYS:O | 1:A:233:SER:C | 2.29 | 0.69 |
| 1:B:11:ASN:O | 1:B:12:THR:C | 2.29 | 0.69 |
| 1:B:95:PHE:HE2 | 1:B:218:ILE:HD11 | 0.93 | 0.69 |
| 1:B:105:SER:HB3 | 1:B:112:VAL:CG1 | 2.21 | 0.69 |
| 1:B:105:SER:HB3 | 1:B:112:VAL:HA | 0.72 | 0.69 |
| 1:B:84:PRO:O | 1:B:85:HIS:CD2 | 2.45 | 0.69 |
| 1:B:105:SER:HB3 | 1:B:112:VAL:CB | 2.21 | 0.69 |
| 1:A:141:ILE:HA | 1:A:153:LYS:O | 1.92 | 0.69 |
| 1:B:49:ILE:CD1 | 1:B:92:TYR:CG | 2.50 | 0.69 |
| 1:B:192:LYS:NZ | 1:B:200:ASN:HD21 | 1.90 | 0.69 |
| 1:B:272:ASP:O | 1:B:275:ILE:HG13 | 1.91 | 0.69 |
| 1:B:1:THR:H3 | 1:B:133:VAL:HG11 | 1.56 | 0.69 |
| 1:A:84:PRO:O | 1:A:85:HIS:CD2 | 2.46 | 0.69 |
| 1:B:4:THR:CG2 | 1:B:19:ILE:HA | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:28:ALA:O | 1:B:29:PHE:HB3 | 1.91 | 0.69 |
| 1:B:141:ILE:HA | 1:B:153:LYS:O | 1.92 | 0.69 |
| 1:A:249:THR:C | 1:A:251:THR:H | 1.95 | 0.69 |
| 1:B:29:PHE:CE1 | 1:B:225:TRP:CD1 | 2.78 | 0.69 |
| 1:B:209:LYS:HG3 | 1:B:213:TYR:CG | 2.28 | 0.69 |
| 1:B:56:LYS:NZ | 1:B:70:GLN:CD | 2.46 | 0.69 |
| 1:B:58:GLU:O | 1:B:59:ILE:HG22 | 1.93 | 0.69 |
| 1:B:158:ASP:CB | 1:B:160:ASN:ND2 | 2.56 | 0.69 |
| 1:A:105:SER:HB2 | 1:A:109:THR:CG2 | 2.20 | 0.69 |
| 1:A:158:ASP:CB | 1:A:160:ASN:ND2 | 2.56 | 0.69 |
| 1:B:112:VAL:O | 1:B:150:THR:OG1 | 2.10 | 0.69 |
| 1:A:19:ILE:O | 1:A:26:VAL:HG12 | 1.90 | 0.68 |
| 1:A:102:PRO:HA | 1:A:113:GLY:O | 1.93 | 0.68 |
| 1:A:278:TRP:HH2 | 1:B:89:ILE:HG13 | 1.56 | 0.68 |
| 1:B:10:LYS:N | 1:B:15:TYR:HB2 | 2.04 | 0.68 |
| 1:B:81:ASN:O | 1:B:82:CYS:C | 2.30 | 0.68 |
| 1:A:42:ILE:HG22 | 1:A:137:LYS:HG2 | 1.72 | 0.68 |
| 1:A:56:LYS:NZ | 1:A:70:GLN:CD | 2.46 | 0.68 |
| 1:B:8:GLY:CA | 1:B:266:LYS:H | 2.05 | 0.68 |
| 1:B:47:VAL:HG22 | 1:B:131:GLY:H | 1.57 | 0.68 |
| 1:B:150:THR:O | 1:B:150:THR:HG22 | 1.94 | 0.68 |
| 1:A:4:THR:CG2 | 1:A:19:ILE:HA | 2.22 | 0.68 |
| 1:A:59:ILE:CG1 | 1:A:59:ILE:O | 2.41 | 0.68 |
| 1:B:102:PRO:HA | 1:B:113:GLY:O | 1.93 | 0.68 |
| 1:B:105:SER:HB2 | 1:B:109:THR:CG2 | 2.20 | 0.68 |
| 1:B:143:ALA:O | 1:B:202:PHE:CD1 | 2.47 | 0.68 |
| 1:B:217:ILE:CG2 | 1:B:218:ILE:N | 2.56 | 0.68 |
| 1:A:209:LYS:HG3 | 1:A:213:TYR:CG | 2.28 | 0.68 |
| 1:B:162:PRO:O | 1:B:163:LEU:HB2 | 1.93 | 0.68 |
| 1:B:49:ILE:CG1 | 1:B:92:TYR:HB3 | 2.24 | 0.68 |
| 1:B:59:ILE:O | 1:B:59:ILE:CG1 | 2.41 | 0.68 |
| 1:B:97:GLN:O | 1:B:225:TRP:CG | 2.47 | 0.68 |
| 1:B:103:ASN:O | 1:B:104:VAL:CB | 2.28 | 0.68 |
| 1:B:174:GLU:C | 1:B:178:PRO:HB3 | 2.05 | 0.68 |
| 1:B:275:ILE:O | 1:B:277:LYS:HB2 | 1.93 | 0.68 |
| 1:A:58:GLU:O | 1:A:59:ILE:HG22 | 1.93 | 0.68 |
| 1:B:23:GLY:O | 1:B:24:LYS:CB | 2.42 | 0.68 |
| 1:A:8:GLY:CA | 1:A:266:LYS:H | 2.05 | 0.68 |
| 1:A:83:PHE:HB3 | 1:A:84:PRO:HD3 | 1.75 | 0.68 |
| 1:A:162:PRO:O | 1:A:163:LEU:HB2 | 1.93 | 0.68 |
| 1:B:83:PHE:HB3 | 1:B:84:PRO:HD3 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:49:ILE:CG1 | 1:A:92:TYR:HB3 | 2.24 | 0.68 |
| 1:A:94:ALA:O | 1:A:96:PRO:HD3 | 1.92 | 0.68 |
| 1:A:115:ASN:O | 1:A:116:ASN:C | 2.32 | 0.68 |
| 1:A:191:TYR:HE2 | 1:A:192:LYS:CE | 2.07 | 0.68 |
| 1:B:92:TYR:CE2 | 1:B:121:LEU:HD21 | 2.29 | 0.68 |
| 1:A:12:THR:O | 1:A:13:LEU:CB | 2.42 | 0.68 |
| 1:A:97:GLN:O | 1:A:225:TRP:CG | 2.47 | 0.68 |
| 1:A:122:GLN:HE22 | 1:A:124:GLY:HA3 | 1.58 | 0.68 |
| 1:A:146:ASP:OD1 | 1:A:147:GLU:OE2 | 2.12 | 0.68 |
| 1:B:12:THR:O | 1:B:13:LEU:CB | 2.42 | 0.68 |
| 1:B:90:HIS:O | 1:B:91:ASN:CB | 2.41 | 0.68 |
| 1:B:92:TYR:HD2 | 1:B:121:LEU:HD23 | 1.58 | 0.68 |
| 1:A:89:ILE:HG13 | 1:B:278:TRP:HH2 | 1.57 | 0.67 |
| 1:A:92:TYR:CE2 | 1:A:121:LEU:HD21 | 2.29 | 0.67 |
| 1:B:81:ASN:HD22 | 1:B:276:ASP:HA | 1.59 | 0.67 |
| 1:A:168:ASN:ND2 | 1:A:168:ASN:C | 2.48 | 0.67 |
| 1:A:241:LEU:O | 1:A:242:THR:C | 2.32 | 0.67 |
| 1:A:7:ILE:HG22 | 1:A:16:LYS:N | 2.04 | 0.67 |
| 1:A:139:LEU:HD12 | 1:A:155:ILE:HG23 | 1.76 | 0.67 |
| 1:B:42:ILE:HG21 | 1:B:159:ILE:HD13 | 1.75 | 0.67 |
| 1:B:241:LEU:O | 1:B:242:THR:C | 2.32 | 0.67 |
| 1:B:191:TYR:HE2 | 1:B:192:LYS:CE | 2.07 | 0.67 |
| 1:B:247:PRO:HB3 | 1:B:252:TYR:CE2 | 2.30 | 0.67 |
| 1:A:143:ALA:O | 1:A:202:PHE:CD1 | 2.47 | 0.67 |
| 1:B:3:THR:O | 1:B:20:GLU:O | 2.12 | 0.67 |
| 1:A:23:GLY:O | 1:A:24:LYS:CB | 2.42 | 0.67 |
| 1:A:217:ILE:CG2 | 1:A:218:ILE:N | 2.56 | 0.67 |
| 1:A:247:PRO:HB3 | 1:A:252:TYR:CE2 | 2.30 | 0.67 |
| 1:B:123:ILE:HD12 | 1:B:177:PHE:HD2 | 1.57 | 0.67 |
| 1:B:168:ASN:ND2 | 1:B:168:ASN:C | 2.48 | 0.67 |
| 1:A:28:ALA:HA | 1:A:32:ILE:HG12 | 1.75 | 0.67 |
| 1:A:147:GLU:CD | 1:A:192:LYS:NZ | 2.48 | 0.67 |
| 1:B:94:ALA:O | 1:B:96:PRO:CD | 2.42 | 0.67 |
| 1:B:115:ASN:O | 1:B:116:ASN:C | 2.32 | 0.67 |
| 1:A:42:ILE:HG21 | 1:A:159:ILE:HD13 | 1.75 | 0.67 |
| 1:A:150:THR:HG22 | 1:A:150:THR:O | 1.94 | 0.67 |
| 1:A:275:ILE:O | 1:A:277:LYS:HB2 | 1.93 | 0.67 |
| 1:B:83:PHE:HB3 | 1:B:84:PRO:CD | 2.25 | 0.67 |
| 1:B:229:ILE:O | 1:B:230:ALA:C | 2.31 | 0.67 |
| 1:A:48:GLU:C | 1:A:49:ILE:CG1 | 2.62 | 0.67 |
| 1:A:229:ILE:O | 1:A:230:ALA:C | 2.31 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:246:LEU:O | 1:A:248:ASP:N | 2.28 | 0.67 |
| 1:B:28:ALA:HA | 1:B:32:ILE:HG12 | 1.75 | 0.67 |
| 1:A:25:PRO:CG | 1:A:257:SER:CA | 2.73 | 0.66 |
| 1:A:83:PHE:HB3 | 1:A:84:PRO:CD | 2.25 | 0.66 |
| 1:A:92:TYR:HD2 | 1:A:121:LEU:HD23 | 1.58 | 0.66 |
| 1:B:34:LEU:O | 1:B:36:ALA:N | 2.24 | 0.66 |
| 1:B:50:PRO:HA | 1:B:128:ALA:HB2 | 1.77 | 0.66 |
| 1:A:56:LYS:HZ2 | 1:A:70:GLN:CD | 1.97 | 0.66 |
| 1:B:93:GLY:N | 1:B:120:VAL:O | 2.28 | 0.66 |
| 1:B:146:ASP:OD1 | 1:B:147:GLU:OE2 | 2.12 | 0.66 |
| 1:A:80:ARG:HD2 | 1:A:279:PHE:HE1 | 1.47 | 0.66 |
| 1:B:139:LEU:HD12 | 1:B:155:ILE:HG23 | 1.76 | 0.66 |
| 1:A:94:ALA:O | 1:A:96:PRO:CD | 2.42 | 0.66 |
| 1:A:152:TRP:C | 1:A:153:LYS:HD2 | 2.15 | 0.66 |
| 1:B:141:ILE:O | 1:B:141:ILE:CG2 | 2.43 | 0.66 |
| 1:B:152:TRP:C | 1:B:153:LYS:HD2 | 2.15 | 0.66 |
| 1:B:163:LEU:HD22 | 1:B:177:PHE:HZ | 1.60 | 0.66 |
| 1:A:3:THR:O | 1:A:20:GLU:O | 2.12 | 0.66 |
| 1:A:123:ILE:HD12 | 1:A:177:PHE:HD2 | 1.57 | 0.66 |
| 1:B:25:PRO:HG2 | 1:B:257:SER:CA | 2.25 | 0.66 |
| 1:B:48:GLU:C | 1:B:49:ILE:CG1 | 2.62 | 0.66 |
| 1:B:59:ILE:HB | 1:B:66:ASN:N | 2.10 | 0.66 |
| 1:A:105:SER:HB2 | 1:A:109:THR:O | 1.95 | 0.66 |
| 1:B:42:ILE:HG22 | 1:B:137:LYS:HG2 | 1.72 | 0.66 |
| 1:A:142:MET:CA | 1:A:153:LYS:HB2 | 2.25 | 0.66 |
| 1:B:30:HIS:CD2 | 1:B:241:LEU:HA | 2.31 | 0.66 |
| 1:A:59:ILE:HB | 1:A:66:ASN:N | 2.10 | 0.66 |
| 1:A:163:LEU:HD23 | 1:A:167:LEU:CD1 | 2.25 | 0.66 |
| 1:B:25:PRO:CG | 1:B:257:SER:CA | 2.73 | 0.66 |
| 1:B:246:LEU:O | 1:B:248:ASP:N | 2.28 | 0.66 |
| 1:A:42:ILE:CG1 | 1:A:159:ILE:HD11 | 2.25 | 0.66 |
| 1:A:50:PRO:HA | 1:A:128:ALA:HB2 | 1.78 | 0.66 |
| 1:A:93:GLY:N | 1:A:120:VAL:O | 2.28 | 0.66 |
| 1:A:141:ILE:HG22 | 1:A:141:ILE:O | 1.95 | 0.66 |
| 1:B:142:MET:CA | 1:B:153:LYS:HB2 | 2.25 | 0.66 |
| 1:B:163:LEU:HD23 | 1:B:167:LEU:CD1 | 2.25 | 0.66 |
| 1:A:25:PRO:HG2 | 1:A:257:SER:CA | 2.25 | 0.65 |
| 1:A:27:SER:HA | 1:A:64:THR:HG22 | 1.72 | 0.65 |
| 1:A:81:ASN:HD22 | 1:A:276:ASP:HA | 1.59 | 0.65 |
| 1:B:141:ILE:O | 1:B:141:ILE:HG22 | 1.95 | 0.65 |
| 1:B:244:VAL:HG23 | 1:B:244:VAL:O | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:42:ILE:CG1 | 1:B:159:ILE:HD11 | 2.25 | 0.65 |
| 1:B:158:ASP:HB3 | 1:B:160:ASN:ND2 | 2.12 | 0.65 |
| 1:B:147:GLU:CD | 1:B:192:LYS:NZ | 2.48 | 0.65 |
| 1:B:190:ILE:CB | 1:B:193:ILE:HG13 | 2.26 | 0.65 |
| 1:A:34:LEU:O | 1:A:36:ALA:N | 2.24 | 0.65 |
| 1:B:1:THR:O | 1:B:2:TYR:CD1 | 2.50 | 0.65 |
| 1:B:105:SER:HB2 | 1:B:109:THR:O | 1.96 | 0.65 |
| 1:A:1:THR:O | 1:A:2:TYR:CD1 | 2.50 | 0.65 |
| 1:A:158:ASP:HB3 | 1:A:160:ASN:ND2 | 2.12 | 0.65 |
| 1:B:58:GLU:C | 1:B:59:ILE:HG23 | 2.16 | 0.65 |
| 1:A:143:ALA:HA | 1:A:152:TRP:HA | 1.78 | 0.65 |
| 1:A:163:LEU:CD2 | 1:A:167:LEU:HD11 | 2.27 | 0.65 |
| 1:B:7:ILE:O | 1:B:15:TYR:HA | 1.96 | 0.65 |
| 1:B:7:ILE:HG22 | 1:B:16:LYS:N | 2.04 | 0.65 |
| 1:B:114:ASP:CB | 1:B:149:GLU:OE1 | 2.45 | 0.65 |
| 1:B:166:LYS:HB3 | 1:B:176:TYR:CE2 | 2.32 | 0.65 |
| 1:A:106:HIS:CB | 1:A:107:PRO:HD2 | 2.27 | 0.65 |
| 1:B:46:VAL:O | 1:B:93:GLY:CA | 2.44 | 0.65 |
| 1:B:53:THR:O | 1:B:88:TYR:CB | 2.26 | 0.65 |
| 1:B:190:ILE:CA | 1:B:193:ILE:HD11 | 2.27 | 0.65 |
| 1:B:220:GLU:O | 1:B:220:GLU:HG2 | 1.96 | 0.65 |
| 1:B:253:SER:O | 1:B:255:ALA:N | 2.30 | 0.65 |
| 1:A:1:THR:CG2 | 1:A:26:VAL:HG21 | 2.27 | 0.64 |
| 1:A:30:HIS:CD2 | 1:A:241:LEU:HA | 2.31 | 0.64 |
| 1:A:80:ARG:CG | 1:A:194:PRO:HB2 | 2.25 | 0.64 |
| 1:A:190:ILE:CB | 1:A:193:ILE:HG13 | 2.26 | 0.64 |
| 1:B:45:MET:HE1 | 1:B:120:VAL:CG1 | 2.12 | 0.64 |
| 1:B:106:HIS:CB | 1:B:107:PRO:HD2 | 2.27 | 0.64 |
| 1:B:139:LEU:O | 1:B:211:LYS:CA | 2.45 | 0.64 |
| 1:B:243:ASN:O | 1:B:252:TYR:HA | 1.97 | 0.64 |
| 1:A:17:VAL:O | 1:A:66:ASN:HB3 | 1.97 | 0.64 |
| 1:A:163:LEU:HA | 1:A:166:LYS:CD | 2.28 | 0.64 |
| 1:A:193:ILE:O | 1:A:195:ASP:N | 2.30 | 0.64 |
| 1:A:7:ILE:O | 1:A:15:TYR:HA | 1.96 | 0.64 |
| 1:A:173:VAL:HG13 | 1:A:177:PHE:HB2 | 1.79 | 0.64 |
| 1:B:17:VAL:O | 1:B:66:ASN:HB3 | 1.97 | 0.64 |
| 1:A:166:LYS:HB3 | 1:A:176:TYR:CE2 | 2.32 | 0.64 |
