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

Jan 31, 2016 – 07:27 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1FNW |
| Title | : | CRYSTAL STRUCTURE OF STREPTOCOCCAL PYROGENIC EXOTOXIN A |
| Authors | : | Earhart, C.A.; Vath, G.M.; Roggiani, M.; Schlivert, P.M.; Ohlendorf, D.H. |
| Deposited on | : | 2000-08-23 |
| Resolution | : | 3.90 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

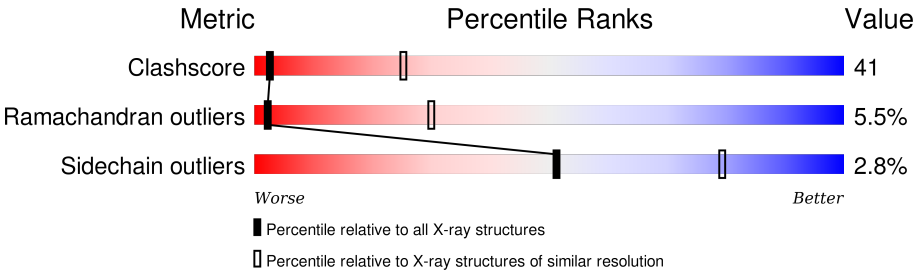
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 102246 | 1031 (4.24-3.56) |
| Ramachandran outliers | 100387 | 1012 (4.26-3.54) |
| Sidechain outliers | 100360 | 1004 (4.26-3.54) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 221 | 43% 48% 10% |
| 1 | B | 221 | 44% 50% 6% |
| 1 | C | 221 | 43% 50% 7% |
| 1 | D | 221 | 41% 52% 7% |
| 1 | E | 221 | 44% 51% 5% |
| 1 | F | 221 | 44% 51% 5% |
| 1 | G | 221 | 41% 53% 6% |

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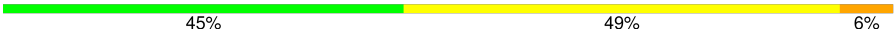
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | H | 221 |   |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14616 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 EXOTOXIN TYPE A PRECURSOR (ALLELE 1).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |
| 1 | B | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |
| 1 | C | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |
| 1 | D | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |
| 1 | E | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |
| 1 | F | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |
| 1 | G | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |
| 1 | H | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1823 | 1166 | 293 | 358 | 6 | | | |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 153 | THR | LEU | CONFLICT | UNP P62560 |
| A | 154 | ILE | THR | CONFLICT | UNP P62560 |
| A | 209 | ASN | SER | CONFLICT | UNP P62560 |
| A | 210 | LYS | ASN | CONFLICT | UNP P62560 |
| B | 453 | THR | LEU | CONFLICT | UNP P62560 |
| B | 454 | ILE | THR | CONFLICT | UNP P62560 |
| B | 509 | ASN | SER | CONFLICT | UNP P62560 |
| B | 510 | LYS | ASN | CONFLICT | UNP P62560 |
| C | 753 | THR | LEU | CONFLICT | UNP P62560 |
| C | 754 | ILE | THR | CONFLICT | UNP P62560 |
| C | 809 | ASN | SER | CONFLICT | UNP P62560 |
| C | 810 | LYS | ASN | CONFLICT | UNP P62560 |
| D | 1053 | THR | LEU | CONFLICT | UNP P62560 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 1054 | ILE | THR | CONFLICT | UNP P62560 |
| D | 1109 | ASN | SER | CONFLICT | UNP P62560 |
| D | 1110 | LYS | ASN | CONFLICT | UNP P62560 |
| E | 1353 | THR | LEU | CONFLICT | UNP P62560 |
| E | 1354 | ILE | THR | CONFLICT | UNP P62560 |
| E | 1409 | ASN | SER | CONFLICT | UNP P62560 |
| E | 1410 | LYS | ASN | CONFLICT | UNP P62560 |
| F | 1653 | THR | LEU | CONFLICT | UNP P62560 |
| F | 1654 | ILE | THR | CONFLICT | UNP P62560 |
| F | 1709 | ASN | SER | CONFLICT | UNP P62560 |
| F | 1710 | LYS | ASN | CONFLICT | UNP P62560 |
| G | 1953 | THR | LEU | CONFLICT | UNP P62560 |
| G | 1954 | ILE | THR | CONFLICT | UNP P62560 |
| G | 2009 | ASN | SER | CONFLICT | UNP P62560 |
| G | 2010 | LYS | ASN | CONFLICT | UNP P62560 |
| H | 2253 | THR | LEU | CONFLICT | UNP P62560 |
| H | 2254 | ILE | THR | CONFLICT | UNP P62560 |
| H | 2309 | ASN | SER | CONFLICT | UNP P62560 |
| H | 2310 | LYS | ASN | CONFLICT | UNP P62560 |

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | G | 4 | Total Cd<br>4 4 | 0 | 0 |
| 2 | D | 4 | Total Cd<br>4 4 | 0 | 0 |
| 2 | E | 4 | Total Cd<br>4 4 | 0 | 0 |
| 2 | H | 3 | Total Cd<br>3 3 | 0 | 0 |
| 2 | B | 4 | Total Cd<br>4 4 | 0 | 0 |
| 2 | C | 4 | Total Cd<br>4 4 | 0 | 0 |
| 2 | A | 4 | Total Cd<br>4 4 | 0 | 0 |
| 2 | F | 5 | Total Cd<br>5 5 | 0 | 0 |

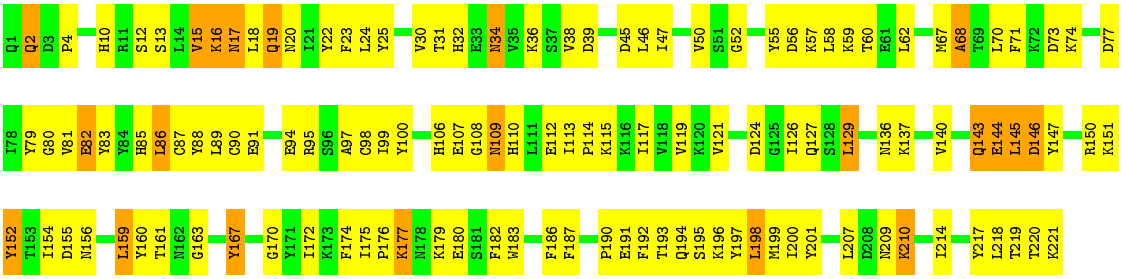
# 3 Residue-property plots (i)

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

Note EDS was not executed.

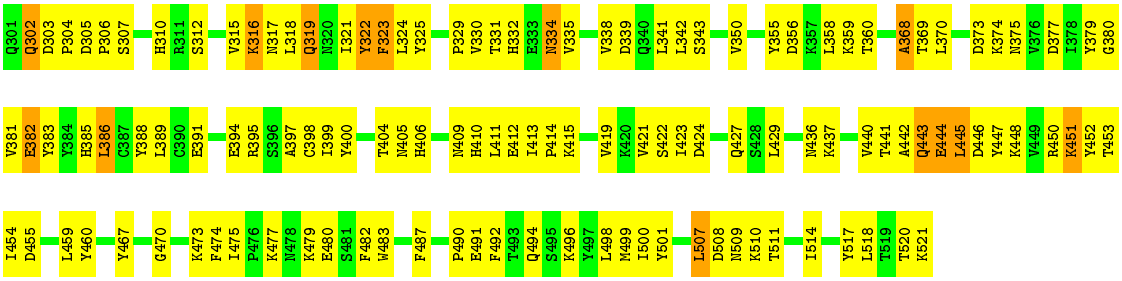
- Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain A:

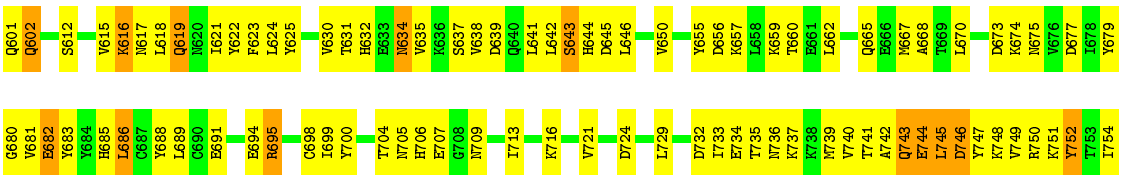
- Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

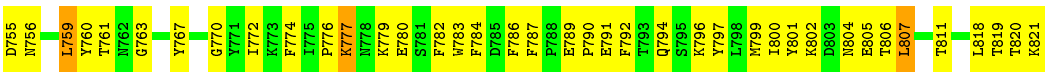
Chain B:

- Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain C:



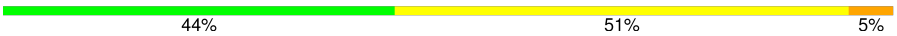

• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

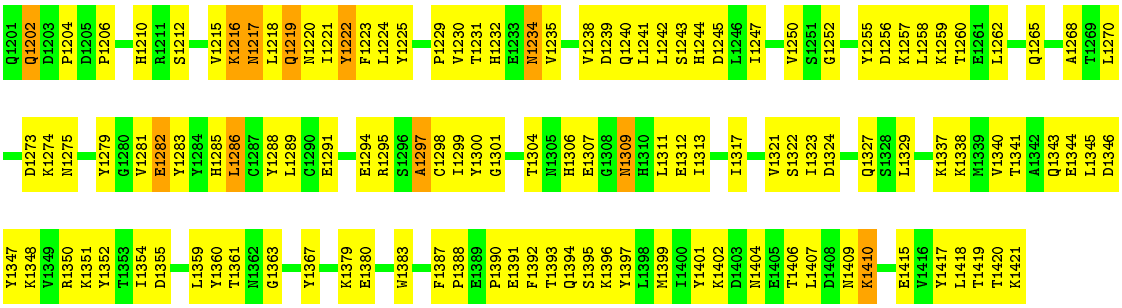
Chain D:



• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

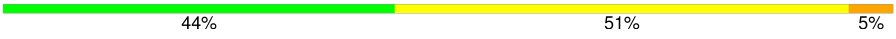
Chain E:

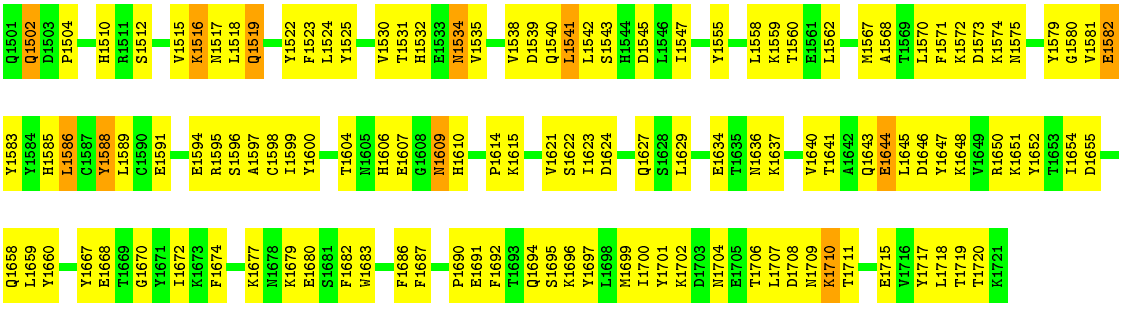



• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

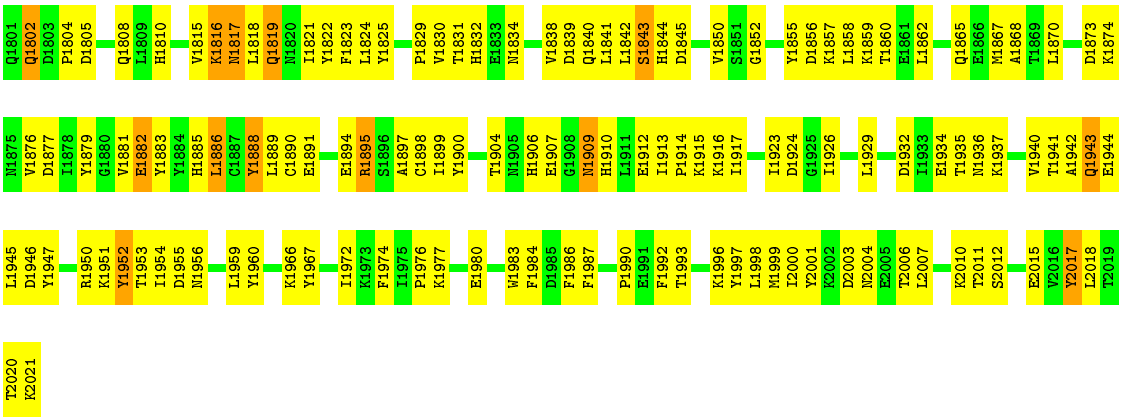
Chain F:



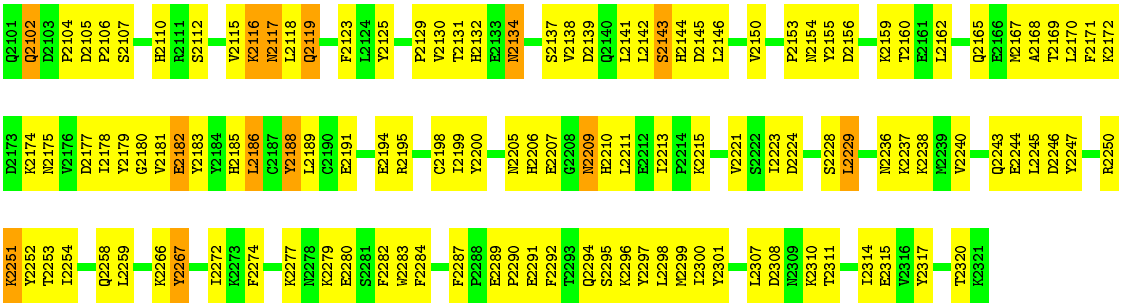

• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain G:




- Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain H:

# 4 Data and refinement statistics (i)

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

| Property | Value | Source |
|---|---|---|
| Space group | P 31 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 226.23Å 226.23Å 81.61Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 20.00 – 3.90 | Depositor |
| % Data completeness<br>(in resolution range) | 77.0 (20.00-3.90) | Depositor |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.213 , 0.305 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 14616 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 26.0 | wwPDB-VP |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.46 | 0/1865 | 0.73 | 0/2522 |
| 1 | B | 0.46 | 0/1865 | 0.71 | 0/2522 |
| 1 | C | 0.45 | 0/1865 | 0.70 | 0/2522 |
| 1 | D | 0.45 | 0/1865 | 0.72 | 0/2522 |
| 1 | E | 0.43 | 0/1865 | 0.69 | 0/2522 |
| 1 | F | 0.46 | 0/1865 | 0.71 | 0/2522 |
| 1 | G | 0.45 | 0/1865 | 0.71 | 0/2522 |
| 1 | H | 0.45 | 0/1865 | 0.71 | 0/2522 |
| All | All | 0.45 | 0/14920 | 0.71 | 0/20176 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1823 | 0 | 1778 | 157 | 0 |
| 1 | B | 1823 | 0 | 1775 | 151 | 0 |
| 1 | C | 1823 | 0 | 1775 | 149 | 0 |
| 1 | D | 1823 | 0 | 1775 | 159 | 0 |
| 1 | E | 1823 | 0 | 1775 | 146 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | F | 1823 | 0 | 1775 | 150 | 0 |
| 1 | G | 1823 | 0 | 1775 | 154 | 0 |
| 1 | H | 1823 | 0 | 1775 | 161 | 0 |
| 2 | A | 4 | 0 | 0 | 0 | 0 |
| 2 | B | 4 | 0 | 0 | 0 | 0 |
| 2 | C | 4 | 0 | 0 | 0 | 0 |
| 2 | D | 4 | 0 | 0 | 0 | 0 |
| 2 | E | 4 | 0 | 0 | 0 | 0 |
| 2 | F | 5 | 0 | 0 | 0 | 0 |
| 2 | G | 4 | 0 | 0 | 0 | 0 |
| 2 | H | 3 | 0 | 0 | 0 | 0 |
| All | All | 14616 | 0 | 14203 | 1180 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (1180) 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:C:619:GLN:H | 1:C:619:GLN:NE2 | 1.55 | 1.03 |
| 1:B:391:GLU:HB3 | 1:D:991:GLU:HB3 | 1.36 | 1.03 |
| 1:H:2119:GLN:NE2 | 1:H:2119:GLN:H | 1.54 | 1.03 |
| 1:E:1291:GLU:HB3 | 1:G:1891:GLU:HB3 | 1.38 | 1.02 |
| 1:E:1219:GLN:H | 1:E:1219:GLN:NE2 | 1.57 | 1.02 |
| 1:A:19:GLN:H | 1:A:19:GLN:NE2 | 1.58 | 1.01 |
| 1:H:2102:GLN:H | 1:H:2102:GLN:NE2 | 1.59 | 0.99 |
| 1:B:479:LYS:HG3 | 1:B:480:GLU:H | 1.27 | 0.98 |
| 1:F:1591:GLU:HB3 | 1:H:2191:GLU:HB3 | 1.41 | 0.98 |
| 1:C:754:ILE:HG12 | 1:C:759:LEU:HB3 | 1.42 | 0.98 |
| 1:A:19:GLN:H | 1:A:19:GLN:HE21 | 1.05 | 0.98 |
| 1:G:1819:GLN:NE2 | 1:G:1819:GLN:H | 1.60 | 0.98 |
| 1:C:619:GLN:H | 1:C:619:GLN:HE21 | 1.04 | 0.97 |
| 1:H:2119:GLN:H | 1:H:2119:GLN:HE21 | 1.09 | 0.96 |
| 1:D:959:LYS:HB2 | 1:D:989:LEU:HD21 | 1.45 | 0.95 |
| 1:A:91:GLU:HB3 | 1:C:691:GLU:HB3 | 1.46 | 0.95 |
| 1:B:359:LYS:HB2 | 1:B:389:LEU:HD21 | 1.46 | 0.94 |
| 1:H:2254:ILE:HG12 | 1:H:2259:LEU:HB3 | 1.48 | 0.94 |
| 1:B:338:VAL:HG23 | 1:B:339:ASP:H | 1.33 | 0.93 |
| 1:G:1838:VAL:HG23 | 1:G:1839:ASP:H | 1.31 | 0.93 |
| 1:D:919:GLN:NE2 | 1:D:919:GLN:H | 1.66 | 0.93 |
| 1:F:1581:VAL:H | 1:F:1643:GLN:HE21 | 1.16 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1819:GLN:HE21 | 1:G:1819:GLN:H | 0.99 | 0.92 |
| 1:E:1354:ILE:HG12 | 1:E:1359:LEU:HB3 | 1.51 | 0.92 |
| 1:B:319:GLN:HE21 | 1:B:319:GLN:H | 0.97 | 0.92 |
| 1:F:1519:GLN:H | 1:F:1519:GLN:HE21 | 1.19 | 0.91 |
| 1:E:1219:GLN:H | 1:E:1219:GLN:HE21 | 1.03 | 0.90 |
| 1:F:1519:GLN:H | 1:F:1519:GLN:NE2 | 1.68 | 0.90 |
| 1:B:319:GLN:NE2 | 1:B:319:GLN:H | 1.69 | 0.90 |
| 1:F:1654:ILE:HG12 | 1:F:1659:LEU:HB3 | 1.56 | 0.88 |
| 1:H:2102:GLN:H | 1:H:2102:GLN:HE21 | 1.20 | 0.88 |
| 1:A:59:LYS:HB2 | 1:A:89:LEU:HD21 | 1.54 | 0.88 |
| 1:B:319:GLN:HE21 | 1:B:319:GLN:N | 1.74 | 0.86 |
| 1:F:1581:VAL:H | 1:F:1643:GLN:NE2 | 1.73 | 0.86 |