| 1:B:140:GLY:HA3 | 1:B:170:ILE:CD1 | 2.28 | 0.64 |
| 1:A:58:GLU:C | 1:A:59:ILE:HG23 | 2.16 | 0.64 |
| 1:A:244:VAL:O | 1:A:244:VAL:HG23 | 1.96 | 0.64 |
| 1:B:163:LEU:CD2 | 1:B:167:LEU:HD11 | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:200:ASN:O | 1:A:201:GLN:HB2 | 1.98 | 0.64 |
| 1:A:253:SER:O | 1:A:255:ALA:N | 2.30 | 0.64 |
| 1:B:122:GLN:HE22 | 1:B:124:GLY:HA3 | 1.58 | 0.64 |
| 1:B:127:ILE:CG2 | 1:B:128:ALA:N | 2.21 | 0.64 |
| 1:B:174:GLU:HA | 1:B:178:PRO:HA | 1.80 | 0.64 |
| 1:A:12:THR:HG23 | 1:A:269:ALA:CB | 2.28 | 0.64 |
| 1:A:226:LYS:O | 1:A:229:ILE:HG13 | 1.98 | 0.64 |
| 1:B:50:PRO:CB | 1:B:128:ALA:HB3 | 2.23 | 0.64 |
| 1:B:143:ALA:HA | 1:B:152:TRP:HA | 1.78 | 0.64 |
| 1:B:83:PHE:O | 1:B:278:TRP:CD1 | 2.51 | 0.64 |
| 1:A:277:LYS:CG | 1:B:125:GLU:CD | 2.67 | 0.64 |
| 1:B:112:VAL:C | 1:B:150:THR:HB | 2.11 | 0.64 |
| 1:B:173:VAL:HG13 | 1:B:177:PHE:HB2 | 1.79 | 0.64 |
| 1:A:42:ILE:CG2 | 1:A:159:ILE:CD1 | 2.76 | 0.64 |
| 1:A:47:VAL:CG2 | 1:A:131:GLY:H | 2.11 | 0.64 |
| 1:A:174:GLU:HA | 1:A:178:PRO:HA | 1.80 | 0.64 |
| 1:B:12:THR:HG23 | 1:B:269:ALA:CB | 2.28 | 0.64 |
| 1:B:12:THR:CG2 | 1:B:269:ALA:HB2 | 2.28 | 0.64 |
| 1:B:29:PHE:O | 1:B:225:TRP:NE1 | 2.31 | 0.64 |
| 1:B:32:ILE:HG22 | 1:B:96:PRO:HG2 | 1.80 | 0.64 |
| 1:B:226:LYS:O | 1:B:229:ILE:HG13 | 1.98 | 0.64 |
| 1:A:46:VAL:O | 1:A:93:GLY:CA | 2.44 | 0.63 |
| 1:B:252:TYR:CE1 | 1:B:254:LYS:HB2 | 2.33 | 0.63 |
| 1:A:177:PHE:HA | 1:B:280:PHE:CE2 | 2.33 | 0.63 |
| 1:A:252:TYR:CE1 | 1:A:254:LYS:HB2 | 2.33 | 0.63 |
| 1:B:193:ILE:O | 1:B:195:ASP:N | 2.30 | 0.63 |
| 1:A:10:LYS:O | 1:A:11:ASN:OD1 | 2.15 | 0.63 |
| 1:A:140:GLY:HA3 | 1:A:170:ILE:CD1 | 2.28 | 0.63 |
| 1:B:8:GLY:O | 1:B:9:ALA:CB | 2.46 | 0.63 |
| 1:B:170:ILE:O | 1:B:171:GLU:C | 2.37 | 0.63 |
| 1:A:8:GLY:O | 1:A:9:ALA:CB | 2.46 | 0.63 |
| 1:A:25:PRO:HG2 | 1:A:257:SER:HA | 1.81 | 0.63 |
| 1:A:139:LEU:O | 1:A:211:LYS:HA | 1.98 | 0.63 |
| 1:B:10:LYS:O | 1:B:11:ASN:OD1 | 2.15 | 0.63 |
| 1:B:82:CYS:SG | 1:B:190:ILE:CD1 | 2.87 | 0.63 |
| 1:B:200:ASN:O | 1:B:201:GLN:HB2 | 1.98 | 0.63 |
| 1:A:50:PRO:CB | 1:A:128:ALA:HB3 | 2.23 | 0.63 |
| 1:A:83:PHE:O | 1:A:278:TRP:CD1 | 2.51 | 0.63 |
| 1:A:163:LEU:HD22 | 1:A:177:PHE:HZ | 1.60 | 0.63 |
| 1:A:190:ILE:CA | 1:A:193:ILE:HD11 | 2.27 | 0.63 |
| 1:A:243:ASN:O | 1:A:252:TYR:HA | 1.97 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:280:PHE:CE2 | 1:B:177:PHE:HA | 2.33 | 0.63 |
| 1:B:11:ASN:HA | 1:B:69:ILE:CD1 | 2.28 | 0.63 |
| 1:B:58:GLU:C | 1:B:59:ILE:CG2 | 2.66 | 0.63 |
| 1:B:98:THR:HG21 | 1:B:221:THR:CG2 | 2.29 | 0.63 |
| 1:A:114:ASP:CB | 1:A:149:GLU:OE1 | 2.45 | 0.63 |
| 1:B:1:THR:CG2 | 1:B:26:VAL:HG21 | 2.27 | 0.63 |
| 1:B:9:ALA:HB1 | 1:B:15:TYR:CB | 2.00 | 0.63 |
| 1:B:25:PRO:HG2 | 1:B:257:SER:HA | 1.81 | 0.63 |
| 1:A:139:LEU:O | 1:A:211:LYS:CA | 2.45 | 0.63 |
| 1:A:220:GLU:HG2 | 1:A:220:GLU:O | 1.96 | 0.63 |
| 1:B:9:ALA:HB2 | 1:B:15:TYR:CA | 2.25 | 0.63 |
| 1:B:54:ASN:HD22 | 1:B:54:ASN:H | 1.46 | 0.63 |
| 1:B:139:LEU:CB | 1:B:155:ILE:HG22 | 2.17 | 0.63 |
| 1:B:158:ASP:C | 1:B:160:ASN:N | 2.49 | 0.63 |
| 1:B:163:LEU:HA | 1:B:166:LYS:CD | 2.28 | 0.63 |
| 1:A:19:ILE:HD13 | 1:A:26:VAL:HG12 | 1.71 | 0.63 |
| 1:A:170:ILE:O | 1:A:171:GLU:C | 2.37 | 0.63 |
| 1:A:26:VAL:CG2 | 1:A:27:SER:N | 2.30 | 0.63 |
| 1:A:32:ILE:HG22 | 1:A:96:PRO:HG2 | 1.80 | 0.63 |
| 1:A:58:GLU:C | 1:A:59:ILE:CG2 | 2.66 | 0.63 |
| 1:A:142:MET:N | 1:A:153:LYS:O | 2.31 | 0.63 |
| 1:A:9:ALA:O | 1:A:10:LYS:CB | 2.36 | 0.62 |
| 1:A:29:PHE:O | 1:A:225:TRP:NE1 | 2.31 | 0.62 |
| 1:A:34:LEU:O | 1:A:43:PHE:HB2 | 1.97 | 0.62 |
| 1:A:125:GLU:CD | 1:B:277:LYS:CG | 2.66 | 0.62 |
| 1:A:11:ASN:HA | 1:A:69:ILE:CD1 | 2.29 | 0.62 |
| 1:A:25:PRO:CG | 1:A:257:SER:HA | 2.29 | 0.62 |
| 1:A:158:ASP:C | 1:A:160:ASN:N | 2.49 | 0.62 |
| 1:B:1:THR:O | 1:B:2:TYR:HD1 | 1.81 | 0.62 |
| 1:B:163:LEU:HG | 1:B:166:LYS:HD2 | 1.81 | 0.62 |
| 1:B:249:THR:HG22 | 1:B:251:THR:OG1 | 1.99 | 0.62 |
| 1:A:9:ALA:HB1 | 1:A:15:TYR:CB | 2.00 | 0.62 |
| 1:B:25:PRO:CG | 1:B:257:SER:HA | 2.29 | 0.62 |
| 1:B:122:GLN:CG | 1:B:157:ILE:HA | 2.29 | 0.62 |
| 1:A:12:THR:CG2 | 1:A:269:ALA:HB2 | 2.28 | 0.62 |
| 1:A:222:HIS:NE2 | 1:A:226:LYS:CG | 2.62 | 0.62 |
| 1:A:229:ILE:HG22 | 1:A:249:THR:HG21 | 1.81 | 0.62 |
| 1:B:140:GLY:HA3 | 1:B:170:ILE:HD11 | 1.82 | 0.62 |
| 1:B:222:HIS:NE2 | 1:B:226:LYS:CG | 2.62 | 0.62 |
| 1:A:98:THR:HG21 | 1:A:221:THR:CG2 | 2.29 | 0.62 |
| 1:A:163:LEU:HG | 1:A:166:LYS:HD2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:222:HIS:CD2 | 1:A:226:LYS:CG | 2.82 | 0.62 |
| 1:B:47:VAL:CG2 | 1:B:131:GLY:H | 2.11 | 0.62 |
| 1:B:142:MET:HB2 | 1:B:153:LYS:HB2 | 1.78 | 0.62 |
| 1:A:1:THR:O | 1:A:2:TYR:HD1 | 1.81 | 0.62 |
| 1:B:13:LEU:HG | 1:B:76:LEU:HD21 | 1.82 | 0.62 |
| 1:B:86:HIS:CG | 1:B:87:GLY:H | 2.18 | 0.62 |
| 1:B:172:ASP:O | 1:B:173:VAL:C | 2.37 | 0.62 |
| 1:A:82:CYS:SG | 1:A:190:ILE:CD1 | 2.87 | 0.62 |
| 1:B:42:ILE:CG2 | 1:B:159:ILE:CD1 | 2.76 | 0.62 |
| 1:B:229:ILE:HG22 | 1:B:249:THR:HG21 | 1.81 | 0.62 |
| 1:A:203:ALA:O | 1:A:206:GLY:N | 2.33 | 0.62 |
| 1:A:9:ALA:HB2 | 1:A:15:TYR:CA | 2.25 | 0.62 |
| 1:A:90:HIS:CE1 | 1:A:184:THR:OG1 | 2.52 | 0.62 |
| 1:A:99:TRP:O | 1:A:224:SER:OG | 2.18 | 0.62 |
| 1:A:106:HIS:HB2 | 1:A:107:PRO:HD2 | 1.82 | 0.62 |
| 1:B:69:ILE:HG21 | 1:B:76:LEU:CB | 2.26 | 0.62 |
| 1:A:105:SER:CB | 1:A:109:THR:HG22 | 2.25 | 0.62 |
| 1:A:230:ALA:CB | 1:A:233:SER:OG | 2.48 | 0.62 |
| 1:B:90:HIS:CE1 | 1:B:184:THR:OG1 | 2.53 | 0.62 |
| 1:B:158:ASP:CG | 1:B:160:ASN:ND2 | 2.49 | 0.62 |
| 1:A:13:LEU:HG | 1:A:76:LEU:HD21 | 1.82 | 0.61 |
| 1:A:53:THR:O | 1:A:88:TYR:CB | 2.26 | 0.61 |
| 1:B:122:GLN:HE21 | 1:B:124:GLY:HA3 | 1.65 | 0.61 |
| 1:B:139:LEU:O | 1:B:211:LYS:HA | 1.98 | 0.61 |
| 1:A:48:GLU:O | 1:A:49:ILE:CG1 | 2.43 | 0.61 |
| 1:B:275:ILE:O | 1:B:276:ASP:C | 2.38 | 0.61 |
| 1:A:97:GLN:HA | 1:A:225:TRP:CE2 | 2.36 | 0.61 |
| 1:A:122:GLN:CG | 1:A:157:ILE:HA | 2.29 | 0.61 |
| 1:A:141:ILE:O | 1:A:141:ILE:CG2 | 2.43 | 0.61 |
| 1:A:172:ASP:O | 1:A:173:VAL:C | 2.37 | 0.61 |
| 1:B:34:LEU:C | 1:B:43:PHE:HB3 | 2.19 | 0.61 |
| 1:A:42:ILE:HG12 | 1:A:43:PHE:H | 0.63 | 0.61 |
| 1:A:249:THR:HG22 | 1:A:251:THR:OG1 | 1.99 | 0.61 |
| 1:B:7:ILE:HB | 1:B:16:LYS:C | 2.19 | 0.61 |
| 1:B:166:LYS:HB3 | 1:B:176:TYR:CZ | 2.36 | 0.61 |
| 1:B:190:ILE:C | 1:B:193:ILE:CG1 | 2.64 | 0.61 |
| 1:B:203:ALA:O | 1:B:206:GLY:N | 2.33 | 0.61 |
| 1:A:209:LYS:HB3 | 1:A:213:TYR:HB2 | 1.82 | 0.61 |
| 1:A:275:ILE:O | 1:A:276:ASP:C | 2.38 | 0.61 |
| 1:B:97:GLN:HA | 1:B:225:TRP:CE2 | 2.36 | 0.61 |
| 1:A:166:LYS:HB3 | 1:A:176:TYR:CZ | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:203:ALA:O | 1:A:204:PHE:C | 2.39 | 0.61 |
| 1:B:203:ALA:O | 1:B:204:PHE:C | 2.39 | 0.61 |
| 1:A:7:ILE:HB | 1:A:16:LYS:C | 2.19 | 0.61 |
| 1:A:190:ILE:C | 1:A:193:ILE:CG1 | 2.64 | 0.61 |
| 1:A:191:TYR:HE2 | 1:A:192:LYS:HE2 | 1.66 | 0.61 |
| 1:A:193:ILE:HA | 1:A:197:LYS:O | 2.01 | 0.61 |
| 1:B:193:ILE:HA | 1:B:197:LYS:O | 2.01 | 0.61 |
| 1:A:86:HIS:CG | 1:A:87:GLY:H | 2.18 | 0.61 |
| 1:B:67:PRO:O | 1:B:68:ILE:CG1 | 2.45 | 0.61 |
| 1:B:209:LYS:HB3 | 1:B:213:TYR:HB2 | 1.82 | 0.61 |
| 1:A:9:ALA:CB | 1:A:15:TYR:N | 2.63 | 0.61 |
| 1:A:141:ILE:HD13 | 1:A:153:LYS:O | 2.01 | 0.61 |
| 1:B:38:LYS:O | 1:B:39:GLU:C | 2.38 | 0.61 |
| 1:B:142:MET:N | 1:B:153:LYS:O | 2.31 | 0.61 |
| 1:A:111:ALA:HB2 | 1:A:145:LEU:HD22 | 1.83 | 0.60 |
| 1:B:5:ARG:CZ | 1:B:25:PRO:HB3 | 2.29 | 0.60 |
| 1:B:38:LYS:CD | 1:B:41:ASN:HB2 | 2.31 | 0.60 |
| 1:B:99:TRP:O | 1:B:224:SER:OG | 2.18 | 0.60 |
| 1:A:4:THR:HG22 | 1:A:19:ILE:CB | 2.31 | 0.60 |
| 1:A:6:GLN:OE1 | 1:A:265:PRO:HB2 | 2.01 | 0.60 |
| 1:A:38:LYS:O | 1:A:39:GLU:C | 2.38 | 0.60 |
| 1:A:101:ASP:O | 1:A:113:GLY:HA3 | 2.02 | 0.60 |
| 1:A:139:LEU:CB | 1:A:155:ILE:HG22 | 2.17 | 0.60 |
| 1:A:253:SER:C | 1:A:255:ALA:N | 2.55 | 0.60 |
| 1:B:34:LEU:O | 1:B:43:PHE:HB2 | 1.97 | 0.60 |
| 1:A:122:GLN:HE21 | 1:A:124:GLY:CA | 2.14 | 0.60 |
| 1:A:140:GLY:HA3 | 1:A:170:ILE:HD11 | 1.82 | 0.60 |
| 1:B:6:GLN:OE1 | 1:B:265:PRO:HB2 | 2.01 | 0.60 |
| 1:A:56:LYS:NZ | 1:A:70:GLN:NE2 | 2.50 | 0.60 |
| 1:A:92:TYR:CD2 | 1:A:121:LEU:HD23 | 2.37 | 0.60 |
| 1:A:98:THR:HA | 1:A:225:TRP:CB | 2.31 | 0.60 |
| 1:B:9:ALA:CB | 1:B:15:TYR:N | 2.63 | 0.60 |
| 1:B:106:HIS:HB2 | 1:B:107:PRO:HD2 | 1.82 | 0.60 |
| 1:B:122:GLN:HE21 | 1:B:124:GLY:CA | 2.14 | 0.60 |
| 1:A:8:GLY:HA3 | 1:A:266:LYS:CG | 2.29 | 0.60 |
| 1:A:104:VAL:O | 1:A:105:SER:C | 2.40 | 0.60 |
| 1:A:54:ASN:H | 1:A:54:ASN:HD22 | 1.46 | 0.60 |
| 1:A:125:GLU:CD | 1:B:277:LYS:HG3 | 2.22 | 0.60 |
| 1:B:4:THR:HG22 | 1:B:19:ILE:CB | 2.31 | 0.60 |
| 1:B:80:ARG:CG | 1:B:194:PRO:HB2 | 2.25 | 0.60 |
| 1:A:27:SER:O | 1:A:31:ASP:N | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:158:ASP:CG | 1:A:160:ASN:ND2 | 2.49 | 0.60 |
| 1:A:179:GLY:O | 1:A:183:ALA:CB | 2.47 | 0.60 |
| 1:B:179:GLY:O | 1:B:183:ALA:CB | 2.47 | 0.60 |
| 1:A:19:ILE:HD12 | 1:A:26:VAL:CG1 | 2.16 | 0.60 |
| 1:A:92:TYR:CD2 | 1:A:121:LEU:CD2 | 2.85 | 0.60 |
| 1:A:188:PHE:O | 1:A:191:TYR:CB | 2.48 | 0.60 |
| 1:B:9:ALA:O | 1:B:10:LYS:CB | 2.36 | 0.60 |
| 1:B:35:TYR:CD2 | 1:B:35:TYR:N | 2.70 | 0.60 |
| 1:B:141:ILE:HD13 | 1:B:153:LYS:O | 2.01 | 0.60 |
| 1:A:5:ARG:CZ | 1:A:25:PRO:HB3 | 2.29 | 0.60 |
| 1:A:129:TYR:O | 1:A:129:TYR:HD1 | 1.85 | 0.60 |
| 1:B:222:HIS:NE2 | 1:B:226:LYS:CD | 2.62 | 0.60 |
| 1:A:157:ILE:HG23 | 1:A:158:ASP:N | 2.17 | 0.59 |
| 1:A:222:HIS:CD2 | 1:A:226:LYS:CE | 2.66 | 0.59 |
| 1:B:29:PHE:H | 1:B:96:PRO:CB | 2.15 | 0.59 |
| 1:B:56:LYS:NZ | 1:B:70:GLN:NE2 | 2.50 | 0.59 |
| 1:B:222:HIS:CD2 | 1:B:226:LYS:CG | 2.82 | 0.59 |
| 1:A:69:ILE:HG21 | 1:A:76:LEU:CB | 2.26 | 0.59 |
| 1:B:27:SER:O | 1:B:31:ASP:N | 2.35 | 0.59 |
| 1:B:92:TYR:CD2 | 1:B:121:LEU:CD2 | 2.85 | 0.59 |
| 1:B:92:TYR:CD2 | 1:B:121:LEU:HD23 | 2.36 | 0.59 |
| 1:A:34:LEU:C | 1:A:43:PHE:HB3 | 2.19 | 0.59 |
| 1:A:38:LYS:C | 1:A:40:ASP:N | 2.53 | 0.59 |
| 1:A:83:PHE:CB | 1:A:84:PRO:CD | 2.80 | 0.59 |
| 1:A:163:LEU:HB3 | 1:A:167:LEU:HD13 | 1.85 | 0.59 |
| 1:A:241:LEU:N | 1:A:241:LEU:HD12 | 2.17 | 0.59 |
| 1:B:38:LYS:C | 1:B:40:ASP:N | 2.53 | 0.59 |
| 1:B:101:ASP:O | 1:B:113:GLY:HA3 | 2.02 | 0.59 |
| 1:B:253:SER:C | 1:B:255:ALA:N | 2.55 | 0.59 |
| 1:B:271:ILE:HB | 1:B:275:ILE:HD12 | 1.84 | 0.59 |
| 1:A:29:PHE:H | 1:A:96:PRO:CB | 2.15 | 0.59 |
| 1:A:158:ASP:C | 1:A:160:ASN:H | 2.06 | 0.59 |
| 1:A:160:ASN:HD22 | 1:A:161:ASP:N | 2.01 | 0.59 |
| 1:A:166:LYS:CD | 1:A:176:TYR:CE2 | 2.81 | 0.59 |
| 1:B:19:ILE:HD12 | 1:B:26:VAL:CG1 | 2.16 | 0.59 |
| 1:B:49:ILE:CD1 | 1:B:92:TYR:HB3 | 2.32 | 0.59 |
| 1:B:59:ILE:O | 1:B:59:ILE:HG13 | 2.02 | 0.59 |
| 1:B:111:ALA:HB2 | 1:B:145:LEU:HD22 | 1.83 | 0.59 |
| 1:B:127:ILE:HG23 | 1:B:128:ALA:H | 1.61 | 0.59 |
| 1:B:181:LEU:O | 1:B:184:THR:N | 2.28 | 0.59 |
| 1:A:38:LYS:CD | 1:A:41:ASN:HB2 | 2.31 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:42:ILE:HG12 | 1:B:43:PHE:CA | 2.23 | 0.59 |
| 1:B:158:ASP:C | 1:B:160:ASN:H | 2.06 | 0.59 |
| 1:B:160:ASN:HD22 | 1:B:161:ASP:N | 2.01 | 0.59 |
| 1:A:59:ILE:CG2 | 1:A:66:ASN:C | 2.66 | 0.59 |
| 1:A:59:ILE:O | 1:A:59:ILE:HG13 | 2.02 | 0.59 |
| 1:A:204:PHE:C | 1:A:206:GLY:N | 2.45 | 0.59 |
| 1:B:192:LYS:C | 1:B:197:LYS:O | 2.40 | 0.59 |
| 1:B:204:PHE:C | 1:B:206:GLY:N | 2.45 | 0.59 |
| 1:B:241:LEU:HD12 | 1:B:241:LEU:N | 2.17 | 0.59 |
| 1:A:150:THR:O | 1:A:150:THR:CG2 | 2.51 | 0.59 |
| 1:B:69:ILE:HD12 | 1:B:76:LEU:HG | 1.85 | 0.59 |
| 1:B:83:PHE:CB | 1:B:84:PRO:CD | 2.80 | 0.59 |
| 1:B:191:TYR:HE2 | 1:B:192:LYS:HE2 | 1.66 | 0.59 |
| 1:B:244:VAL:O | 1:B:244:VAL:CG2 | 2.51 | 0.59 |
| 1:A:67:PRO:O | 1:A:68:ILE:CG1 | 2.45 | 0.59 |
| 1:A:192:LYS:CB | 1:A:197:LYS:HB3 | 2.30 | 0.59 |
| 1:B:65:LEU:C | 1:B:66:ASN:CG | 2.62 | 0.59 |
| 1:B:122:GLN:CG | 1:B:156:ALA:O | 2.51 | 0.59 |
| 1:B:141:ILE:HG13 | 1:B:217:ILE:HG21 | 1.85 | 0.59 |
| 1:B:157:ILE:HG23 | 1:B:158:ASP:N | 2.17 | 0.59 |
| 1:B:246:LEU:C | 1:B:248:ASP:N | 2.56 | 0.59 |
| 1:A:7:ILE:CG2 | 1:A:14:GLU:O | 2.51 | 0.58 |
| 1:A:146:ASP:HB2 | 1:A:147:GLU:OE1 | 2.03 | 0.58 |
| 1:A:277:LYS:HG3 | 1:B:125:GLU:CD | 2.22 | 0.58 |
| 1:B:129:TYR:O | 1:B:129:TYR:HD1 | 1.85 | 0.58 |
| 1:B:41:ASN:HD21 | 1:B:137:LYS:CE | 2.10 | 0.58 |
| 1:B:58:GLU:O | 1:B:59:ILE:CG2 | 2.52 | 0.58 |
| 1:A:51:ARG:CG | 1:A:90:HIS:N | 2.64 | 0.58 |
| 1:B:7:ILE:CG2 | 1:B:14:GLU:O | 2.51 | 0.58 |
| 1:B:19:ILE:HD13 | 1:B:19:ILE:C | 2.24 | 0.58 |
| 1:A:192:LYS:C | 1:A:197:LYS:O | 2.40 | 0.58 |
| 1:A:69:ILE:HD12 | 1:A:76:LEU:HG | 1.85 | 0.58 |
| 1:A:122:GLN:CG | 1:A:156:ALA:O | 2.51 | 0.58 |
| 1:B:150:THR:O | 1:B:150:THR:CG2 | 2.51 | 0.58 |
| 1:A:141:ILE:HG13 | 1:A:217:ILE:HG21 | 1.85 | 0.58 |
| 1:A:244:VAL:O | 1:A:244:VAL:CG2 | 2.51 | 0.58 |
| 1:B:98:THR:HA | 1:B:225:TRP:CB | 2.31 | 0.58 |
| 1:B:104:VAL:O | 1:B:105:SER:C | 2.40 | 0.58 |
| 1:B:163:LEU:HB3 | 1:B:167:LEU:HD13 | 1.85 | 0.58 |
| 1:A:217:ILE:HG23 | 1:A:218:ILE:N | 2.18 | 0.58 |
| 1:A:49:ILE:CD1 | 1:A:92:TYR:HB3 | 2.32 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:63:GLU:OE2 | 1:A:256:ALA:HB1 | 2.04 | 0.58 |
| 1:A:110:LYS:C | 1:A:112:VAL:N | 2.37 | 0.58 |
| 1:B:80:ARG:HA | 1:B:80:ARG:NE | 2.19 | 0.58 |
| 1:B:98:THR:OG1 | 1:B:221:THR:HG23 | 2.04 | 0.58 |
| 1:B:122:GLN:HG2 | 1:B:157:ILE:HA | 1.86 | 0.58 |
| 1:B:164:ALA:C | 1:B:166:LYS:H | 2.07 | 0.58 |
| 1:A:34:LEU:C | 1:A:36:ALA:H | 2.06 | 0.58 |
| 1:A:41:ASN:HD21 | 1:A:137:LYS:CE | 2.10 | 0.58 |
| 1:A:80:ARG:HD3 | 1:A:279:PHE:CD1 | 2.37 | 0.58 |
| 1:A:127:ILE:HG23 | 1:A:128:ALA:H | 1.61 | 0.58 |
| 1:A:18:TYR:CE1 | 1:A:260:ILE:HD12 | 2.39 | 0.58 |
| 1:A:65:LEU:C | 1:A:66:ASN:CG | 2.62 | 0.58 |
| 1:A:74:GLY:O | 1:A:75:LYS:HG2 | 1.96 | 0.58 |
| 1:B:48:GLU:O | 1:B:49:ILE:CG1 | 2.43 | 0.58 |
| 1:B:71:ASN:C | 1:B:72:THR:OG1 | 2.43 | 0.58 |
| 1:B:97:GLN:C | 1:B:225:TRP:CG | 2.78 | 0.58 |
| 1:B:99:TRP:CZ2 | 1:B:115:ASN:OD1 | 2.57 | 0.58 |
| 1:B:103:ASN:HA | 1:B:112:VAL:CG1 | 2.33 | 0.58 |
| 1:A:19:ILE:HD13 | 1:A:19:ILE:C | 2.24 | 0.57 |
| 1:A:193:ILE:CA | 1:A:197:LYS:O | 2.52 | 0.57 |
| 1:B:63:GLU:OE2 | 1:B:256:ALA:HB1 | 2.04 | 0.57 |
| 1:A:99:TRP:CZ2 | 1:A:115:ASN:OD1 | 2.57 | 0.57 |
| 1:A:141:ILE:HG13 | 1:A:214:ALA:HA | 1.86 | 0.57 |
| 1:A:157:ILE:HG23 | 1:A:158:ASP:H | 1.69 | 0.57 |
| 1:A:246:LEU:C | 1:A:248:ASP:N | 2.56 | 0.57 |
| 1:B:110:LYS:C | 1:B:112:VAL:N | 2.37 | 0.57 |
| 1:A:142:MET:HB2 | 1:A:153:LYS:HB2 | 1.78 | 0.57 |
| 1:A:225:TRP:CE3 | 1:A:226:LYS:N | 2.73 | 0.57 |
| 1:A:225:TRP:CH2 | 1:A:229:ILE:HD11 | 2.39 | 0.57 |
| 1:A:271:ILE:HB | 1:A:275:ILE:HD12 | 1.84 | 0.57 |
| 1:B:80:ARG:HD3 | 1:B:279:PHE:CD1 | 2.37 | 0.57 |
| 1:B:225:TRP:CH2 | 1:B:229:ILE:HD11 | 2.39 | 0.57 |
| 1:A:54:ASN:HB2 | 1:A:275:ILE:HG21 | 1.86 | 0.57 |
| 1:B:54:ASN:OD1 | 1:B:81:ASN:CG | 2.43 | 0.57 |
| 1:B:90:HIS:CE1 | 1:B:184:THR:HG23 | 2.40 | 0.57 |
| 1:A:9:ALA:HB3 | 1:A:15:TYR:CD1 | 2.39 | 0.57 |
| 1:A:86:HIS:CG | 1:A:87:GLY:N | 2.71 | 0.57 |
| 1:A:97:GLN:C | 1:A:225:TRP:CG | 2.78 | 0.57 |
| 1:A:98:THR:OG1 | 1:A:221:THR:HG23 | 2.04 | 0.57 |
| 1:A:107:PRO:O | 1:A:108:GLU:CB | 2.52 | 0.57 |
| 1:A:122:GLN:HE21 | 1:A:124:GLY:HA3 | 1.65 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:187:TRP:O | 1:A:187:TRP:CE3 | 2.57 | 0.57 |
| 1:A:228:LEU:CD1 | 1:A:234:SER:OG | 2.53 | 0.57 |
| 1:B:107:PRO:O | 1:B:108:GLU:CB | 2.52 | 0.57 |
| 1:A:58:GLU:O | 1:A:59:ILE:CG2 | 2.52 | 0.57 |
| 1:A:158:ASP:OD2 | 1:A:160:ASN:ND2 | 2.38 | 0.57 |
| 1:B:9:ALA:HB3 | 1:B:15:TYR:CD1 | 2.39 | 0.57 |
| 1:B:146:ASP:HB2 | 1:B:147:GLU:OE1 | 2.03 | 0.57 |
| 1:A:57:LEU:HB3 | 1:A:68:ILE:H | 1.69 | 0.57 |
| 1:B:228:LEU:CD1 | 1:B:234:SER:OG | 2.53 | 0.57 |
| 1:B:18:TYR:CE1 | 1:B:260:ILE:HD12 | 2.39 | 0.57 |
| 1:B:86:HIS:CG | 1:B:87:GLY:N | 2.71 | 0.57 |
| 1:B:158:ASP:CB | 1:B:161:ASP:HB3 | 2.35 | 0.57 |
| 1:B:187:TRP:O | 1:B:187:TRP:CE3 | 2.57 | 0.57 |
| 1:B:193:ILE:CA | 1:B:197:LYS:O | 2.52 | 0.57 |
| 1:B:230:ALA:CB | 1:B:233:SER:OG | 2.48 | 0.57 |
| 1:A:222:HIS:NE2 | 1:A:226:LYS:CD | 2.62 | 0.56 |
| 1:B:5:ARG:HH12 | 1:B:260:ILE:HG21 | 0.72 | 0.56 |
| 1:B:8:GLY:H | 1:B:265:PRO:HA | 1.69 | 0.56 |
| 1:B:19:ILE:HD13 | 1:B:26:VAL:HG12 | 1.71 | 0.56 |
| 1:B:58:GLU:CD | 1:B:116:ASN:OD1 | 2.43 | 0.56 |
| 1:B:158:ASP:OD2 | 1:B:160:ASN:ND2 | 2.38 | 0.56 |
| 1:B:225:TRP:CE3 | 1:B:226:LYS:N | 2.73 | 0.56 |
| 1:A:242:THR:CA | 1:A:251:THR:HB | 2.32 | 0.56 |
| 1:B:98:THR:HG22 | 1:B:221:THR:OG1 | 1.93 | 0.56 |
| 1:A:54:ASN:OD1 | 1:A:81:ASN:CG | 2.43 | 0.56 |
| 1:A:112:VAL:C | 1:A:150:THR:HB | 2.11 | 0.56 |
| 1:A:137:LYS:HE3 | 1:A:159:ILE:HG23 | 1.88 | 0.56 |
| 1:A:229:ILE:O | 1:A:231:GLY:N | 2.38 | 0.56 |
| 1:B:54:ASN:HB2 | 1:B:275:ILE:HG21 | 1.86 | 0.56 |
| 1:B:137:LYS:HE3 | 1:B:159:ILE:HG23 | 1.88 | 0.56 |
| 1:B:141:ILE:HG13 | 1:B:214:ALA:HA | 1.86 | 0.56 |
| 1:B:157:ILE:HG23 | 1:B:158:ASP:H | 1.69 | 0.56 |
| 1:A:90:HIS:CE1 | 1:A:184:THR:HG23 | 2.40 | 0.56 |
| 1:A:122:GLN:HG2 | 1:A:157:ILE:HA | 1.86 | 0.56 |
| 1:A:164:ALA:C | 1:A:166:LYS:H | 2.07 | 0.56 |
| 1:B:33:PRO:HA | 1:B:97:GLN:NE2 | 2.20 | 0.56 |
| 1:A:218:ILE:HG22 | 1:A:219:LYS:N | 2.19 | 0.56 |
| 1:B:64:THR:C | 1:B:65:LEU:CD2 | 2.72 | 0.56 |
| 1:B:229:ILE:O | 1:B:231:GLY:N | 2.38 | 0.56 |
| 1:A:42:ILE:HG12 | 1:A:43:PHE:CA | 2.23 | 0.56 |
| 1:A:58:GLU:CD | 1:A:116:ASN:OD1 | 2.43 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:9:ALA:CB | 1:A:15:TYR:HA | 2.31 | 0.56 |
| 1:A:90:HIS:O | 1:A:91:ASN:CB | 2.41 | 0.56 |
| 1:B:82:CYS:HG | 1:B:190:ILE:HG13 | 1.66 | 0.56 |
| 1:B:217:ILE:HG23 | 1:B:218:ILE:N | 2.18 | 0.56 |
| 1:A:8:GLY:H | 1:A:265:PRO:HA | 1.70 | 0.56 |
| 1:A:80:ARG:NE | 1:A:80:ARG:HA | 2.19 | 0.56 |
| 1:A:12:THR:OG1 | 1:A:13:LEU:N | 2.39 | 0.56 |
| 1:A:139:LEU:HD12 | 1:A:155:ILE:HG21 | 1.89 | 0.56 |
| 1:B:45:MET:HE2 | 1:B:120:VAL:CG1 | 2.21 | 0.56 |
| 1:B:158:ASP:O | 1:B:159:ILE:C | 2.44 | 0.56 |
| 1:B:218:ILE:HG22 | 1:B:219:LYS:N | 2.19 | 0.56 |
| 1:B:20:GLU:HA | 1:B:26:VAL:HG12 | 1.88 | 0.55 |
| 1:B:59:ILE:CG2 | 1:B:66:ASN:C | 2.66 | 0.55 |
| 1:B:192:LYS:CB | 1:B:197:LYS:HB3 | 2.30 | 0.55 |
| 1:A:32:ILE:O | 1:A:32:ILE:HG22 | 2.06 | 0.55 |