| 1:B:454:ILE:HG12 | 1:B:459:LEU:HB3 | 1.57 | 0.85 |
| 1:H:2131:THR:HG22 | 1:H:2179:TYR:CD1 | 2.12 | 0.84 |
| 1:G:1996:LYS:HD3 | 1:G:1997:TYR:N | 1.92 | 0.84 |
| 1:H:2102:GLN:N | 1:H:2102:GLN:HE21 | 1.75 | 0.84 |
| 1:H:2296:LYS:HD3 | 1:H:2297:TYR:N | 1.93 | 0.83 |
| 1:G:1859:LYS:HB2 | 1:G:1889:LEU:HD21 | 1.59 | 0.83 |
| 1:F:1559:LYS:HB2 | 1:F:1589:LEU:HD21 | 1.59 | 0.82 |
| 1:B:338:VAL:HG23 | 1:B:339:ASP:N | 1.95 | 0.82 |
| 1:A:38:VAL:HG23 | 1:A:39:ASP:H | 1.44 | 0.82 |
| 1:C:625:TYR:CE2 | 1:C:750:ARG:HD2 | 2.15 | 0.82 |
| 1:D:925:TYR:CE2 | 1:D:1050:ARG:HD2 | 2.15 | 0.82 |
| 1:G:1858:LEU:HD12 | 1:G:1897:ALA:O | 1.78 | 0.81 |
| 1:A:38:VAL:HG23 | 1:A:39:ASP:N | 1.94 | 0.81 |
| 1:B:325:TYR:CE2 | 1:B:450:ARG:HD2 | 2.16 | 0.81 |
| 1:A:179:LYS:HG3 | 1:A:180:GLU:H | 1.45 | 0.81 |
| 1:B:379:TYR:CE2 | 1:B:444:GLU:HG3 | 2.15 | 0.81 |
| 1:B:383:TYR:CE1 | 1:B:398:CYS:HB2 | 2.15 | 0.81 |
| 1:D:981:VAL:H | 1:D:1043:GLN:NE2 | 1.79 | 0.81 |
| 1:H:2130:VAL:HG21 | 1:H:2182:GLU:HB3 | 1.62 | 0.80 |
| 1:H:2159:LYS:HB2 | 1:H:2189:LEU:HD21 | 1.63 | 0.80 |
| 1:F:1562:LEU:HD12 | 1:F:1568:ALA:HA | 1.65 | 0.79 |
| 1:H:2237:LYS:HB2 | 1:H:2240:VAL:HG12 | 1.63 | 0.79 |
| 1:G:1838:VAL:HG23 | 1:G:1839:ASP:N | 1.98 | 0.78 |
| 1:E:1351:LYS:HE2 | 1:E:1355:ASP:OD2 | 1.83 | 0.78 |
| 1:D:1037:LYS:HB2 | 1:D:1040:VAL:HG12 | 1.65 | 0.78 |
| 1:B:400:TYR:CE2 | 1:B:499:MET:HG2 | 2.17 | 0.78 |
| 1:D:962:LEU:HD12 | 1:D:968:ALA:HA | 1.64 | 0.78 |
| 1:H:2195:ARG:NH1 | 1:H:2195:ARG:HB3 | 1.99 | 0.78 |
| 1:E:1291:GLU:HB3 | 1:G:1891:GLU:CB | 2.14 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:154:ILE:HG12 | 1:A:159:LEU:HB3 | 1.65 | 0.77 |
| 1:C:616:LYS:HD3 | 1:C:791:GLU:HG2 | 1.65 | 0.77 |
| 1:E:1295:ARG:HB3 | 1:E:1295:ARG:NH1 | 2.00 | 0.77 |
| 1:B:391:GLU:HB3 | 1:D:991:GLU:CB | 2.15 | 0.77 |
| 1:F:1538:VAL:HG23 | 1:F:1539:ASP:H | 1.48 | 0.77 |
| 1:G:1819:GLN:HE21 | 1:G:1819:GLN:N | 1.79 | 0.76 |
| 1:H:2254:ILE:HA | 1:H:2259:LEU:H | 1.50 | 0.76 |
| 1:A:15:VAL:HG11 | 1:A:18:LEU:HD13 | 1.68 | 0.76 |
| 1:F:1560:THR:HA | 1:F:1599:ILE:O | 1.86 | 0.76 |
| 1:E:1396:LYS:HD3 | 1:E:1397:TYR:N | 2.01 | 0.76 |
| 1:H:2116:LYS:HE2 | 1:H:2292:PHE:H | 1.49 | 0.76 |
| 1:F:1516:LYS:HG3 | 1:F:1517:ASN:H | 1.50 | 0.76 |
| 1:D:919:GLN:H | 1:D:919:GLN:HE21 | 1.29 | 0.76 |
| 1:F:1679:LYS:HG3 | 1:F:1680:GLU:H | 1.49 | 0.76 |
| 1:E:1225:TYR:CE2 | 1:E:1350:ARG:HD2 | 2.21 | 0.76 |
| 1:F:1516:LYS:HE2 | 1:F:1691:GLU:HA | 1.66 | 0.76 |
| 1:A:196:LYS:HD3 | 1:A:197:TYR:N | 2.00 | 0.75 |
| 1:E:1238:VAL:HG23 | 1:E:1239:ASP:N | 2.01 | 0.75 |
| 1:H:2125:TYR:CE2 | 1:H:2250:ARG:HD2 | 2.21 | 0.75 |
| 1:A:196:LYS:C | 1:A:196:LYS:HD3 | 2.07 | 0.75 |
| 1:F:1541:LEU:HG | 1:F:1542:LEU:HG | 1.69 | 0.75 |
| 1:G:1825:TYR:CE2 | 1:G:1950:ARG:HD2 | 2.22 | 0.75 |
| 1:C:659:LYS:HB2 | 1:C:689:LEU:HD21 | 1.69 | 0.75 |
| 1:G:1882:GLU:HA | 1:G:1899:ILE:HG22 | 1.69 | 0.75 |
| 1:B:391:GLU:CB | 1:D:991:GLU:HB3 | 2.13 | 0.75 |
| 1:C:751:LYS:HE2 | 1:C:755:ASP:OD2 | 1.87 | 0.75 |
| 1:H:2138:VAL:HG23 | 1:H:2139:ASP:H | 1.51 | 0.75 |
| 1:A:19:GLN:NE2 | 1:A:19:GLN:N | 2.35 | 0.74 |
| 1:A:30:VAL:HG21 | 1:A:82:GLU:HB3 | 1.68 | 0.74 |
| 1:G:1802:GLN:NE2 | 1:G:1802:GLN:H | 1.85 | 0.74 |
| 1:G:1916:LYS:HG2 | 1:G:1934:GLU:HG2 | 1.69 | 0.74 |
| 1:H:2115:VAL:HG13 | 1:H:2292:PHE:HE2 | 1.52 | 0.74 |
| 1:F:1538:VAL:HG23 | 1:F:1539:ASP:N | 2.02 | 0.74 |
| 1:E:1291:GLU:CB | 1:G:1891:GLU:HB3 | 2.17 | 0.74 |
| 1:B:373:ASP:C | 1:B:374:LYS:HD2 | 2.08 | 0.74 |
| 1:A:91:GLU:HB3 | 1:C:691:GLU:CB | 2.18 | 0.73 |
| 1:E:1285:HIS:CD2 | 1:F:1594:GLU:HG2 | 2.23 | 0.73 |
| 1:E:1219:GLN:HE21 | 1:E:1219:GLN:N | 1.84 | 0.73 |
| 1:E:1219:GLN:NE2 | 1:E:1219:GLN:N | 2.34 | 0.73 |