| 1:A:33:PRO:HA | 1:A:97:GLN:NE2 | 2.20 | 0.55 |
| 1:A:35:TYR:N | 1:A:35:TYR:CD2 | 2.70 | 0.55 |
| 1:A:103:ASN:O | 1:A:104:VAL:CB | 2.28 | 0.55 |
| 1:B:105:SER:CB | 1:B:109:THR:HG22 | 2.25 | 0.55 |
| 1:A:4:THR:CA | 1:A:19:ILE:HA | 2.37 | 0.55 |
| 1:A:103:ASN:HA | 1:A:112:VAL:CG1 | 2.33 | 0.55 |
| 1:B:12:THR:OG1 | 1:B:13:LEU:N | 2.39 | 0.55 |
| 1:B:107:PRO:O | 1:B:108:GLU:HB2 | 2.07 | 0.55 |
| 1:B:225:TRP:HE3 | 1:B:226:LYS:N | 2.04 | 0.55 |
| 1:B:34:LEU:C | 1:B:36:ALA:H | 2.06 | 0.55 |
| 1:B:59:ILE:HG22 | 1:B:67:PRO:CD | 2.34 | 0.55 |
| 1:A:25:PRO:HG3 | 1:A:257:SER:CA | 2.37 | 0.55 |
| 1:A:30:HIS:HB3 | 1:A:243:ASN:OD1 | 2.06 | 0.55 |
| 1:A:158:ASP:CB | 1:A:161:ASP:HB3 | 2.35 | 0.55 |
| 1:A:232:LYS:O | 1:A:234:SER:O | 2.25 | 0.55 |
| 1:A:211:LYS:HD3 | 1:A:212:LYS:NZ | 2.22 | 0.55 |
| 1:A:241:LEU:O | 1:A:243:ASN:CG | 2.44 | 0.55 |
| 1:B:4:THR:CA | 1:B:19:ILE:HA | 2.37 | 0.55 |
| 1:A:7:ILE:HG22 | 1:A:15:TYR:CA | 2.35 | 0.55 |
| 1:A:225:TRP:HE3 | 1:A:226:LYS:N | 2.04 | 0.55 |
| 1:B:6:GLN:HB3 | 1:B:265:PRO:HB3 | 1.88 | 0.55 |
| 1:B:8:GLY:HA3 | 1:B:266:LYS:CG | 2.29 | 0.55 |
| 1:B:30:HIS:HB3 | 1:B:243:ASN:OD1 | 2.06 | 0.55 |
| 1:B:181:LEU:O | 1:B:183:ALA:N | 2.40 | 0.55 |
| 1:A:61:LYS:HG3 | 1:A:239:ILE:HG22 | 1.88 | 0.55 |
| 1:A:95:PHE:CE2 | 1:A:154:VAL:HG11 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:139:LEU:CD1 | 1:A:155:ILE:HG21 | 2.37 | 0.55 |
| 1:B:57:LEU:HB3 | 1:B:68:ILE:H | 1.69 | 0.55 |
| 1:B:139:LEU:HD12 | 1:B:155:ILE:HG21 | 1.89 | 0.55 |
| 1:B:232:LYS:O | 1:B:234:SER:O | 2.25 | 0.55 |
| 1:A:6:GLN:HB3 | 1:A:265:PRO:HB3 | 1.88 | 0.55 |
| 1:A:107:PRO:O | 1:A:108:GLU:HB2 | 2.07 | 0.55 |
| 1:A:158:ASP:O | 1:A:159:ILE:C | 2.44 | 0.55 |
| 1:B:95:PHE:CE2 | 1:B:154:VAL:HG11 | 2.42 | 0.55 |
| 1:B:166:LYS:CD | 1:B:176:TYR:CE2 | 2.81 | 0.55 |
| 1:A:25:PRO:HG3 | 1:A:257:SER:O | 2.07 | 0.54 |
| 1:A:58:GLU:N | 1:A:68:ILE:H | 2.05 | 0.54 |
| 1:A:139:LEU:CG | 1:A:155:ILE:CG2 | 2.86 | 0.54 |
| 1:A:226:LYS:C | 1:A:228:LEU:H | 2.11 | 0.54 |
| 1:B:11:ASN:O | 1:B:13:LEU:N | 2.40 | 0.54 |
| 1:B:25:PRO:HG3 | 1:B:257:SER:CA | 2.37 | 0.54 |
| 1:B:58:GLU:N | 1:B:68:ILE:H | 2.05 | 0.54 |
| 1:A:71:ASN:C | 1:A:72:THR:OG1 | 2.43 | 0.54 |
| 1:B:211:LYS:HD3 | 1:B:212:LYS:NZ | 2.22 | 0.54 |
| 1:B:241:LEU:O | 1:B:243:ASN:CG | 2.44 | 0.54 |
| 1:B:147:GLU:O | 1:B:148:GLY:C | 2.45 | 0.54 |
| 1:A:142:MET:HE2 | 1:A:202:PHE:HE1 | 1.64 | 0.54 |
| 1:B:9:ALA:CB | 1:B:15:TYR:HA | 2.31 | 0.54 |
| 1:B:139:LEU:CD1 | 1:B:155:ILE:HG21 | 2.37 | 0.54 |
| 1:B:173:VAL:HA | 1:B:177:PHE:HD1 | 1.73 | 0.54 |
| 1:A:181:LEU:O | 1:A:183:ALA:N | 2.40 | 0.54 |
| 1:A:11:ASN:O | 1:A:13:LEU:N | 2.40 | 0.54 |
| 1:B:11:ASN:HA | 1:B:69:ILE:HD11 | 1.89 | 0.54 |
| 1:B:40:ASP:N | 1:B:40:ASP:OD2 | 2.41 | 0.54 |
| 1:B:61:LYS:HG3 | 1:B:239:ILE:HG22 | 1.88 | 0.54 |
| 1:B:153:LYS:HE2 | 1:B:188:PHE:CZ | 2.43 | 0.54 |
| 1:B:184:THR:O | 1:B:185:ASP:C | 2.46 | 0.54 |
| 1:A:147:GLU:O | 1:A:148:GLY:C | 2.45 | 0.54 |
| 1:A:153:LYS:HE2 | 1:A:188:PHE:CZ | 2.43 | 0.54 |
| 1:B:54:ASN:N | 1:B:54:ASN:ND2 | 2.56 | 0.54 |
| 1:A:228:LEU:HD12 | 1:A:234:SER:OG | 2.08 | 0.54 |
| 1:B:173:VAL:O | 1:B:176:TYR:N | 2.41 | 0.54 |
| 1:A:92:TYR:HA | 1:A:120:VAL:O | 2.08 | 0.54 |
| 1:A:129:TYR:O | 1:A:131:GLY:N | 2.41 | 0.54 |
| 1:B:92:TYR:HA | 1:B:120:VAL:O | 2.08 | 0.54 |
| 1:B:92:TYR:HE2 | 1:B:121:LEU:HD21 | 1.73 | 0.54 |
| 1:B:139:LEU:CG | 1:B:155:ILE:CG2 | 2.86 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:7:ILE:CB | 1:A:16:LYS:H | 2.15 | 0.54 |
| 1:A:11:ASN:HA | 1:A:69:ILE:HD11 | 1.89 | 0.54 |
| 1:A:64:THR:C | 1:A:65:LEU:CD2 | 2.72 | 0.54 |
| 1:A:98:THR:C | 1:A:225:TRP:HB2 | 2.29 | 0.54 |
| 1:A:139:LEU:CD1 | 1:A:155:ILE:CG2 | 2.85 | 0.54 |
| 1:A:173:VAL:O | 1:A:176:TYR:N | 2.41 | 0.54 |
| 1:A:173:VAL:HA | 1:A:177:PHE:HD1 | 1.73 | 0.54 |
| 1:A:20:GLU:HA | 1:A:26:VAL:HG12 | 1.88 | 0.53 |
| 1:A:176:TYR:HB3 | 1:A:177:PHE:CD1 | 2.43 | 0.53 |
| 1:B:176:TYR:HB3 | 1:B:177:PHE:CD1 | 2.43 | 0.53 |
| 1:A:229:ILE:HG22 | 1:A:249:THR:CG2 | 2.38 | 0.53 |
| 1:A:244:VAL:HG21 | 1:A:254:LYS:HG3 | 1.90 | 0.53 |
| 1:A:5:ARG:HH12 | 1:A:260:ILE:HG21 | 0.72 | 0.53 |
| 1:A:98:THR:HG22 | 1:A:221:THR:OG1 | 1.93 | 0.53 |
| 1:B:25:PRO:HG3 | 1:B:257:SER:O | 2.07 | 0.53 |
| 1:B:49:ILE:CG1 | 1:B:92:TYR:CB | 2.86 | 0.53 |
| 1:A:1:THR:CB | 1:A:133:VAL:HG21 | 2.38 | 0.53 |
| 1:B:89:ILE:O | 1:B:90:HIS:CG | 2.61 | 0.53 |
| 1:B:228:LEU:HD12 | 1:B:234:SER:OG | 2.08 | 0.53 |
| 1:A:54:ASN:N | 1:A:54:ASN:ND2 | 2.56 | 0.53 |
| 1:A:122:GLN:HB2 | 1:A:156:ALA:O | 2.07 | 0.53 |
| 1:A:184:THR:HA | 1:A:187:TRP:HD1 | 1.74 | 0.53 |
| 1:B:32:ILE:O | 1:B:32:ILE:HG22 | 2.06 | 0.53 |
| 1:B:188:PHE:O | 1:B:191:TYR:CB | 2.48 | 0.53 |
| 1:B:229:ILE:HG22 | 1:B:249:THR:CG2 | 2.38 | 0.53 |
| 1:B:254:LYS:HG2 | 1:B:254:LYS:O | 2.08 | 0.53 |
| 1:A:182:ARG:HH11 | 1:A:185:ASP:HB2 | 1.72 | 0.53 |
| 1:B:1:THR:CB | 1:B:133:VAL:HG21 | 2.38 | 0.53 |
| 1:B:129:TYR:O | 1:B:131:GLY:N | 2.41 | 0.53 |
| 1:B:222:HIS:CD2 | 1:B:226:LYS:CE | 2.66 | 0.53 |
| 1:A:9:ALA:HB2 | 1:A:15:TYR:N | 2.24 | 0.53 |
| 1:A:40:ASP:N | 1:A:40:ASP:OD2 | 2.41 | 0.53 |
| 1:A:184:THR:O | 1:A:185:ASP:C | 2.46 | 0.53 |
| 1:B:29:PHE:N | 1:B:96:PRO:HB2 | 2.24 | 0.53 |
| 1:B:32:ILE:O | 1:B:33:PRO:O | 2.27 | 0.53 |
| 1:B:184:THR:HA | 1:B:187:TRP:HD1 | 1.74 | 0.53 |
| 1:A:89:ILE:O | 1:A:90:HIS:CG | 2.61 | 0.53 |
| 1:A:159:ILE:O | 1:A:159:ILE:HG22 | 2.09 | 0.53 |
| 1:B:226:LYS:C | 1:B:228:LEU:H | 2.11 | 0.53 |
| 1:B:54:ASN:OD1 | 1:B:81:ASN:OD1 | 2.27 | 0.53 |
| 1:B:81:ASN:ND2 | 1:B:276:ASP:HA | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:90:HIS:CE1 | 1:B:184:THR:HG1 | 2.26 | 0.53 |
| 1:A:81:ASN:ND2 | 1:A:276:ASP:HA | 2.24 | 0.52 |
| 1:A:254:LYS:O | 1:A:254:LYS:HG2 | 2.09 | 0.52 |
| 1:A:49:ILE:CG1 | 1:A:92:TYR:CB | 2.86 | 0.52 |
| 1:A:142:MET:HG3 | 1:A:208:ALA:HB2 | 1.91 | 0.52 |
| 1:A:181:LEU:O | 1:A:184:THR:N | 2.28 | 0.52 |
| 1:B:7:ILE:HG22 | 1:B:15:TYR:CA | 2.35 | 0.52 |
| 1:A:2:TYR:CB | 1:A:22:ASP:H | 2.22 | 0.52 |
| 1:A:54:ASN:OD1 | 1:A:81:ASN:OD1 | 2.27 | 0.52 |
| 1:A:59:ILE:HG22 | 1:A:67:PRO:CD | 2.34 | 0.52 |
| 1:B:29:PHE:HE1 | 1:B:225:TRP:HD1 | 1.53 | 0.52 |
| 1:B:32:ILE:CG2 | 1:B:96:PRO:CG | 2.79 | 0.52 |
| 1:B:48:GLU:HB3 | 1:B:67:PRO:HB3 | 1.91 | 0.52 |
| 1:B:51:ARG:CB | 1:B:51:ARG:CZ | 2.87 | 0.52 |
| 1:A:32:ILE:O | 1:A:33:PRO:O | 2.27 | 0.52 |
| 1:B:7:ILE:CB | 1:B:16:LYS:H | 2.15 | 0.52 |
| 1:B:118:ILE:HG23 | 1:B:119:ASP:N | 2.23 | 0.52 |
| 1:B:122:GLN:HG3 | 1:B:157:ILE:HA | 1.91 | 0.52 |
| 1:A:27:SER:OG | 1:A:30:HIS:HB2 | 2.10 | 0.52 |
| 1:B:50:PRO:HA | 1:B:128:ALA:CB | 2.39 | 0.52 |
| 1:B:98:THR:C | 1:B:225:TRP:HB2 | 2.29 | 0.52 |
| 1:B:106:HIS:CG | 1:B:107:PRO:HD2 | 2.45 | 0.52 |
| 1:A:122:GLN:HG3 | 1:A:157:ILE:HA | 1.91 | 0.52 |
| 1:B:27:SER:OG | 1:B:30:HIS:HB2 | 2.10 | 0.52 |
| 1:B:159:ILE:HG22 | 1:B:159:ILE:O | 2.09 | 0.52 |
| 1:B:209:LYS:CB | 1:B:213:TYR:HB2 | 2.39 | 0.52 |
| 1:B:64:THR:HG22 | 1:B:64:THR:O | 2.09 | 0.52 |
| 1:B:244:VAL:HG21 | 1:B:254:LYS:HG3 | 1.90 | 0.52 |
| 1:A:238:GLY:O | 1:A:239:ILE:HD13 | 2.10 | 0.52 |
| 1:B:21:LYS:HB3 | 1:B:26:VAL:HB | 1.92 | 0.52 |
| 1:B:122:GLN:HB2 | 1:B:156:ALA:O | 2.07 | 0.52 |
| 1:B:190:ILE:O | 1:B:193:ILE:HG12 | 2.10 | 0.52 |
| 1:A:21:LYS:HB3 | 1:A:26:VAL:HB | 1.92 | 0.52 |
| 1:A:48:GLU:HB3 | 1:A:67:PRO:HB3 | 1.91 | 0.52 |
| 1:A:116:ASN:O | 1:A:117:PRO:O | 2.28 | 0.52 |
| 1:A:171:GLU:O | 1:A:172:ASP:C | 2.48 | 0.52 |
| 1:B:142:MET:HG3 | 1:B:208:ALA:HB2 | 1.91 | 0.52 |
| 1:B:69:ILE:HG22 | 1:B:77:ARG:N | 2.20 | 0.52 |
| 1:B:139:LEU:CD1 | 1:B:155:ILE:CG2 | 2.85 | 0.52 |
| 1:B:249:THR:C | 1:B:251:THR:N | 2.59 | 0.52 |
| 1:A:16:LYS:CE | 1:A:62:GLU:OE2 | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:59:ILE:CG2 | 1:A:67:PRO:CA | 2.83 | 0.51 |
| 1:A:92:TYR:HE2 | 1:A:121:LEU:HD21 | 1.73 | 0.51 |
| 1:A:54:ASN:HD22 | 1:A:54:ASN:N | 2.08 | 0.51 |
| 1:B:51:ARG:HA | 1:B:88:TYR:O | 2.10 | 0.51 |
| 1:B:54:ASN:HD22 | 1:B:54:ASN:N | 2.08 | 0.51 |
| 1:B:2:TYR:CB | 1:B:22:ASP:H | 2.22 | 0.51 |
| 1:B:16:LYS:CE | 1:B:62:GLU:OE2 | 2.58 | 0.51 |
| 1:B:74:GLY:O | 1:B:75:LYS:HG2 | 1.96 | 0.51 |
| 1:A:29:PHE:N | 1:A:96:PRO:HB2 | 2.24 | 0.51 |
| 1:A:105:SER:CB | 1:A:109:THR:O | 2.57 | 0.51 |
| 1:A:209:LYS:CB | 1:A:213:TYR:HB2 | 2.39 | 0.51 |
| 1:B:161:ASP:CG | 1:B:162:PRO:HD2 | 2.31 | 0.51 |
| 1:B:238:GLY:O | 1:B:239:ILE:HD13 | 2.10 | 0.51 |
| 1:A:50:PRO:HA | 1:A:128:ALA:CB | 2.39 | 0.51 |
| 1:A:51:ARG:HA | 1:A:88:TYR:O | 2.10 | 0.51 |
| 1:B:46:VAL:HG13 | 1:B:96:PRO:HG3 | 1.92 | 0.51 |
| 1:B:51:ARG:CG | 1:B:90:HIS:N | 2.64 | 0.51 |
| 1:B:58:GLU:O | 1:B:66:ASN:O | 2.29 | 0.51 |
| 1:B:171:GLU:O | 1:B:172:ASP:C | 2.48 | 0.51 |
| 1:A:65:LEU:C | 1:A:66:ASN:ND2 | 2.63 | 0.51 |
| 1:A:106:HIS:CG | 1:A:107:PRO:HD2 | 2.45 | 0.51 |
| 1:B:9:ALA:HB2 | 1:B:15:TYR:N | 2.24 | 0.51 |
| 1:A:51:ARG:HB2 | 1:A:51:ARG:CZ | 2.40 | 0.51 |
| 1:B:38:LYS:HG2 | 1:B:41:ASN:N | 2.26 | 0.51 |
| 1:B:51:ARG:HB2 | 1:B:51:ARG:CZ | 2.40 | 0.51 |
| 1:B:192:LYS:HE3 | 1:B:200:ASN:OD1 | 2.11 | 0.51 |
| 1:B:242:THR:CA | 1:B:251:THR:HB | 2.32 | 0.51 |
| 1:A:89:ILE:O | 1:A:90:HIS:ND1 | 2.44 | 0.51 |
| 1:B:111:ALA:HB1 | 1:B:149:GLU:N | 2.26 | 0.51 |
| 1:A:46:VAL:HG13 | 1:A:96:PRO:HG3 | 1.93 | 0.51 |
| 1:A:64:THR:CG2 | 1:A:64:THR:O | 2.59 | 0.51 |
| 1:B:5:ARG:HH11 | 1:B:260:ILE:CG2 | 1.87 | 0.51 |
| 1:B:105:SER:CB | 1:B:109:THR:O | 2.57 | 0.51 |
| 1:B:115:ASN:C | 1:B:116:ASN:O | 2.49 | 0.51 |
| 1:A:47:VAL:O | 1:A:131:GLY:N | 2.44 | 0.51 |
| 1:A:90:HIS:CE1 | 1:A:184:THR:HG1 | 2.27 | 0.51 |
| 1:A:192:LYS:O | 1:A:193:ILE:C | 2.49 | 0.51 |
| 1:A:1:THR:H3 | 1:A:133:VAL:CG1 | 2.23 | 0.50 |
| 1:A:64:THR:HG22 | 1:A:64:THR:O | 2.09 | 0.50 |
| 1:A:86:HIS:ND1 | 1:A:87:GLY:N | 2.59 | 0.50 |
| 1:B:47:VAL:O | 1:B:131:GLY:N | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:173:VAL:O | 1:B:174:GLU:C | 2.49 | 0.50 |
| 1:B:192:LYS:O | 1:B:193:ILE:C | 2.50 | 0.50 |
| 1:A:38:LYS:HG2 | 1:A:41:ASN:N | 2.26 | 0.50 |
| 1:A:129:TYR:CD2 | 1:A:132:GLN:CD | 2.85 | 0.50 |
| 1:B:38:LYS:HG2 | 1:B:38:LYS:O | 2.11 | 0.50 |
| 1:B:142:MET:HE1 | 1:B:202:PHE:CZ | 2.34 | 0.50 |
| 1:A:38:LYS:HG2 | 1:A:38:LYS:O | 2.11 | 0.50 |
| 1:A:190:ILE:O | 1:A:193:ILE:HG12 | 2.10 | 0.50 |
| 1:B:89:ILE:O | 1:B:90:HIS:ND1 | 2.44 | 0.50 |
| 1:A:161:ASP:CG | 1:A:162:PRO:HD2 | 2.31 | 0.50 |
| 1:A:173:VAL:O | 1:A:174:GLU:C | 2.49 | 0.50 |
| 1:B:11:ASN:HA | 1:B:69:ILE:HD12 | 1.94 | 0.50 |
| 1:B:116:ASN:O | 1:B:117:PRO:O | 2.28 | 0.50 |
| 1:A:62:GLU:O | 1:A:63:GLU:CB | 2.44 | 0.50 |
| 1:B:69:ILE:C | 1:B:70:GLN:O | 2.45 | 0.50 |
| 1:B:129:TYR:CD2 | 1:B:132:GLN:CD | 2.85 | 0.50 |
| 1:A:192:LYS:HE3 | 1:A:200:ASN:OD1 | 2.11 | 0.50 |
| 1:A:252:TYR:HE1 | 1:A:254:LYS:HB2 | 1.76 | 0.50 |
| 1:B:8:GLY:CA | 1:B:266:LYS:N | 2.73 | 0.50 |
| 1:B:241:LEU:O | 1:B:242:THR:O | 2.30 | 0.50 |
| 1:A:8:GLY:CA | 1:A:266:LYS:N | 2.73 | 0.50 |
| 1:A:58:GLU:O | 1:A:66:ASN:O | 2.29 | 0.50 |
| 1:A:115:ASN:C | 1:A:116:ASN:O | 2.49 | 0.50 |
| 1:A:65:LEU:O | 1:A:66:ASN:CG | 2.50 | 0.49 |
| 1:B:42:ILE:HG13 | 1:B:136:VAL:C | 2.10 | 0.49 |
| 1:B:51:ARG:CA | 1:B:88:TYR:O | 2.59 | 0.49 |
| 1:B:164:ALA:C | 1:B:166:LYS:N | 2.65 | 0.49 |
| 1:B:197:LYS:O | 1:B:198:PRO:O | 2.30 | 0.49 |
| 1:A:3:THR:O | 1:A:20:GLU:CA | 2.60 | 0.49 |
| 1:A:142:MET:HE2 | 1:A:202:PHE:HZ | 1.56 | 0.49 |
| 1:A:142:MET:HB2 | 1:A:153:LYS:CB | 2.38 | 0.49 |
| 1:B:86:HIS:ND1 | 1:B:87:GLY:N | 2.59 | 0.49 |
| 1:B:142:MET:CE | 1:B:202:PHE:HE1 | 2.16 | 0.49 |
| 1:B:142:MET:HE2 | 1:B:202:PHE:HE1 | 1.73 | 0.49 |
| 1:A:4:THR:HG22 | 1:A:19:ILE:HA | 1.93 | 0.49 |
| 1:A:51:ARG:CA | 1:A:88:TYR:O | 2.59 | 0.49 |
| 1:A:97:GLN:O | 1:A:225:TRP:CE3 | 2.65 | 0.49 |
| 1:A:111:ALA:HB1 | 1:A:149:GLU:N | 2.26 | 0.49 |
| 1:A:127:ILE:CG2 | 1:A:128:ALA:N | 2.21 | 0.49 |
| 1:B:64:THR:CG2 | 1:B:64:THR:O | 2.59 | 0.49 |
| 1:B:141:ILE:O | 1:B:208:ALA:HB1 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:147:GLU:O | 1:B:149:GLU:HG2 | 2.12 | 0.49 |
| 1:B:244:VAL:CG1 | 1:B:254:LYS:HA | 2.42 | 0.49 |
| 1:A:125:GLU:CD | 1:B:277:LYS:HG2 | 2.33 | 0.49 |
| 1:A:241:LEU:O | 1:A:242:THR:O | 2.30 | 0.49 |
| 1:B:34:LEU:HG | 1:B:96:PRO:O | 2.12 | 0.49 |
| 1:B:43:PHE:CZ | 1:B:218:ILE:HD13 | 2.47 | 0.49 |
| 1:A:213:TYR:O | 1:A:217:ILE:HB | 2.13 | 0.49 |
| 1:B:47:VAL:C | 1:B:48:GLU:HG3 | 2.32 | 0.49 |
| 1:A:34:LEU:HG | 1:A:96:PRO:O | 2.12 | 0.49 |
| 1:A:69:ILE:C | 1:A:70:GLN:O | 2.45 | 0.49 |
| 1:A:94:ALA:O | 1:A:95:PHE:C | 2.51 | 0.49 |
| 1:B:226:LYS:C | 1:B:228:LEU:N | 2.65 | 0.49 |
| 1:A:111:ALA:HB3 | 1:A:145:LEU:CD2 | 2.43 | 0.49 |
| 1:B:97:GLN:O | 1:B:225:TRP:CE3 | 2.65 | 0.49 |
| 1:A:70:GLN:O | 1:A:77:ARG:HB2 | 2.13 | 0.49 |
| 1:A:147:GLU:O | 1:A:149:GLU:HG2 | 2.12 | 0.49 |
| 1:A:164:ALA:C | 1:A:166:LYS:N | 2.65 | 0.49 |
| 1:B:5:ARG:HH22 | 1:B:25:PRO:CB | 2.20 | 0.49 |
| 1:B:59:ILE:CG2 | 1:B:67:PRO:CA | 2.83 | 0.49 |
| 1:B:111:ALA:HB3 | 1:B:145:LEU:CD2 | 2.43 | 0.49 |
| 1:B:177:PHE:N | 1:B:177:PHE:HD1 | 2.08 | 0.49 |
| 1:B:217:ILE:HG22 | 1:B:218:ILE:N | 2.27 | 0.49 |
| 1:A:109:THR:CG2 | 1:A:150:THR:OG1 | 2.49 | 0.49 |
| 1:A:181:LEU:C | 1:A:183:ALA:N | 2.66 | 0.49 |
| 1:B:213:TYR:O | 1:B:217:ILE:HB | 2.13 | 0.49 |
| 1:A:118:ILE:HG23 | 1:A:119:ASP:N | 2.23 | 0.49 |
| 1:B:3:THR:O | 1:B:20:GLU:CA | 2.60 | 0.49 |
| 1:B:27:SER:HB3 | 1:B:31:ASP:OD2 | 2.13 | 0.49 |
| 1:B:49:ILE:HG13 | 1:B:92:TYR:CB | 2.35 | 0.49 |
| 1:B:182:ARG:HH11 | 1:B:185:ASP:HB2 | 1.72 | 0.49 |
| 1:A:43:PHE:CZ | 1:A:218:ILE:HD13 | 2.47 | 0.48 |
| 1:A:158:ASP:HB3 | 1:A:160:ASN:HD22 | 1.78 | 0.48 |
| 1:A:177:PHE:N | 1:A:177:PHE:HD1 | 2.07 | 0.48 |
| 1:A:83:PHE:CD2 | 1:A:84:PRO:N | 2.81 | 0.48 |
| 1:A:188:PHE:O | 1:A:191:TYR:CD2 | 2.67 | 0.48 |
| 1:B:63:GLU:O | 1:B:240:ASP:HB3 | 2.13 | 0.48 |
| 1:B:99:TRP:HZ2 | 1:B:115:ASN:OD1 | 1.96 | 0.48 |
| 1:B:142:MET:HB2 | 1:B:153:LYS:CB | 2.38 | 0.48 |
| 1:B:190:ILE:N | 1:B:193:ILE:HD11 | 2.28 | 0.48 |
| 1:A:47:VAL:C | 1:A:48:GLU:HG3 | 2.32 | 0.48 |
| 1:A:137:LYS:HG3 | 1:A:159:ILE:CD1 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:226:LYS:C | 1:A:228:LEU:N | 2.65 | 0.48 |
| 1:B:160:ASN:ND2 | 1:B:160:ASN:H | 2.10 | 0.48 |
| 1:B:225:TRP:CE3 | 1:B:225:TRP:C | 2.87 | 0.48 |
| 1:A:141:ILE:O | 1:A:208:ALA:HB1 | 2.12 | 0.48 |
| 1:A:225:TRP:CE3 | 1:A:225:TRP:C | 2.87 | 0.48 |
| 1:B:177:PHE:N | 1:B:178:PRO:CD | 2.76 | 0.48 |
| 1:B:190:ILE:O | 1:B:193:ILE:CG1 | 2.61 | 0.48 |
| 1:A:1:THR:N | 1:A:133:VAL:CG1 | 2.60 | 0.48 |
| 1:A:177:PHE:N | 1:A:178:PRO:CD | 2.76 | 0.48 |
| 1:A:190:ILE:N | 1:A:193:ILE:HD11 | 2.29 | 0.48 |
| 1:B:94:ALA:O | 1:B:95:PHE:C | 2.51 | 0.48 |
| 1:B:105:SER:HB2 | 1:B:112:VAL:CA | 2.24 | 0.48 |
| 1:B:209:LYS:CB | 1:B:213:TYR:CB | 2.92 | 0.48 |
| 1:A:37:ASP:O | 1:A:38:LYS:HB3 | 2.12 | 0.48 |
| 1:A:83:PHE:CA | 1:A:278:TRP:CD1 | 2.94 | 0.48 |
| 1:A:209:LYS:CB | 1:A:213:TYR:CB | 2.92 | 0.48 |
| 1:B:70:GLN:O | 1:B:77:ARG:HB2 | 2.13 | 0.48 |
| 1:A:5:ARG:HH11 | 1:A:260:ILE:CG2 | 1.87 | 0.48 |
| 1:B:41:ASN:C | 1:B:42:ILE:HG22 | 2.33 | 0.48 |
| 1:B:83:PHE:CD2 | 1:B:84:PRO:N | 2.81 | 0.48 |
| 1:B:84:PRO:O | 1:B:85:HIS:HB2 | 2.12 | 0.48 |
| 1:B:158:ASP:HB3 | 1:B:160:ASN:HD22 | 1.78 | 0.48 |
| 1:A:11:ASN:HA | 1:A:69:ILE:HD12 | 1.94 | 0.48 |
| 1:A:63:GLU:O | 1:A:240:ASP:HB3 | 2.13 | 0.48 |
| 1:A:122:GLN:HG3 | 1:A:136:VAL:HG21 | 1.96 | 0.48 |
| 1:A:217:ILE:HG22 | 1:A:218:ILE:N | 2.27 | 0.48 |
| 1:B:1:THR:HG22 | 1:B:26:VAL:HG11 | 1.91 | 0.48 |
| 1:A:4:THR:HG22 | 1:A:19:ILE:CA | 2.44 | 0.48 |
| 1:A:27:SER:HB3 | 1:A:31:ASP:OD2 | 2.13 | 0.48 |
| 1:A:69:ILE:HG22 | 1:A:77:ARG:N | 2.20 | 0.48 |
| 1:A:244:VAL:CG1 | 1:A:254:LYS:HA | 2.43 | 0.48 |
| 1:B:4:THR:HG22 | 1:B:19:ILE:HA | 1.93 | 0.48 |
| 1:B:37:ASP:O | 1:B:38:LYS:HB3 | 2.12 | 0.48 |
| 1:A:41:ASN:C | 1:A:42:ILE:HG22 | 2.33 | 0.48 |
| 1:A:190:ILE:O | 1:A:193:ILE:CG1 | 2.61 | 0.48 |
| 1:B:111:ALA:CB | 1:B:145:LEU:HD22 | 2.44 | 0.48 |
| 1:B:129:TYR:O | 1:B:129:TYR:CD1 | 2.67 | 0.48 |
| 1:B:136:VAL:HA | 1:B:159:ILE:H | 1.79 | 0.48 |
| 1:B:163:LEU:HD22 | 1:B:177:PHE:CE1 | 2.48 | 0.48 |
| 1:A:136:VAL:HA | 1:A:159:ILE:H | 1.79 | 0.47 |
| 1:A:168:ASN:ND2 | 1:A:169:ASP:HB2 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:277:LYS:HG2 | 1:B:125:GLU:CD | 2.33 | 0.47 |
| 1:A:49:ILE:HG13 | 1:A:92:TYR:CB | 2.35 | 0.47 |
| 1:A:116:ASN:H | 1:A:116:ASN:HD22 | 1.62 | 0.47 |
| 1:A:160:ASN:ND2 | 1:A:160:ASN:H | 2.10 | 0.47 |
| 1:A:176:TYR:CB | 1:A:177:PHE:CD1 | 2.97 | 0.47 |
| 1:A:176:TYR:CB | 1:A:177:PHE:CE1 | 2.94 | 0.47 |
| 1:A:1:THR:HG22 | 1:A:26:VAL:HG11 | 1.91 | 0.47 |
| 1:A:38:LYS:C | 1:A:40:ASP:H | 2.17 | 0.47 |
| 1:A:197:LYS:O | 1:A:198:PRO:O | 2.30 | 0.47 |
| 1:B:137:LYS:HG3 | 1:B:159:ILE:CD1 | 2.44 | 0.47 |
| 1:B:252:TYR:HE1 | 1:B:254:LYS:HB2 | 1.76 | 0.47 |
| 1:B:168:ASN:ND2 | 1:B:169:ASP:HB2 | 2.29 | 0.47 |
| 1:B:176:TYR:CB | 1:B:177:PHE:CD1 | 2.97 | 0.47 |
| 1:B:188:PHE:O | 1:B:191:TYR:CD2 | 2.67 | 0.47 |
| 1:A:83:PHE:CB | 1:A:84:PRO:HD3 | 2.42 | 0.47 |
| 1:B:122:GLN:HG3 | 1:B:136:VAL:HG21 | 1.96 | 0.47 |
| 1:B:186:GLU:HA | 1:B:189:ARG:HG3 | 1.96 | 0.47 |
| 1:B:222:HIS:CE1 | 1:B:225:TRP:CZ3 | 3.02 | 0.47 |
| 1:A:59:ILE:HA | 1:A:66:ASN:C | 2.34 | 0.47 |
| 1:B:4:THR:HG22 | 1:B:19:ILE:CA | 2.44 | 0.47 |
| 1:B:34:LEU:C | 1:B:36:ALA:N | 2.67 | 0.47 |
| 1:B:51:ARG:HG3 | 1:B:90:HIS:N | 2.06 | 0.47 |
| 1:B:118:ILE:O | 1:B:118:ILE:HG22 | 2.14 | 0.47 |
| 1:A:25:PRO:HG3 | 1:A:257:SER:HA | 1.97 | 0.47 |
| 1:A:129:TYR:O | 1:A:129:TYR:CD1 | 2.67 | 0.47 |
| 1:A:176:TYR:C | 1:A:178:PRO:HD3 | 2.35 | 0.47 |
| 1:B:83:PHE:CA | 1:B:278:TRP:CD1 | 2.94 | 0.47 |
| 1:B:89:ILE:O | 1:B:89:ILE:HD13 | 2.14 | 0.47 |
| 1:B:176:TYR:C | 1:B:178:PRO:HD3 | 2.35 | 0.47 |
| 1:B:211:LYS:HD3 | 1:B:212:LYS:HZ3 | 1.80 | 0.47 |
| 1:A:58:GLU:OE2 | 1:A:116:ASN:OD1 | 2.33 | 0.47 |
| 1:A:137:LYS:HE3 | 1:A:159:ILE:CG2 | 2.45 | 0.47 |
| 1:B:19:ILE:CD1 | 1:B:26:VAL:HG13 | 2.33 | 0.47 |
| 1:A:122:GLN:NE2 | 1:A:124:GLY:N | 2.63 | 0.47 |
| 1:A:144:LEU:O | 1:A:151:ASP:HB2 | 2.14 | 0.47 |
| 1:A:222:HIS:CE1 | 1:A:225:TRP:CZ3 | 3.02 | 0.47 |