| 1:B:454:ILE:HA | 1:B:459:LEU:H | 1.53 | 0.73 |
| 1:D:973:ASP:C | 1:D:974:LYS:HD2 | 2.08 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1579:TYR:CE2 | 1:F:1644:GLU:HG3 | 2.23 | 0.73 |
| 1:H:2131:THR:HG22 | 1:H:2179:TYR:HD1 | 1.54 | 0.73 |
| 1:E:1282:GLU:HA | 1:E:1299:ILE:HG22 | 1.71 | 0.73 |
| 1:G:1819:GLN:NE2 | 1:G:1819:GLN:N | 2.34 | 0.72 |
| 1:H:2277:LYS:HD3 | 1:H:2277:LYS:O | 1.88 | 0.72 |
| 1:F:1709:ASN:CG | 1:F:1710:LYS:H | 1.92 | 0.72 |
| 1:F:1516:LYS:HG3 | 1:F:1517:ASN:N | 2.02 | 0.72 |
| 1:B:334:ASN:HB2 | 1:B:406:HIS:CD2 | 2.24 | 0.72 |
| 1:B:335:VAL:O | 1:B:375:ASN:HA | 1.89 | 0.72 |
| 1:E:1291:GLU:HG2 | 1:G:1891:GLU:OE1 | 1.90 | 0.72 |
| 1:E:1281:VAL:H | 1:E:1343:GLN:NE2 | 1.88 | 0.72 |
| 1:E:1217:ASN:HB3 | 1:E:1219:GLN:OE1 | 1.88 | 0.72 |
| 1:H:2138:VAL:HG23 | 1:H:2139:ASP:N | 2.03 | 0.72 |
| 1:E:1273:ASP:C | 1:E:1274:LYS:HD2 | 2.10 | 0.72 |
| 1:C:619:GLN:HE21 | 1:C:619:GLN:N | 1.84 | 0.71 |
| 1:A:19:GLN:HE21 | 1:A:19:GLN:N | 1.83 | 0.71 |
| 1:D:916:LYS:HG3 | 1:D:917:ASN:N | 2.06 | 0.71 |
| 1:G:1862:LEU:HD12 | 1:G:1868:ALA:HA | 1.72 | 0.71 |
| 1:F:1525:TYR:CE2 | 1:F:1650:ARG:HD2 | 2.25 | 0.71 |
| 1:E:1258:LEU:HD12 | 1:E:1297:ALA:O | 1.90 | 0.71 |
| 1:E:1291:GLU:OE1 | 1:G:1891:GLU:HG2 | 1.90 | 0.71 |
| 1:C:616:LYS:HE2 | 1:C:791:GLU:HA | 1.72 | 0.71 |
| 1:H:2130:VAL:CG2 | 1:H:2182:GLU:HB3 | 2.19 | 0.71 |
| 1:C:619:GLN:NE2 | 1:C:619:GLN:N | 2.36 | 0.70 |
| 1:A:24:LEU:HD13 | 1:A:198:LEU:HD21 | 1.73 | 0.70 |
| 1:D:956:ASP:O | 1:D:957:LYS:HD3 | 1.89 | 0.70 |
| 1:D:916:LYS:HG3 | 1:D:917:ASN:H | 1.56 | 0.70 |
| 1:A:16:LYS:HE2 | 1:A:192:PHE:H | 1.55 | 0.70 |
| 1:E:1281:VAL:H | 1:E:1343:GLN:HE21 | 1.38 | 0.70 |
| 1:B:496:LYS:C | 1:B:496:LYS:HD3 | 2.12 | 0.70 |
| 1:D:1054:ILE:HG12 | 1:D:1059:LEU:HB3 | 1.74 | 0.70 |
| 1:D:979:TYR:CE2 | 1:D:1044:GLU:HG3 | 2.26 | 0.70 |
| 1:D:1079:LYS:HG3 | 1:D:1080:GLU:H | 1.56 | 0.70 |
| 1:H:2134:ASN:HB2 | 1:H:2206:HIS:CD2 | 2.26 | 0.70 |
| 1:B:338:VAL:CG2 | 1:B:339:ASP:H | 2.05 | 0.70 |
| 1:H:2221:VAL:HB | 1:H:2229:LEU:HD12 | 1.73 | 0.69 |
| 1:A:2:GLN:H | 1:A:2:GLN:NE2 | 1.90 | 0.69 |
| 1:H:2119:GLN:N | 1:H:2119:GLN:HE21 | 1.87 | 0.69 |
| 1:E:1230:VAL:HG13 | 1:E:1255:TYR:OH | 1.93 | 0.69 |
| 1:E:1234:ASN:HB2 | 1:E:1306:HIS:CD2 | 2.27 | 0.69 |
| 1:A:91:GLU:HG2 | 1:C:691:GLU:OE1 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1259:LYS:HB2 | 1:E:1289:LEU:HD21 | 1.75 | 0.69 |
| 1:G:1877:ASP:OD2 | 1:G:1906:HIS:HA | 1.93 | 0.69 |
| 1:B:312:SER:HB3 | 1:B:487:PHE:CE2 | 2.28 | 0.69 |
| 1:G:1816:LYS:HE2 | 1:G:1992:PHE:H | 1.58 | 0.69 |
| 1:H:2296:LYS:C | 1:H:2296:LYS:HD3 | 2.12 | 0.69 |
| 1:A:73:ASP:C | 1:A:74:LYS:HD2 | 2.13 | 0.69 |
| 1:C:681:VAL:H | 1:C:743:GLN:HE21 | 1.39 | 0.69 |
| 1:F:1519:GLN:N | 1:F:1519:GLN:NE2 | 2.40 | 0.69 |
| 1:F:1558:LEU:HD12 | 1:F:1597:ALA:O | 1.92 | 0.69 |
| 1:G:1977:LYS:HB2 | 1:G:2011:THR:HB | 1.75 | 0.69 |
| 1:B:451:LYS:HE2 | 1:B:455:ASP:OD2 | 1.93 | 0.69 |
| 1:H:2112:SER:HB3 | 1:H:2287:PHE:CE2 | 2.27 | 0.69 |
| 1:C:631:THR:HG22 | 1:C:679:TYR:CD1 | 2.29 | 0.68 |
| 1:G:2007:LEU:O | 1:G:2007:LEU:HD12 | 1.93 | 0.68 |
| 1:E:1283:TYR:CE1 | 1:E:1298:CYS:HB2 | 2.29 | 0.68 |
| 1:E:1379:LYS:HG3 | 1:E:1380:GLU:H | 1.59 | 0.68 |
| 1:H:2181:VAL:H | 1:H:2243:GLN:HE21 | 1.39 | 0.68 |
| 1:G:1817:ASN:HB3 | 1:G:1819:GLN:OE1 | 1.94 | 0.67 |
| 1:D:1051:LYS:HE2 | 1:D:1055:ASP:OD2 | 1.93 | 0.67 |
| 1:H:2179:TYR:CD2 | 1:H:2244:GLU:HG3 | 2.29 | 0.67 |
| 1:A:38:VAL:CG2 | 1:A:39:ASP:H | 2.07 | 0.67 |
| 1:D:916:LYS:HE2 | 1:D:1092:PHE:H | 1.59 | 0.67 |
| 1:B:370:LEU:O | 1:B:370:LEU:HD23 | 1.95 | 0.67 |
| 1:G:1805:ASP:H | 1:G:1808:GLN:NE2 | 1.92 | 0.67 |