| 1:B:4:THR:HA | 1:B:20:GLU:H | 1.80 | 0.47 |
| 1:B:144:LEU:O | 1:B:151:ASP:HB2 | 2.14 | 0.47 |
| 1:B:176:TYR:CB | 1:B:177:PHE:CE1 | 2.94 | 0.47 |
| 1:A:34:LEU:C | 1:A:36:ALA:N | 2.67 | 0.47 |
| 1:B:58:GLU:HG3 | 1:B:70:GLN:HE22 | 1.61 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:137:LYS:HE3 | 1:B:159:ILE:CG2 | 2.45 | 0.47 |
| 1:B:247:PRO:CA | 1:B:252:TYR:CD2 | 2.93 | 0.47 |
| 1:A:20:GLU:CA | 1:A:26:VAL:HG12 | 2.45 | 0.46 |
| 1:A:111:ALA:CB | 1:A:145:LEU:HD22 | 2.44 | 0.46 |
| 1:A:186:GLU:HA | 1:A:189:ARG:HG3 | 1.96 | 0.46 |
| 1:B:12:THR:CG2 | 1:B:269:ALA:CB | 2.91 | 0.46 |
| 1:B:116:ASN:H | 1:B:116:ASN:HD22 | 1.62 | 0.46 |
| 1:B:219:LYS:C | 1:B:221:THR:H | 2.18 | 0.46 |
| 1:A:4:THR:HA | 1:A:20:GLU:H | 1.80 | 0.46 |
| 1:A:99:TRP:HZ2 | 1:A:115:ASN:OD1 | 1.96 | 0.46 |
| 1:A:139:LEU:H | 1:A:155:ILE:HG22 | 1.81 | 0.46 |
| 1:A:247:PRO:CA | 1:A:252:TYR:CD2 | 2.93 | 0.46 |
| 1:B:57:LEU:HB3 | 1:B:68:ILE:CA | 2.46 | 0.46 |
| 1:B:59:ILE:HA | 1:B:66:ASN:C | 2.34 | 0.46 |
| 1:B:142:MET:HE2 | 1:B:202:PHE:HZ | 1.55 | 0.46 |
| 1:A:89:ILE:O | 1:A:89:ILE:HD13 | 2.14 | 0.46 |
| 1:A:161:ASP:OD1 | 1:A:162:PRO:CD | 2.60 | 0.46 |
| 1:A:168:ASN:C | 1:A:168:ASN:HD22 | 2.18 | 0.46 |
| 1:B:122:GLN:NE2 | 1:B:124:GLY:N | 2.63 | 0.46 |
| 1:A:19:ILE:CD1 | 1:A:26:VAL:HG13 | 2.33 | 0.46 |
| 1:B:20:GLU:CA | 1:B:26:VAL:HG12 | 2.45 | 0.46 |
| 1:B:142:MET:O | 1:B:152:TRP:C | 2.48 | 0.46 |
| 1:A:4:THR:CG2 | 1:A:19:ILE:CB | 2.94 | 0.46 |
| 1:A:29:PHE:HE1 | 1:A:225:TRP:HD1 | 1.54 | 0.46 |
| 1:A:142:MET:HE1 | 1:A:202:PHE:CZ | 2.35 | 0.46 |
| 1:A:188:PHE:C | 1:A:191:TYR:HB3 | 2.35 | 0.46 |
| 1:B:106:HIS:CD2 | 1:B:107:PRO:HD2 | 2.51 | 0.46 |
| 1:B:71:ASN:O | 1:B:72:THR:HB | 2.09 | 0.46 |
| 1:A:12:THR:CG2 | 1:A:269:ALA:CB | 2.91 | 0.46 |
| 1:A:54:ASN:CB | 1:A:275:ILE:HG21 | 2.46 | 0.46 |
| 1:B:54:ASN:CB | 1:B:275:ILE:HG21 | 2.46 | 0.46 |
| 1:B:136:VAL:HG11 | 1:B:156:ALA:CB | 2.36 | 0.46 |
| 1:A:10:LYS:N | 1:A:15:TYR:CG | 2.84 | 0.46 |
| 1:A:54:ASN:CB | 1:A:275:ILE:CG2 | 2.94 | 0.46 |
| 1:A:106:HIS:CD2 | 1:A:107:PRO:HD2 | 2.51 | 0.46 |
| 1:B:22:ASP:HB3 | 1:B:23:GLY:H | 1.58 | 0.46 |
| 1:B:38:LYS:C | 1:B:40:ASP:H | 2.17 | 0.46 |
| 1:B:54:ASN:CB | 1:B:275:ILE:CG2 | 2.94 | 0.46 |
| 1:B:174:GLU:OE2 | 1:B:181:LEU:HD12 | 2.16 | 0.46 |
| 1:A:91:ASN:OD1 | 1:A:128:ALA:HB2 | 2.16 | 0.46 |
| 1:B:4:THR:CG2 | 1:B:19:ILE:CB | 2.94 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:83:PHE:CB | 1:B:84:PRO:HD3 | 2.42 | 0.46 |
| 1:A:118:ILE:O | 1:A:118:ILE:HG22 | 2.14 | 0.46 |
| 1:A:19:ILE:HG23 | 1:A:26:VAL:HG13 | 1.99 | 0.45 |
| 1:A:29:PHE:HA | 1:A:96:PRO:CB | 2.46 | 0.45 |
| 1:A:167:LEU:HD11 | 1:A:177:PHE:HE1 | 1.81 | 0.45 |
| 1:A:182:ARG:CD | 1:A:185:ASP:OD2 | 2.58 | 0.45 |
| 1:A:219:LYS:C | 1:A:221:THR:H | 2.18 | 0.45 |
| 1:B:58:GLU:OE2 | 1:B:116:ASN:OD1 | 2.33 | 0.45 |
| 1:B:181:LEU:C | 1:B:183:ALA:N | 2.66 | 0.45 |
| 1:A:225:TRP:HZ3 | 1:A:226:LYS:CG | 2.13 | 0.45 |
| 1:B:10:LYS:N | 1:B:15:TYR:CG | 2.84 | 0.45 |
| 1:B:19:ILE:HD13 | 1:B:26:VAL:HG13 | 1.75 | 0.45 |
| 1:B:63:GLU:HA | 1:B:240:ASP:CG | 2.36 | 0.45 |
| 1:A:163:LEU:HD22 | 1:A:177:PHE:CE1 | 2.48 | 0.45 |
| 1:B:61:LYS:HG3 | 1:B:239:ILE:CG2 | 2.47 | 0.45 |
| 1:B:106:HIS:CB | 1:B:107:PRO:CD | 2.94 | 0.45 |
| 1:B:222:HIS:O | 1:B:226:LYS:N | 2.47 | 0.45 |
| 1:A:63:GLU:HA | 1:A:240:ASP:CG | 2.36 | 0.45 |
| 1:A:174:GLU:OE2 | 1:A:181:LEU:HD12 | 2.16 | 0.45 |
| 1:B:25:PRO:HG3 | 1:B:257:SER:C | 2.37 | 0.45 |
| 1:A:10:LYS:CD | 1:A:268:ASP:OD2 | 2.64 | 0.45 |
| 1:A:57:LEU:HB3 | 1:A:68:ILE:CA | 2.46 | 0.45 |
| 1:A:180:LEU:O | 1:A:184:THR:OG1 | 2.34 | 0.45 |
| 1:B:19:ILE:HG23 | 1:B:26:VAL:HG13 | 1.99 | 0.45 |
| 1:B:27:SER:O | 1:B:31:ASP:HB2 | 2.16 | 0.45 |
| 1:B:91:ASN:OD1 | 1:B:128:ALA:HB2 | 2.16 | 0.45 |
| 1:B:139:LEU:H | 1:B:155:ILE:HG22 | 1.81 | 0.45 |
| 1:A:27:SER:O | 1:A:31:ASP:HB2 | 2.16 | 0.45 |
| 1:A:28:ALA:O | 1:A:29:PHE:CB | 2.63 | 0.45 |
| 1:A:100:GLU:CG | 1:A:117:PRO:O | 2.64 | 0.45 |
| 1:A:106:HIS:CB | 1:A:107:PRO:CD | 2.94 | 0.45 |
| 1:A:130:THR:O | 1:A:130:THR:HG23 | 2.15 | 0.45 |
| 1:B:9:ALA:HB3 | 1:B:15:TYR:HA | 1.88 | 0.45 |
| 1:B:181:LEU:O | 1:B:182:ARG:C | 2.55 | 0.45 |
| 1:A:146:ASP:O | 1:A:147:GLU:C | 2.54 | 0.45 |
| 1:B:10:LYS:CD | 1:B:268:ASP:OD2 | 2.64 | 0.45 |
| 1:B:19:ILE:C | 1:B:26:VAL:CG1 | 2.85 | 0.45 |
| 1:B:111:ALA:CB | 1:B:145:LEU:CD2 | 2.94 | 0.45 |
| 1:B:167:LEU:HD11 | 1:B:177:PHE:HE1 | 1.81 | 0.45 |
| 1:B:180:LEU:O | 1:B:184:THR:OG1 | 2.34 | 0.45 |
| 1:A:4:THR:HA | 1:A:20:GLU:N | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:25:PRO:HG3 | 1:A:257:SER:C | 2.37 | 0.45 |
| 1:A:111:ALA:CB | 1:A:145:LEU:CD2 | 2.94 | 0.45 |
| 1:A:174:GLU:CD | 1:A:181:LEU:HD12 | 2.36 | 0.45 |
| 1:B:42:ILE:HG12 | 1:B:43:PHE:H | 0.63 | 0.45 |
| 1:B:65:LEU:O | 1:B:66:ASN:CG | 2.50 | 0.45 |
| 1:A:225:TRP:CE3 | 1:A:226:LYS:CA | 3.00 | 0.45 |
| 1:B:100:GLU:CG | 1:B:117:PRO:O | 2.64 | 0.45 |
| 1:B:161:ASP:OD1 | 1:B:162:PRO:CD | 2.60 | 0.45 |
| 1:B:217:ILE:O | 1:B:221:THR:HB | 2.17 | 0.45 |
| 1:A:177:PHE:O | 1:A:179:GLY:N | 2.50 | 0.45 |
| 1:A:181:LEU:O | 1:A:182:ARG:C | 2.55 | 0.45 |
| 1:B:29:PHE:HA | 1:B:96:PRO:CB | 2.47 | 0.45 |
| 1:B:237:LYS:HD3 | 1:B:241:LEU:HD21 | 1.99 | 0.45 |
| 1:A:9:ALA:HB2 | 1:A:15:TYR:HA | 1.98 | 0.44 |
| 1:A:139:LEU:CG | 1:A:155:ILE:HG21 | 2.43 | 0.44 |
| 1:B:92:TYR:CD2 | 1:B:121:LEU:HD21 | 2.51 | 0.44 |
| 1:B:168:ASN:C | 1:B:168:ASN:HD22 | 2.18 | 0.44 |
| 1:B:174:GLU:CD | 1:B:181:LEU:HD12 | 2.36 | 0.44 |
| 1:B:190:ILE:H | 1:B:190:ILE:HG23 | 1.56 | 0.44 |
| 1:A:237:LYS:HD3 | 1:A:241:LEU:HD21 | 1.99 | 0.44 |
| 1:B:4:THR:HA | 1:B:20:GLU:N | 2.31 | 0.44 |
| 1:B:47:VAL:HG22 | 1:B:131:GLY:N | 2.26 | 0.44 |
| 1:B:146:ASP:O | 1:B:147:GLU:C | 2.54 | 0.44 |
| 1:A:12:THR:O | 1:A:76:LEU:HD21 | 2.17 | 0.44 |
| 1:A:71:ASN:O | 1:A:72:THR:HB | 2.09 | 0.44 |
| 1:A:84:PRO:O | 1:A:85:HIS:HB2 | 2.12 | 0.44 |
| 1:B:225:TRP:CE3 | 1:B:226:LYS:CA | 3.00 | 0.44 |
| 1:A:83:PHE:HA | 1:A:278:TRP:CG | 2.52 | 0.44 |
| 1:B:60:THR:O | 1:B:61:LYS:HB2 | 2.17 | 0.44 |
| 1:B:134:LYS:CE | 1:B:158:ASP:OD1 | 2.52 | 0.44 |
| 1:A:60:THR:O | 1:A:61:LYS:HB2 | 2.17 | 0.44 |
| 1:A:65:LEU:HD22 | 1:A:65:LEU:N | 2.32 | 0.44 |
| 1:A:95:PHE:HD2 | 1:A:218:ILE:HG12 | 1.83 | 0.44 |
| 1:A:98:THR:CA | 1:A:225:TRP:CB | 2.96 | 0.44 |
| 1:A:222:HIS:O | 1:A:226:LYS:N | 2.47 | 0.44 |
| 1:B:12:THR:O | 1:B:76:LEU:HD21 | 2.17 | 0.44 |
| 1:A:168:ASN:O | 1:A:168:ASN:CG | 2.56 | 0.44 |
| 1:A:217:ILE:O | 1:A:221:THR:HB | 2.17 | 0.44 |
| 1:B:42:ILE:HD11 | 1:B:136:VAL:H | 1.83 | 0.44 |
| 1:B:146:ASP:CB | 1:B:147:GLU:OE1 | 2.65 | 0.44 |
| 1:A:47:VAL:HG22 | 1:A:131:GLY:N | 2.26 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:61:LYS:HG3 | 1:A:239:ILE:CG2 | 2.47 | 0.44 |
| 1:A:102:PRO:HA | 1:A:113:GLY:C | 2.38 | 0.44 |
| 1:A:136:VAL:HG11 | 1:A:156:ALA:CB | 2.36 | 0.44 |
| 1:A:142:MET:O | 1:A:152:TRP:HA | 2.18 | 0.44 |
| 1:A:146:ASP:CB | 1:A:147:GLU:OE1 | 2.65 | 0.44 |
| 1:A:174:GLU:O | 1:A:178:PRO:CA | 2.57 | 0.44 |
| 1:B:9:ALA:HB2 | 1:B:15:TYR:HA | 1.98 | 0.44 |
| 1:B:95:PHE:HD2 | 1:B:218:ILE:HG12 | 1.83 | 0.44 |
| 1:B:102:PRO:HA | 1:B:113:GLY:C | 2.38 | 0.44 |
| 1:B:182:ARG:HD3 | 1:B:182:ARG:HA | 1.72 | 0.44 |
| 1:A:6:GLN:O | 1:A:265:PRO:N | 2.51 | 0.44 |
| 1:A:19:ILE:C | 1:A:26:VAL:CG1 | 2.85 | 0.44 |
| 1:A:27:SER:HB3 | 1:A:31:ASP:CG | 2.39 | 0.44 |
| 1:A:38:LYS:CG | 1:A:38:LYS:O | 2.66 | 0.44 |
| 1:B:142:MET:O | 1:B:152:TRP:HA | 2.18 | 0.44 |
| 1:B:29:PHE:N | 1:B:96:PRO:CB | 2.81 | 0.44 |
| 1:B:65:LEU:HD22 | 1:B:65:LEU:N | 2.32 | 0.44 |
| 1:B:177:PHE:O | 1:B:179:GLY:N | 2.50 | 0.44 |
| 1:B:192:LYS:CE | 1:B:200:ASN:HD21 | 2.29 | 0.44 |
| 1:A:192:LYS:CE | 1:A:200:ASN:HD21 | 2.29 | 0.43 |
| 1:B:1:THR:H3 | 1:B:133:VAL:CG1 | 2.25 | 0.43 |
| 1:B:6:GLN:O | 1:B:265:PRO:N | 2.51 | 0.43 |
| 1:B:135:GLU:O | 1:B:136:VAL:CB | 2.38 | 0.43 |
| 1:A:52:TRP:HB3 | 1:A:86:HIS:CD2 | 2.53 | 0.43 |
| 1:A:58:GLU:HG3 | 1:A:70:GLN:HE22 | 1.62 | 0.43 |
| 1:A:143:ALA:O | 1:A:202:PHE:HD1 | 1.99 | 0.43 |
| 1:B:80:ARG:HG3 | 1:B:194:PRO:CG | 2.48 | 0.43 |
| 1:B:193:ILE:HG12 | 1:B:193:ILE:H | 1.55 | 0.43 |
| 1:A:98:THR:HG22 | 1:A:99:TRP:N | 2.33 | 0.43 |
| 1:B:27:SER:HB3 | 1:B:31:ASP:CG | 2.38 | 0.43 |
| 1:B:57:LEU:CB | 1:B:68:ILE:H | 2.31 | 0.43 |
| 1:B:62:GLU:O | 1:B:63:GLU:CB | 2.44 | 0.43 |
| 1:B:98:THR:CA | 1:B:225:TRP:CB | 2.96 | 0.43 |
| 1:B:188:PHE:C | 1:B:191:TYR:HB3 | 2.35 | 0.43 |
| 1:A:42:ILE:HD11 | 1:A:136:VAL:H | 1.83 | 0.43 |
| 1:A:83:PHE:CZ | 1:B:179:GLY:HA3 | 2.53 | 0.43 |
| 1:A:163:LEU:HB3 | 1:A:167:LEU:CD1 | 2.49 | 0.43 |
| 1:A:182:ARG:HD3 | 1:A:182:ARG:HA | 1.72 | 0.43 |
| 1:B:52:TRP:HB3 | 1:B:86:HIS:CD2 | 2.53 | 0.43 |
| 1:B:209:LYS:HB2 | 1:B:213:TYR:CB | 2.49 | 0.43 |
| 1:B:232:LYS:O | 1:B:234:SER:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:142:MET:O | 1:A:152:TRP:C | 2.48 | 0.43 |
| 1:A:170:ILE:CG1 | 1:A:210:ASN:HA | 2.48 | 0.43 |
| 1:A:179:GLY:HA3 | 1:B:83:PHE:CZ | 2.53 | 0.43 |
| 1:A:51:ARG:HG3 | 1:A:90:HIS:N | 2.06 | 0.43 |