| 1:E:1300:TYR:CE2 | 1:E:1399:MET:HG2 | 2.28 | 0.67 |
| 1:C:634:ASN:HB2 | 1:C:706:HIS:CD2 | 2.30 | 0.67 |
| 1:H:2243:GLN:HG3 | 1:H:2301:TYR:CD1 | 2.30 | 0.67 |
| 1:A:25:TYR:CE2 | 1:A:150:ARG:HD2 | 2.29 | 0.67 |
| 1:A:100:TYR:CE2 | 1:A:199:MET:HG2 | 2.31 | 0.66 |
| 1:C:698:CYS:O | 1:C:699:ILE:HG23 | 1.95 | 0.66 |
| 1:H:2267:TYR:CD1 | 1:H:2267:TYR:N | 2.63 | 0.66 |
| 1:F:1610:HIS:CD2 | 1:F:1636:ASN:HB3 | 2.30 | 0.66 |
| 1:A:83:TYR:HB2 | 1:A:194:GLN:HE21 | 1.60 | 0.66 |
| 1:D:985:HIS:CD2 | 1:D:986:LEU:HG | 2.31 | 0.66 |
| 1:H:2307:LEU:HD12 | 1:H:2307:LEU:O | 1.95 | 0.66 |
| 1:A:91:GLU:H | 1:C:691:GLU:CD | 1.98 | 0.66 |
| 1:B:437:LYS:HB2 | 1:B:440:VAL:HG12 | 1.78 | 0.66 |
| 1:B:325:TYR:CD2 | 1:B:450:ARG:HD2 | 2.30 | 0.66 |
| 1:D:931:THR:HG22 | 1:D:979:TYR:CD1 | 2.31 | 0.66 |
| 1:E:1238:VAL:HG23 | 1:E:1239:ASP:H | 1.59 | 0.66 |
| 1:B:316:LYS:HD3 | 1:B:491:GLU:HG2 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1696:LYS:HD3 | 1:F:1696:LYS:C | 2.15 | 0.66 |
| 1:B:507:LEU:HD12 | 1:B:507:LEU:O | 1.96 | 0.65 |
| 1:F:1707:LEU:O | 1:F:1707:LEU:HD12 | 1.96 | 0.65 |
| 1:F:1709:ASN:CG | 1:F:1710:LYS:N | 2.50 | 0.65 |
| 1:A:2:GLN:H | 1:A:2:GLN:HE21 | 1.42 | 0.65 |
| 1:B:316:LYS:HG3 | 1:B:317:ASN:H | 1.60 | 0.65 |
| 1:D:904:PRO:HB3 | 1:D:1083:TRP:CZ2 | 2.31 | 0.65 |
| 1:D:1045:LEU:O | 1:D:1049:VAL:HG23 | 1.96 | 0.65 |
| 1:B:316:LYS:HG3 | 1:B:317:ASN:N | 2.11 | 0.65 |
| 1:A:179:LYS:HG3 | 1:A:180:GLU:N | 2.12 | 0.65 |
| 1:D:1043:GLN:HG3 | 1:D:1101:TYR:CD1 | 2.31 | 0.65 |
| 1:C:673:ASP:C | 1:C:674:LYS:HD2 | 2.16 | 0.65 |
| 1:C:674:LYS:N | 1:C:674:LYS:HD2 | 2.11 | 0.65 |
| 1:D:915:VAL:HA | 1:D:1090:PRO:HA | 1.79 | 0.65 |
| 1:C:700:TYR:CE2 | 1:C:799:MET:HG2 | 2.31 | 0.65 |
| 1:A:119:VAL:HG13 | 1:A:214:ILE:HG22 | 1.78 | 0.65 |
| 1:A:137:LYS:HB2 | 1:A:140:VAL:HG12 | 1.79 | 0.65 |
| 1:C:602:GLN:H | 1:C:602:GLN:NE2 | 1.94 | 0.65 |
| 1:F:1519:GLN:O | 1:F:1522:TYR:HB3 | 1.97 | 0.65 |
| 1:B:391:GLU:HG2 | 1:D:991:GLU:OE1 | 1.97 | 0.64 |
| 1:H:2119:GLN:NE2 | 1:H:2119:GLN:N | 2.37 | 0.64 |
| 1:B:479:LYS:HG3 | 1:B:480:GLU:N | 2.06 | 0.64 |
| 1:B:360:THR:HA | 1:B:399:ILE:O | 1.98 | 0.64 |
| 1:C:681:VAL:H | 1:C:743:GLN:NE2 | 1.96 | 0.64 |
| 1:A:81:VAL:H | 1:A:143:GLN:NE2 | 1.95 | 0.64 |
| 1:A:83:TYR:CE1 | 1:A:98:CYS:HB2 | 2.32 | 0.64 |
| 1:D:1043:GLN:HG3 | 1:D:1101:TYR:CE1 | 2.32 | 0.64 |
| 1:G:1860:THR:HA | 1:G:1899:ILE:O | 1.96 | 0.64 |
| 1:B:500:ILE:HG13 | 1:B:501:TYR:CD2 | 2.31 | 0.64 |
| 1:A:150:ARG:O | 1:A:151:LYS:C | 2.36 | 0.64 |
| 1:A:16:LYS:O | 1:A:18:LEU:N | 2.31 | 0.64 |
| 1:E:1294:GLU:HG2 | 1:F:1585:HIS:CD2 | 2.32 | 0.64 |
| 1:H:2112:SER:HB3 | 1:H:2287:PHE:CD2 | 2.32 | 0.64 |
| 1:B:316:LYS:HE2 | 1:B:491:GLU:HA | 1.80 | 0.64 |
| 1:C:779:LYS:HG3 | 1:C:780:GLU:H | 1.63 | 0.64 |
| 1:F:1535:VAL:O | 1:F:1575:ASN:HA | 1.98 | 0.64 |
| 1:E:1359:LEU:HG | 1:E:1360:TYR:CD2 | 2.33 | 0.64 |
| 1:F:1670:GLY:HA3 | 1:F:1718:LEU:HD23 | 1.80 | 0.63 |
| 1:H:2116:LYS:HG3 | 1:H:2117:ASN:N | 2.12 | 0.63 |
| 1:F:1547:ILE:HD13 | 1:F:1589:LEU:HD22 | 1.80 | 0.63 |
| 1:G:1829:PRO:HD3 | 1:G:1947:TYR:CZ | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:79:TYR:CE2 | 1:A:144:GLU:HG3 | 2.33 | 0.63 |
| 1:H:2300:ILE:HG13 | 1:H:2301:TYR:CD2 | 2.33 | 0.63 |
| 1:D:931:THR:HG22 | 1:D:979:TYR:HD1 | 1.63 | 0.63 |
| 1:G:1910:HIS:CD2 | 1:G:1936:ASN:HB3 | 2.34 | 0.63 |
| 1:D:1072:ILE:HB | 1:D:1086:PHE:CE2 | 2.34 | 0.63 |
| 1:C:638:VAL:HG23 | 1:C:639:ASP:H | 1.63 | 0.63 |
| 1:B:391:GLU:OE1 | 1:D:991:GLU:HG2 | 1.99 | 0.63 |
| 1:G:1881:VAL:H | 1:G:1943:GLN:HE21 | 1.46 | 0.63 |
| 1:F:1570:LEU:HD23 | 1:F:1570:LEU:O | 1.98 | 0.63 |
| 1:A:177:LYS:O | 1:A:177:LYS:HD3 | 1.99 | 0.63 |
| 1:D:935:VAL:O | 1:D:975:ASN:HA | 1.99 | 0.63 |
| 1:A:95:ARG:NH1 | 1:A:95:ARG:HB3 | 2.14 | 0.62 |
| 1:F:1583:TYR:CE1 | 1:F:1598:CYS:HB2 | 2.34 | 0.62 |
| 1:E:1225:TYR:CD2 | 1:E:1350:ARG:HD2 | 2.35 | 0.62 |
| 1:B:383:TYR:CE1 | 1:B:398:CYS:CB | 2.82 | 0.62 |
| 1:G:1804:PRO:HD3 | 1:G:1983:TRP:CD1 | 2.34 | 0.62 |
| 1:A:45:ASP:O | 1:A:46:LEU:HD23 | 1.98 | 0.62 |
| 1:B:470:GLY:HA2 | 1:B:517:TYR:O | 2.00 | 0.62 |
| 1:D:925:TYR:CD2 | 1:D:1050:ARG:HD2 | 2.34 | 0.62 |
| 1:A:38:VAL:CG2 | 1:A:39:ASP:N | 2.62 | 0.62 |
| 1:C:612:SER:HB3 | 1:C:787:PHE:CE2 | 2.34 | 0.62 |
| 1:F:1525:TYR:CD2 | 1:F:1650:ARG:HD2 | 2.35 | 0.62 |
| 1:C:777:LYS:O | 1:C:777:LYS:HD3 | 1.98 | 0.62 |
| 1:B:319:GLN:NE2 | 1:B:319:GLN:N | 2.38 | 0.62 |
| 1:D:959:LYS:HB2 | 1:D:989:LEU:CD2 | 2.27 | 0.62 |
| 1:B:450:ARG:O | 1:B:451:LYS:C | 2.38 | 0.62 |
| 1:D:974:LYS:HD2 | 1:D:974:LYS:N | 2.14 | 0.62 |
| 1:G:1977:LYS:CB | 1:G:2011:THR:HB | 2.30 | 0.62 |
| 1:E:1229:PRO:HD3 | 1:E:1347:TYR:CE2 | 2.34 | 0.62 |
| 1:E:1291:GLU:CD | 1:G:1891:GLU:H | 2.03 | 0.61 |
| 1:F:1583:TYR:HB2 | 1:F:1694:GLN:HE21 | 1.65 | 0.61 |
| 1:D:981:VAL:H | 1:D:1043:GLN:HE21 | 1.45 | 0.61 |
| 1:E:1252:GLY:HA3 | 1:E:1255:TYR:CZ | 2.35 | 0.61 |
| 1:E:1223:PHE:CE2 | 1:F:1595:ARG:NH2 | 2.67 | 0.61 |
| 1:C:800:ILE:HG13 | 1:C:801:TYR:CD2 | 2.34 | 0.61 |
| 1:F:1696:LYS:HD3 | 1:F:1697:TYR:N | 2.16 | 0.61 |
| 1:F:1609:ASN:O | 1:F:1637:LYS:HA | 2.00 | 0.61 |
| 1:F:1538:VAL:CG2 | 1:F:1539:ASP:H | 2.13 | 0.61 |
| 1:E:1279:TYR:CE2 | 1:E:1344:GLU:HG3 | 2.36 | 0.61 |
| 1:C:630:VAL:HG21 | 1:C:682:GLU:HB3 | 1.83 | 0.61 |
| 1:G:1943:GLN:OE1 | 1:G:2001:TYR:HB3 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:115:LYS:HD3 | 1:A:210:LYS:NZ | 2.15 | 0.61 |
| 1:G:1838:VAL:CG2 | 1:G:1839:ASP:H | 2.08 | 0.61 |
| 1:D:970:LEU:HD23 | 1:D:970:LEU:O | 2.00 | 0.61 |
| 1:G:1879:TYR:CE2 | 1:G:1944:GLU:HG3 | 2.35 | 0.61 |
| 1:C:638:VAL:HG23 | 1:C:639:ASP:N | 2.16 | 0.61 |
| 1:E:1216:LYS:HG3 | 1:E:1217:ASN:N | 2.16 | 0.61 |
| 1:F:1650:ARG:O | 1:F:1654:ILE:HG13 | 1.99 | 0.61 |
| 1:A:143:GLN:O | 1:A:144:GLU:C | 2.39 | 0.61 |
| 1:E:1279:TYR:CD2 | 1:E:1344:GLU:HG3 | 2.35 | 0.61 |
| 1:C:743:GLN:HG3 | 1:C:801:TYR:CD1 | 2.36 | 0.61 |
| 1:B:359:LYS:HB2 | 1:B:389:LEU:CD2 | 2.26 | 0.60 |
| 1:H:2160:THR:O | 1:H:2160:THR:HG23 | 2.01 | 0.60 |
| 1:G:1829:PRO:HD3 | 1:G:1947:TYR:CE2 | 2.36 | 0.60 |
| 1:G:1996:LYS:HD3 | 1:G:1996:LYS:C | 2.21 | 0.60 |
| 1:F:1679:LYS:HG3 | 1:F:1680:GLU:N | 2.16 | 0.60 |
| 1:B:395:ARG:HB3 | 1:B:395:ARG:NH1 | 2.16 | 0.60 |
| 1:E:1396:LYS:HD3 | 1:E:1396:LYS:C | 2.21 | 0.60 |
| 1:A:60:THR:HA | 1:A:99:ILE:O | 2.01 | 0.60 |
| 1:H:2179:TYR:CE2 | 1:H:2244:GLU:HG3 | 2.37 | 0.60 |
| 1:G:1860:THR:O | 1:G:1860:THR:HG23 | 2.01 | 0.60 |
| 1:E:1229:PRO:HD3 | 1:E:1347:TYR:CZ | 2.37 | 0.60 |
| 1:H:2102:GLN:N | 1:H:2102:GLN:NE2 | 2.35 | 0.60 |
| 1:D:1000:TYR:CE2 | 1:D:1099:MET:HG2 | 2.36 | 0.60 |
| 1:G:1915:LYS:HE3 | 1:G:2010:LYS:HD3 | 1.82 | 0.60 |
| 1:D:1061:THR:O | 1:D:1063:GLY:N | 2.34 | 0.60 |
| 1:A:34:ASN:HB2 | 1:A:106:HIS:CD2 | 2.37 | 0.60 |
| 1:A:91:GLU:OE1 | 1:C:691:GLU:HG2 | 2.01 | 0.60 |
| 1:F:1677:LYS:HB2 | 1:F:1711:THR:HB | 1.84 | 0.59 |
| 1:C:616:LYS:HG3 | 1:C:617:ASN:N | 2.17 | 0.59 |
| 1:G:1804:PRO:HD3 | 1:G:1983:TRP:NE1 | 2.18 | 0.59 |
| 1:C:685:HIS:CD2 | 1:D:994:GLU:HG2 | 2.37 | 0.59 |
| 1:F:1573:ASP:C | 1:F:1574:LYS:HD2 | 2.23 | 0.59 |
| 1:C:820:THR:O | 1:C:821:LYS:C | 2.40 | 0.59 |
| 1:F:1591:GLU:HB3 | 1:H:2191:GLU:CB | 2.26 | 0.59 |
| 1:D:916:LYS:HD3 | 1:D:1091:GLU:HG2 | 1.83 | 0.59 |
| 1:G:1951:LYS:HE2 | 1:G:1955:ASP:OD2 | 2.03 | 0.59 |
| 1:A:62:LEU:HD12 | 1:A:68:ALA:HA | 1.83 | 0.59 |
| 1:B:316:LYS:HE2 | 1:B:492:PHE:H | 1.66 | 0.59 |