| 1:A:95:PHE:HD2 | 1:A:218:ILE:CG1 | 2.32 | 0.43 |
| 1:A:209:LYS:HB2 | 1:A:213:TYR:CB | 2.49 | 0.43 |
| 1:B:81:ASN:OD1 | 1:B:87:GLY:N | 2.51 | 0.43 |
| 1:A:8:GLY:HA3 | 1:A:266:LYS:N | 2.34 | 0.43 |
| 1:A:81:ASN:OD1 | 1:A:87:GLY:N | 2.51 | 0.43 |
| 1:A:83:PHE:CE1 | 1:A:280:PHE:CZ | 2.98 | 0.43 |
| 1:B:168:ASN:O | 1:B:168:ASN:CG | 2.56 | 0.43 |
| 1:B:238:GLY:O | 1:B:239:ILE:CG2 | 2.56 | 0.43 |
| 1:A:105:SER:HB2 | 1:A:112:VAL:CA | 2.24 | 0.43 |
| 1:A:215:LEU:O | 1:A:219:LYS:HB2 | 2.19 | 0.43 |
| 1:B:176:TYR:C | 1:B:178:PRO:CD | 2.88 | 0.43 |
| 1:B:215:LEU:O | 1:B:219:LYS:HB2 | 2.19 | 0.43 |
| 1:A:176:TYR:C | 1:A:178:PRO:CD | 2.87 | 0.42 |
| 1:A:232:LYS:O | 1:A:234:SER:N | 2.51 | 0.42 |
| 1:B:34:LEU:HD21 | 1:B:95:PHE:CA | 2.49 | 0.42 |
| 1:B:95:PHE:HD2 | 1:B:218:ILE:CG1 | 2.32 | 0.42 |
| 1:B:98:THR:HG22 | 1:B:99:TRP:N | 2.33 | 0.42 |
| 1:B:111:ALA:O | 1:B:112:VAL:C | 2.57 | 0.42 |
| 1:B:170:ILE:CG1 | 1:B:210:ASN:HA | 2.48 | 0.42 |
| 1:B:174:GLU:O | 1:B:178:PRO:CA | 2.57 | 0.42 |
| 1:A:29:PHE:N | 1:A:96:PRO:CB | 2.81 | 0.42 |
| 1:A:34:LEU:HD21 | 1:A:95:PHE:CA | 2.49 | 0.42 |
| 1:A:36:ALA:O | 1:A:43:PHE:HA | 2.19 | 0.42 |
| 1:A:57:LEU:CB | 1:A:68:ILE:H | 2.31 | 0.42 |
| 1:A:238:GLY:O | 1:A:239:ILE:CG2 | 2.56 | 0.42 |
| 1:B:142:MET:HB3 | 1:B:153:LYS:CG | 2.50 | 0.42 |
| 1:B:182:ARG:CD | 1:B:185:ASP:OD2 | 2.58 | 0.42 |
| 1:B:244:VAL:CG2 | 1:B:254:LYS:HG3 | 2.49 | 0.42 |
| 1:A:30:HIS:CD2 | 1:A:241:LEU:O | 2.72 | 0.42 |
| 1:A:83:PHE:HZ | 1:B:179:GLY:C | 2.22 | 0.42 |
| 1:A:117:PRO:HB2 | 1:A:118:ILE:H | 1.67 | 0.42 |
| 1:A:179:GLY:C | 1:B:83:PHE:HZ | 2.22 | 0.42 |
| 1:B:30:HIS:CD2 | 1:B:241:LEU:O | 2.72 | 0.42 |
| 1:B:95:PHE:CD2 | 1:B:218:ILE:CG1 | 3.02 | 0.42 |
| 1:A:69:ILE:CG2 | 1:A:77:ARG:H | 2.24 | 0.42 |
| 1:A:80:ARG:HG3 | 1:A:194:PRO:CG | 2.48 | 0.42 |
| 1:A:111:ALA:O | 1:A:112:VAL:C | 2.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:226:LYS:O | 1:A:228:LEU:N | 2.53 | 0.42 |
| 1:B:8:GLY:HA3 | 1:B:266:LYS:N | 2.34 | 0.42 |
| 1:B:142:MET:HB3 | 1:B:153:LYS:HG2 | 2.01 | 0.42 |
| 1:A:142:MET:HB3 | 1:A:153:LYS:CG | 2.50 | 0.42 |
| 1:A:277:LYS:HG2 | 1:B:125:GLU:OE2 | 2.10 | 0.42 |
| 1:B:105:SER:H | 1:B:112:VAL:CG1 | 2.20 | 0.42 |
| 1:B:215:LEU:HD23 | 1:B:215:LEU:HA | 1.84 | 0.42 |
| 1:B:226:LYS:O | 1:B:228:LEU:N | 2.53 | 0.42 |
| 1:A:19:ILE:HD13 | 1:A:26:VAL:HG13 | 1.75 | 0.42 |
| 1:A:118:ILE:HD12 | 1:A:221:THR:CB | 2.49 | 0.42 |
| 1:A:125:GLU:OE2 | 1:B:277:LYS:HG2 | 2.10 | 0.42 |
| 1:A:164:ALA:O | 1:A:166:LYS:N | 2.53 | 0.42 |
| 1:B:36:ALA:O | 1:B:43:PHE:HA | 2.19 | 0.42 |
| 1:B:83:PHE:HA | 1:B:278:TRP:CG | 2.52 | 0.42 |
| 1:A:95:PHE:CD2 | 1:A:218:ILE:CG1 | 3.02 | 0.42 |
| 1:A:134:LYS:CE | 1:A:158:ASP:OD1 | 2.52 | 0.42 |
| 1:B:252:TYR:CD1 | 1:B:252:TYR:C | 2.92 | 0.42 |
| 1:A:9:ALA:HB3 | 1:A:15:TYR:HA | 1.88 | 0.42 |
| 1:A:42:ILE:CB | 1:A:159:ILE:HD11 | 2.50 | 0.42 |
| 1:A:136:VAL:C | 1:A:159:ILE:HG13 | 2.40 | 0.42 |
| 1:A:244:VAL:CG2 | 1:A:254:LYS:HG3 | 2.49 | 0.42 |
| 1:B:41:ASN:HB3 | 1:B:42:ILE:H | 1.72 | 0.42 |
| 1:B:136:VAL:HG22 | 1:B:157:ILE:H | 1.14 | 0.42 |
| 1:A:59:ILE:HG13 | 1:A:65:LEU:HB3 | 2.02 | 0.42 |
| 1:A:177:PHE:HD1 | 1:A:177:PHE:H | 1.68 | 0.42 |
| 1:B:10:LYS:O | 1:B:11:ASN:ND2 | 2.53 | 0.42 |
| 1:B:59:ILE:HB | 1:B:66:ASN:CA | 2.49 | 0.42 |
| 1:B:118:ILE:HD12 | 1:B:221:THR:CB | 2.49 | 0.42 |
| 1:B:214:ALA:O | 1:B:218:ILE:N | 2.41 | 0.42 |
| 1:A:59:ILE:HB | 1:A:66:ASN:CA | 2.49 | 0.42 |
| 1:A:241:LEU:N | 1:A:241:LEU:CD1 | 2.83 | 0.42 |
| 1:A:252:TYR:CD1 | 1:A:252:TYR:C | 2.92 | 0.42 |
| 1:A:275:ILE:O | 1:A:277:LYS:CB | 2.66 | 0.42 |
| 1:A:7:ILE:C | 1:A:8:GLY:O | 2.50 | 0.41 |
| 1:A:10:LYS:C | 1:A:11:ASN:CG | 2.77 | 0.41 |
| 1:B:25:PRO:HG3 | 1:B:257:SER:HA | 1.97 | 0.41 |
| 1:B:38:LYS:CG | 1:B:38:LYS:O | 2.66 | 0.41 |
| 1:B:136:VAL:C | 1:B:159:ILE:HG13 | 2.40 | 0.41 |
| 1:A:16:LYS:HE2 | 1:A:62:GLU:OE2 | 2.20 | 0.41 |
| 1:A:45:MET:HB3 | 1:A:95:PHE:HE1 | 1.86 | 0.41 |
| 1:B:16:LYS:HE2 | 1:B:62:GLU:OE2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:32:ILE:HG21 | 1:B:96:PRO:HG3 | 2.00 | 0.41 |
| 1:B:122:GLN:HG2 | 1:B:156:ALA:O | 2.20 | 0.41 |
| 1:B:200:ASN:HD22 | 1:B:200:ASN:HA | 1.60 | 0.41 |
| 1:A:10:LYS:O | 1:A:11:ASN:ND2 | 2.53 | 0.41 |
| 1:A:41:ASN:HB3 | 1:A:42:ILE:H | 1.72 | 0.41 |
| 1:A:42:ILE:CD1 | 1:A:136:VAL:H | 2.33 | 0.41 |
| 1:A:122:GLN:HG2 | 1:A:156:ALA:O | 2.20 | 0.41 |
| 1:A:139:LEU:N | 1:A:155:ILE:HG22 | 2.36 | 0.41 |
| 1:A:148:GLY:O | 1:A:149:GLU:HG2 | 2.20 | 0.41 |
| 1:B:34:LEU:C | 1:B:43:PHE:CB | 2.82 | 0.41 |
| 1:B:42:ILE:CB | 1:B:159:ILE:HD11 | 2.50 | 0.41 |
| 1:B:218:ILE:O | 1:B:218:ILE:HG23 | 2.17 | 0.41 |
| 1:A:142:MET:HB3 | 1:A:153:LYS:HG2 | 2.01 | 0.41 |
| 1:A:175:LYS:C | 1:A:178:PRO:HD3 | 2.41 | 0.41 |
| 1:A:193:ILE:HG12 | 1:A:193:ILE:H | 1.55 | 0.41 |
| 1:B:42:ILE:CD1 | 1:B:136:VAL:H | 2.33 | 0.41 |
| 1:B:64:THR:O | 1:B:65:LEU:HD22 | 2.20 | 0.41 |
| 1:B:112:VAL:HB | 1:B:113:GLY:H | 1.51 | 0.41 |
| 1:B:113:GLY:HA2 | 1:B:150:THR:HB | 2.02 | 0.41 |
| 1:B:139:LEU:N | 1:B:155:ILE:HG22 | 2.36 | 0.41 |
| 1:B:160:ASN:HD22 | 1:B:161:ASP:H | 1.67 | 0.41 |
| 1:B:164:ALA:O | 1:B:166:LYS:N | 2.53 | 0.41 |
| 1:B:225:TRP:CE3 | 1:B:226:LYS:HA | 2.55 | 0.41 |
| 1:B:275:ILE:O | 1:B:277:LYS:CB | 2.66 | 0.41 |
| 1:A:28:ALA:HA | 1:A:32:ILE:CG1 | 2.48 | 0.41 |
| 1:A:113:GLY:HA2 | 1:A:150:THR:HB | 2.03 | 0.41 |
| 1:A:177:PHE:CA | 1:B:280:PHE:CE2 | 3.03 | 0.41 |
| 1:A:242:THR:HA | 1:A:251:THR:O | 2.20 | 0.41 |
| 1:B:147:GLU:OE1 | 1:B:147:GLU:N | 2.54 | 0.41 |
| 1:B:163:LEU:HB3 | 1:B:167:LEU:CD1 | 2.49 | 0.41 |
| 1:B:189:ARG:C | 1:B:191:TYR:N | 2.74 | 0.41 |
| 1:B:191:TYR:CD2 | 1:B:192:LYS:N | 2.89 | 0.41 |
| 1:A:81:ASN:O | 1:A:278:TRP:HD1 | 2.04 | 0.41 |
| 1:A:225:TRP:CE3 | 1:A:226:LYS:HA | 2.55 | 0.41 |
| 1:A:249:THR:C | 1:A:251:THR:N | 2.59 | 0.41 |
| 1:B:134:LYS:HE3 | 1:B:158:ASP:CG | 2.37 | 0.41 |
| 1:A:92:TYR:CD2 | 1:A:121:LEU:HD21 | 2.51 | 0.41 |
| 1:A:142:MET:CE | 1:A:202:PHE:HE1 | 2.16 | 0.41 |
| 1:A:228:LEU:O | 1:A:229:ILE:C | 2.59 | 0.41 |
| 1:B:242:THR:HA | 1:B:251:THR:O | 2.20 | 0.41 |
| 1:A:200:ASN:C | 1:A:201:GLN:CG | 2.63 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:218:ILE:O | 1:A:218:ILE:HG23 | 2.17 | 0.41 |
| 1:B:139:LEU:O | 1:B:211:LYS:HB2 | 2.21 | 0.41 |
| 1:B:148:GLY:O | 1:B:149:GLU:HG2 | 2.20 | 0.41 |
| 1:B:182:ARG:NH1 | 1:B:185:ASP:CB | 2.66 | 0.41 |
| 1:A:4:THR:HA | 1:A:19:ILE:HA | 2.03 | 0.41 |
| 1:A:59:ILE:CG2 | 1:A:67:PRO:CD | 2.96 | 0.41 |
| 1:A:112:VAL:O | 1:A:150:THR:CG2 | 2.61 | 0.41 |
| 1:A:147:GLU:OE1 | 1:A:147:GLU:N | 2.54 | 0.41 |
| 1:A:191:TYR:CD2 | 1:A:192:LYS:N | 2.89 | 0.41 |
| 1:B:64:THR:O | 1:B:65:LEU:CD2 | 2.69 | 0.41 |
| 1:B:65:LEU:C | 1:B:66:ASN:ND2 | 2.63 | 0.41 |
| 1:B:192:LYS:O | 1:B:193:ILE:O | 2.39 | 0.41 |
| 1:A:33:PRO:O | 1:A:97:GLN:HG3 | 2.21 | 0.41 |
| 1:A:34:LEU:C | 1:A:43:PHE:CB | 2.82 | 0.41 |
| 1:A:51:ARG:CG | 1:A:89:ILE:HA | 2.19 | 0.41 |
| 1:A:92:TYR:HD2 | 1:A:121:LEU:CD2 | 2.25 | 0.41 |
| 1:A:193:ILE:CB | 1:A:194:PRO:HD2 | 2.46 | 0.41 |
| 1:A:214:ALA:O | 1:A:218:ILE:N | 2.41 | 0.41 |
| 1:B:59:ILE:HG22 | 1:B:67:PRO:HA | 1.93 | 0.41 |
| 1:B:59:ILE:HG13 | 1:B:65:LEU:HB3 | 2.02 | 0.41 |
| 1:B:141:ILE:CA | 1:B:153:LYS:O | 2.67 | 0.41 |
| 1:B:175:LYS:C | 1:B:178:PRO:HD3 | 2.41 | 0.41 |
| 1:B:193:ILE:CB | 1:B:194:PRO:HD2 | 2.46 | 0.41 |
| 1:A:50:PRO:HB3 | 1:A:128:ALA:CB | 2.29 | 0.40 |
| 1:A:64:THR:O | 1:A:65:LEU:CD2 | 2.69 | 0.40 |
| 1:B:5:ARG:HH22 | 1:B:25:PRO:CG | 2.35 | 0.40 |
| 1:B:81:ASN:HD21 | 1:B:86:HIS:CE1 | 2.39 | 0.40 |
| 1:B:129:TYR:HD2 | 1:B:132:GLN:CD | 2.25 | 0.40 |
| 1:B:130:THR:O | 1:B:130:THR:HG23 | 2.15 | 0.40 |
| 1:B:137:LYS:CG | 1:B:159:ILE:CD1 | 3.00 | 0.40 |
| 1:A:139:LEU:O | 1:A:211:LYS:HB2 | 2.21 | 0.40 |
| 1:A:170:ILE:HG13 | 1:A:210:ASN:HA | 2.03 | 0.40 |
| 1:A:234:SER:HB2 | 1:A:237:LYS:HG3 | 2.03 | 0.40 |
| 1:B:4:THR:HA | 1:B:19:ILE:HA | 2.03 | 0.40 |
| 1:B:173:VAL:HA | 1:B:177:PHE:CD1 | 2.55 | 0.40 |
| 1:B:217:ILE:HD12 | 1:B:220:GLU:CD | 2.42 | 0.40 |
| 1:A:80:ARG:HD3 | 1:A:279:PHE:HD1 | 1.84 | 0.40 |
| 1:A:83:PHE:N | 1:A:84:PRO:HD2 | 2.37 | 0.40 |
| 1:B:33:PRO:O | 1:B:97:GLN:HG3 | 2.21 | 0.40 |
| 1:B:83:PHE:N | 1:B:84:PRO:HD2 | 2.37 | 0.40 |
| 1:B:102:PRO:O | 1:B:112:VAL:CB | 2.63 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:177:PHE:HD1 | 1:B:177:PHE:H | 1.68 | 0.40 |
| 1:A:22:ASP:HB3 | 1:A:23:GLY:H | 1.58 | 0.40 |
| 1:A:32:ILE:HG21 | 1:A:96:PRO:HG3 | 2.00 | 0.40 |
| 1:A:190:ILE:H | 1:A:190:ILE:HG23 | 1.56 | 0.40 |
| 1:B:51:ARG:CG | 1:B:89:ILE:HA | 2.19 | 0.40 |
| 1:B:80:ARG:HG2 | 1:B:194:PRO:O | 2.21 | 0.40 |
| 1:A:111:ALA:C | 1:A:112:VAL:HG23 | 2.42 | 0.40 |
| 1:A:219:LYS:C | 1:A:221:THR:N | 2.75 | 0.40 |
| 1:B:45:MET:HB3 | 1:B:95:PHE:HE1 | 1.86 | 0.40 |
| 1:B:59:ILE:CG2 | 1:B:67:PRO:CD | 2.96 | 0.40 |
| 1:B:81:ASN:O | 1:B:278:TRP:HD1 | 2.04 | 0.40 |
| 1:B:82:CYS:HB3 | 1:B:190:ILE:CD1 | 2.52 | 0.40 |
| 1:B:234:SER:HB2 | 1:B:237:LYS:HG3 | 2.04 | 0.40 |

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:247:PRO:CG | 1:B:108:GLU:OE2[1_445] | 1.56 | 0.64 |
| 1:A:115:ASN:ND2 | 1:B:75:LYS:NZ[1_455] | 1.71 | 0.49 |
| 1:A:174:GLU:OE1 | 1:B:248:ASP:CG[2_775] | 1.72 | 0.48 |
| 1:B:2:TYR:OH | 1:B:199:GLU:OE2[2_774] | 1.82 | 0.38 |
| 1:A:247:PRO:CG | 1:B:108:GLU:CG[1_445] | 1.84 | 0.36 |
| 1:A:147:GLU:O | 1:B:73:LYS:NZ[1_455] | 1.85 | 0.35 |
| 1:A:174:GLU:OE1 | 1:B:248:ASP:OD1[2_775] | 1.85 | 0.35 |
| 1:B:24:LYS:NZ | 1:B:182:ARG:NE[2_774] | 1.92 | 0.28 |
| 1:B:24:LYS:CE | 1:B:182:ARG:NH2[2_774] | 1.95 | 0.25 |
| 1:A:247:PRO:CG | 1:B:108:GLU:CD[1_445] | 2.05 | 0.15 |
| 1:A:252:TYR:OH | 1:B:106:HIS:CD2[1_445] | 2.07 | 0.13 |
| 1:A:174:GLU:OE1 | 1:B:248:ASP:OD2[2_775] | 2.15 | 0.05 |
| 1:A:149:GLU:CG | 1:B:73:LYS:NZ[1_455] | 2.18 | 0.02 |

## 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 | 279/285 (98%) | 151 (54%) | 53 (19%) | 75 (27%) | 0 | 0 |
| 1 | B | 279/285 (98%) | 152 (54%) | 53 (19%) | 74 (26%) | 0 | 0 |
| All | All | 558/570 (98%) | 303 (54%) | 106 (19%) | 149 (27%) | 0 | 0 |

All (149) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | TYR |
| 1 | A | 8 | GLY |
| 1 | A | 9 | ALA |
| 1 | A | 12 | THR |
| 1 | A | 13 | LEU |
| 1 | A | 24 | LYS |
| 1 | A | 33 | PRO |
| 1 | A | 37 | ASP |
| 1 | A | 39 | GLU |
| 1 | A | 63 | GLU |
| 1 | A | 70 | GLN |
| 1 | A | 82 | CYS |
| 1 | A | 85 | HIS |
| 1 | A | 91 | ASN |
| 1 | A | 94 | ALA |
| 1 | A | 104 | VAL |
| 1 | A | 111 | ALA |
| 1 | A | 116 | ASN |
| 1 | A | 117 | PRO |
| 1 | A | 130 | THR |
| 1 | A | 136 | VAL |
| 1 | A | 159 | ILE |
| 1 | A | 172 | ASP |
| 1 | A | 173 | VAL |
| 1 | A | 181 | LEU |
| 1 | A | 185 | ASP |
| 1 | A | 186 | GLU |
| 1 | A | 187 | TRP |
| 1 | A | 193 | ILE |
| 1 | A | 195 | ASP |
| 1 | A | 198 | PRO |
| 1 | A | 201 | GLN |
| 1 | A | 205 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 233 | SER |
| 1 | A | 275 | ILE |
| 1 | A | 276 | ASP |
| 1 | B | 2 | TYR |
| 1 | B | 8 | GLY |
| 1 | B | 9 | ALA |
| 1 | B | 12 | THR |
| 1 | B | 13 | LEU |
| 1 | B | 24 | LYS |
| 1 | B | 33 | PRO |
| 1 | B | 37 | ASP |
| 1 | B | 39 | GLU |
| 1 | B | 63 | GLU |
| 1 | B | 70 | GLN |
| 1 | B | 82 | CYS |
| 1 | B | 85 | HIS |
| 1 | B | 91 | ASN |
| 1 | B | 94 | ALA |
| 1 | B | 104 | VAL |
| 1 | B | 111 | ALA |
| 1 | B | 116 | ASN |
| 1 | B | 117 | PRO |
| 1 | B | 130 | THR |
| 1 | B | 136 | VAL |
| 1 | B | 159 | ILE |
| 1 | B | 172 | ASP |
| 1 | B | 173 | VAL |
| 1 | B | 181 | LEU |
| 1 | B | 185 | ASP |
| 1 | B | 186 | GLU |
| 1 | B | 187 | TRP |
| 1 | B | 193 | ILE |
| 1 | B | 195 | ASP |
| 1 | B | 198 | PRO |
| 1 | B | 201 | GLN |
| 1 | B | 205 | SER |
| 1 | B | 233 | SER |
| 1 | B | 275 | ILE |
| 1 | B | 276 | ASP |
| 1 | A | 10 | LYS |
| 1 | A | 11 | ASN |
| 1 | A | 26 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 34 | LEU |
| 1 | A | 35 | TYR |
| 1 | A | 62 | GLU |
| 1 | A | 72 | THR |
| 1 | A | 75 | LYS |
| 1 | A | 90 | HIS |
| 1 | A | 92 | TYR |
| 1 | A | 97 | GLN |
| 1 | A | 108 | GLU |
| 1 | A | 182 | ARG |
| 1 | A | 230 | ALA |
| 1 | A | 239 | ILE |
| 1 | A | 242 | THR |
| 1 | A | 254 | LYS |
| 1 | B | 10 | LYS |
| 1 | B | 11 | ASN |
| 1 | B | 26 | VAL |
| 1 | B | 34 | LEU |
| 1 | B | 35 | TYR |
| 1 | B | 62 | GLU |
| 1 | B | 72 | THR |
| 1 | B | 75 | LYS |
| 1 | B | 90 | HIS |
| 1 | B | 92 | TYR |
| 1 | B | 97 | GLN |
| 1 | B | 108 | GLU |
| 1 | B | 182 | ARG |
| 1 | B | 230 | ALA |
| 1 | B | 239 | ILE |
| 1 | B | 242 | THR |
| 1 | B | 254 | LYS |
| 1 | A | 42 | ILE |
| 1 | A | 112 | VAL |
| 1 | A | 171 | GLU |
| 1 | B | 42 | ILE |
| 1 | B | 112 | VAL |
| 1 | B | 171 | GLU |
| 1 | A | 25 | PRO |
| 1 | A | 74 | GLY |
| 1 | A | 95 | PHE |
| 1 | A | 148 | GLY |
| 1 | A | 164 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 204 | PHE |
| 1 | A | 247 | PRO |
| 1 | B | 25 | PRO |
| 1 | B | 74 | GLY |
| 1 | B | 95 | PHE |
| 1 | B | 148 | GLY |
| 1 | B | 164 | ALA |
| 1 | B | 204 | PHE |
| 1 | B | 247 | PRO |
| 1 | A | 65 | LEU |
| 1 | A | 194 | PRO |
| 1 | A | 203 | ALA |
| 1 | A | 250 | PRO |
| 1 | B | 65 | LEU |
| 1 | B | 194 | PRO |
| 1 | B | 203 | ALA |
| 1 | B | 250 | PRO |
| 1 | A | 15 | TYR |
| 1 | A | 49 | ILE |
| 1 | A | 68 | ILE |
| 1 | A | 105 | SER |
| 1 | A | 178 | PRO |
| 1 | B | 15 | TYR |
| 1 | B | 49 | ILE |
| 1 | B | 68 | ILE |
| 1 | B | 178 | PRO |
| 1 | A | 127 | ILE |
| 1 | B | 127 | ILE |
| 1 | A | 59 | ILE |
| 1 | B | 59 | ILE |
| 1 | A | 83 | PHE |
| 1 | B | 83 | PHE |

### 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 | 243/247 (98%) | 158 (65%) | 85 (35%) | 0 1 |
| 1 | B | 243/247 (98%) | 158 (65%) | 85 (35%) | 0 1 |
| All | All | 486/494 (98%) | 316 (65%) | 170 (35%) | 0 1 |

All (170) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3 | THR |
| 1 | A | 7 | ILE |
| 1 | A | 17 | VAL |
| 1 | A | 19 | ILE |
| 1 | A | 26 | VAL |
| 1 | A | 27 | SER |
| 1 | A | 35 | TYR |
| 1 | A | 40 | ASP |
| 1 | A | 41 | ASN |
| 1 | A | 42 | ILE |
| 1 | A | 43 | PHE |
| 1 | A | 44 | ASN |
| 1 | A | 45 | MET |
| 1 | A | 48 | GLU |
| 1 | A | 49 | ILE |
| 1 | A | 51 | ARG |
| 1 | A | 53 | THR |
| 1 | A | 54 | ASN |
| 1 | A | 57 | LEU |
| 1 | A | 60 | THR |
| 1 | A | 62 | GLU |
| 1 | A | 63 | GLU |
| 1 | A | 65 | LEU |
| 1 | A | 66 | ASN |
| 1 | A | 79 | VAL |
| 1 | A | 80 | ARG |
| 1 | A | 83 | PHE |
| 1 | A | 86 | HIS |
| 1 | A | 89 | ILE |
| 1 | A | 92 | TYR |
| 1 | A | 99 | TRP |
| 1 | A | 100 | GLU |
| 1 | A | 104 | VAL |
| 1 | A | 106 | HIS |
| 1 | A | 109 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 112 | VAL |
| 1 | A | 115 | ASN |
| 1 | A | 118 | ILE |
| 1 | A | 121 | LEU |
| 1 | A | 123 | ILE |
| 1 | A | 125 | GLU |
| 1 | A | 126 | THR |
| 1 | A | 130 | THR |
| 1 | A | 135 | GLU |
| 1 | A | 136 | VAL |
| 1 | A | 141 | ILE |
| 1 | A | 144 | LEU |
| 1 | A | 150 | THR |
| 1 | A | 151 | ASP |
| 1 | A | 153 | LYS |
| 1 | A | 155 | ILE |
| 1 | A | 158 | ASP |
| 1 | A | 160 | ASN |
| 1 | A | 161 | ASP |
| 1 | A | 163 | LEU |
| 1 | A | 168 | ASN |
| 1 | A | 169 | ASP |
| 1 | A | 171 | GLU |
| 1 | A | 177 | PHE |
| 1 | A | 182 | ARG |
| 1 | A | 187 | TRP |
| 1 | A | 189 | ARG |
| 1 | A | 191 | TYR |
| 1 | A | 193 | ILE |
| 1 | A | 200 | ASN |
| 1 | A | 210 | ASN |
| 1 | A | 211 | LYS |
| 1 | A | 212 | LYS |
| 1 | A | 213 | TYR |
| 1 | A | 217 | ILE |
| 1 | A | 218 | ILE |
| 1 | A | 220 | GLU |
| 1 | A | 223 | ASN |
| 1 | A | 224 | SER |
| 1 | A | 225 | TRP |
| 1 | A | 229 | ILE |
| 1 | A | 239 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 240 | ASP |
| 1 | A | 242 | THR |
| 1 | A | 251 | THR |
| 1 | A | 258 | ASP |
| 1 | A | 271 | ILE |
| 1 | A | 272 | ASP |
| 1 | A | 276 | ASP |
| 1 | A | 278 | TRP |
| 1 | B | 3 | THR |
| 1 | B | 7 | ILE |
| 1 | B | 17 | VAL |
| 1 | B | 19 | ILE |
| 1 | B | 26 | VAL |
| 1 | B | 27 | SER |
| 1 | B | 35 | TYR |
| 1 | B | 40 | ASP |
| 1 | B | 41 | ASN |
| 1 | B | 42 | ILE |
| 1 | B | 43 | PHE |
| 1 | B | 44 | ASN |
| 1 | B | 45 | MET |
| 1 | B | 48 | GLU |
| 1 | B | 49 | ILE |
| 1 | B | 51 | ARG |
| 1 | B | 53 | THR |
| 1 | B | 54 | ASN |
| 1 | B | 57 | LEU |
| 1 | B | 60 | THR |
| 1 | B | 62 | GLU |
| 1 | B | 63 | GLU |
| 1 | B | 65 | LEU |
| 1 | B | 66 | ASN |
| 1 | B | 79 | VAL |
| 1 | B | 80 | ARG |
| 1 | B | 83 | PHE |
| 1 | B | 86 | HIS |
| 1 | B | 89 | ILE |
| 1 | B | 92 | TYR |
| 1 | B | 99 | TRP |
| 1 | B | 100 | GLU |
| 1 | B | 104 | VAL |
| 1 | B | 106 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 109 | THR |
| 1 | B | 112 | VAL |
| 1 | B | 115 | ASN |
| 1 | B | 118 | ILE |
| 1 | B | 121 | LEU |
| 1 | B | 123 | ILE |
| 1 | B | 125 | GLU |
| 1 | B | 126 | THR |
| 1 | B | 130 | THR |
| 1 | B | 135 | GLU |
| 1 | B | 136 | VAL |
| 1 | B | 141 | ILE |
| 1 | B | 144 | LEU |
| 1 | B | 150 | THR |
| 1 | B | 151 | ASP |
| 1 | B | 153 | LYS |
| 1 | B | 155 | ILE |
| 1 | B | 158 | ASP |
| 1 | B | 160 | ASN |
| 1 | B | 161 | ASP |
| 1 | B | 163 | LEU |
| 1 | B | 168 | ASN |
| 1 | B | 169 | ASP |
| 1 | B | 171 | GLU |
| 1 | B | 177 | PHE |
| 1 | B | 182 | ARG |
| 1 | B | 187 | TRP |
| 1 | B | 189 | ARG |
| 1 | B | 191 | TYR |
| 1 | B | 193 | ILE |
| 1 | B | 200 | ASN |
| 1 | B | 210 | ASN |
| 1 | B | 211 | LYS |
| 1 | B | 212 | LYS |
| 1 | B | 213 | TYR |
| 1 | B | 217 | ILE |
| 1 | B | 218 | ILE |
| 1 | B | 220 | GLU |
| 1 | B | 223 | ASN |
| 1 | B | 224 | SER |
| 1 | B | 225 | TRP |
| 1 | B | 229 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 239 | ILE |
| 1 | B | 240 | ASP |
| 1 | B | 242 | THR |
| 1 | B | 251 | THR |
| 1 | B | 258 | ASP |
| 1 | B | 271 | ILE |
| 1 | B | 272 | ASP |
| 1 | B | 276 | ASP |
| 1 | B | 278 | TRP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 41 | ASN |
| 1 | A | 66 | ASN |
| 1 | A | 122 | GLN |
| 1 | A | 160 | ASN |
| 1 | A | 168 | ASN |
| 1 | A | 200 | ASN |
| 1 | B | 41 | ASN |
| 1 | B | 66 | ASN |
| 1 | B | 122 | GLN |
| 1 | B | 160 | ASN |
| 1 | B | 168 | ASN |
| 1 | B | 200 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.