| 1:G:1841:LEU:HG | 1:G:1842:LEU:HG | 1.84 | 0.59 |
| 1:A:60:THR:HG23 | 1:A:60:THR:O | 2.02 | 0.59 |
| 1:G:1885:HIS:CD2 | 1:H:2194:GLU:HG2 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:12:SER:HB3 | 1:A:187:PHE:CE2 | 2.38 | 0.59 |
| 1:D:1029:LEU:HD12 | 1:D:1029:LEU:C | 2.23 | 0.59 |
| 1:C:754:ILE:CG1 | 1:C:759:LEU:HB3 | 2.25 | 0.59 |
| 1:C:677:ASP:OD1 | 1:C:706:HIS:HD2 | 1.84 | 0.59 |
| 1:C:602:GLN:HE21 | 1:C:602:GLN:N | 2.00 | 0.59 |
| 1:B:330:VAL:HG21 | 1:B:382:GLU:HB3 | 1.85 | 0.59 |
| 1:F:1581:VAL:N | 1:F:1643:GLN:NE2 | 2.48 | 0.59 |
| 1:D:934:ASN:OD1 | 1:D:975:ASN:HB3 | 2.02 | 0.59 |
| 1:D:904:PRO:HD3 | 1:D:1083:TRP:CE2 | 2.38 | 0.58 |
| 1:G:1945:LEU:HD12 | 1:G:1974:PHE:HE2 | 1.68 | 0.58 |
| 1:D:929:PRO:HD3 | 1:D:1047:TYR:CZ | 2.38 | 0.58 |
| 1:A:94:GLU:HG2 | 1:B:385:HIS:CD2 | 2.38 | 0.58 |
| 1:D:932:HIS:CE1 | 1:D:950:VAL:HB | 2.38 | 0.58 |
| 1:D:983:TYR:CE1 | 1:D:998:CYS:CB | 2.87 | 0.58 |
| 1:F:1534:ASN:HB2 | 1:F:1606:HIS:CD2 | 2.38 | 0.58 |
| 1:D:942:LEU:O | 1:D:944:HIS:N | 2.35 | 0.58 |
| 1:E:1420:THR:O | 1:E:1421:LYS:C | 2.41 | 0.58 |
| 1:D:1117:TYR:O | 1:D:1118:LEU:HD23 | 2.04 | 0.58 |
| 1:G:1870:LEU:O | 1:G:1874:LYS:HD3 | 2.04 | 0.58 |
| 1:G:1937:LYS:HB2 | 1:G:1940:VAL:HG12 | 1.84 | 0.58 |
| 1:D:960:THR:O | 1:D:960:THR:HG23 | 2.03 | 0.58 |
| 1:F:1594:GLU:O | 1:F:1595:ARG:HB2 | 2.03 | 0.58 |
| 1:E:1235:VAL:O | 1:E:1275:ASN:HA | 2.02 | 0.58 |
| 1:D:977:ASP:OD2 | 1:D:1006:HIS:HA | 2.04 | 0.58 |
| 1:C:721:VAL:HB | 1:C:729:LEU:HD12 | 1.85 | 0.58 |
| 1:C:660:THR:O | 1:C:660:THR:HG23 | 2.04 | 0.58 |
| 1:G:1862:LEU:HB3 | 1:G:1867:MET:SD | 2.44 | 0.58 |
| 1:E:1304:THR:HG23 | 1:E:1341:THR:HG22 | 1.86 | 0.58 |
| 1:H:2141:LEU:HG | 1:H:2142:LEU:HG | 1.84 | 0.58 |
| 1:H:2142:LEU:C | 1:H:2144:HIS:H | 2.06 | 0.58 |
| 1:G:1967:TYR:CD1 | 1:G:1967:TYR:N | 2.72 | 0.58 |
| 1:A:77:ASP:OD1 | 1:A:106:HIS:HD2 | 1.87 | 0.58 |
| 1:D:983:TYR:HB2 | 1:D:1094:GLN:HE21 | 1.69 | 0.57 |
| 1:G:1825:TYR:CD2 | 1:G:1950:ARG:HD2 | 2.39 | 0.57 |
| 1:E:1217:ASN:HA | 1:E:1219:GLN:HE22 | 1.69 | 0.57 |
| 1:C:625:TYR:CD2 | 1:C:750:ARG:HD2 | 2.39 | 0.57 |
| 1:C:750:ARG:O | 1:C:754:ILE:HG13 | 2.04 | 0.57 |
| 1:A:83:TYR:HB2 | 1:A:194:GLN:NE2 | 2.18 | 0.57 |
| 1:F:1516:LYS:HD3 | 1:F:1691:GLU:HG2 | 1.86 | 0.57 |
| 1:F:1650:ARG:O | 1:F:1651:LYS:C | 2.41 | 0.57 |
| 1:F:1581:VAL:N | 1:F:1643:GLN:HE21 | 1.94 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1519:GLN:N | 1:F:1519:GLN:HE21 | 1.95 | 0.57 |
| 1:F:1516:LYS:CG | 1:F:1517:ASN:H | 2.12 | 0.57 |
| 1:G:1804:PRO:HB3 | 1:G:1983:TRP:CZ2 | 2.39 | 0.57 |
| 1:H:2131:THR:HA | 1:H:2178:ILE:O | 2.05 | 0.57 |
| 1:F:1562:LEU:HD12 | 1:F:1568:ALA:CA | 2.33 | 0.57 |
| 1:E:1283:TYR:CE1 | 1:E:1298:CYS:CB | 2.88 | 0.57 |
| 1:G:1855:TYR:C | 1:G:1895:ARG:HH12 | 2.08 | 0.57 |
| 1:D:960:THR:HA | 1:D:999:ILE:O | 2.03 | 0.57 |
| 1:B:410:HIS:CD2 | 1:B:436:ASN:HB3 | 2.40 | 0.57 |
| 1:E:1415:GLU:OE1 | 1:E:1417:TYR:OH | 2.20 | 0.57 |
| 1:G:1816:LYS:HG3 | 1:G:1817:ASN:N | 2.19 | 0.57 |
| 1:F:1670:GLY:HA3 | 1:F:1718:LEU:CD2 | 2.35 | 0.57 |
| 1:C:743:GLN:O | 1:C:744:GLU:C | 2.41 | 0.57 |
| 1:B:321:ILE:HG22 | 1:B:460:TYR:CE1 | 2.39 | 0.57 |
| 1:F:1717:TYR:O | 1:F:1718:LEU:HD23 | 2.04 | 0.57 |
| 1:C:796:LYS:HD3 | 1:C:796:LYS:C | 2.26 | 0.57 |
| 1:E:1241:LEU:HG | 1:E:1242:LEU:HG | 1.87 | 0.57 |
| 1:D:983:TYR:CE1 | 1:D:998:CYS:HB3 | 2.40 | 0.56 |
| 1:H:2138:VAL:CG2 | 1:H:2139:ASP:H | 2.16 | 0.56 |
| 1:A:4:PRO:HD3 | 1:A:183:TRP:NE1 | 2.19 | 0.56 |
| 1:A:82:GLU:HA | 1:A:99:ILE:HG22 | 1.87 | 0.56 |
| 1:H:2243:GLN:HG3 | 1:H:2301:TYR:CE1 | 2.40 | 0.56 |
| 1:D:934:ASN:HB2 | 1:D:1006:HIS:CD2 | 2.40 | 0.56 |
| 1:E:1407:LEU:O | 1:E:1407:LEU:HD12 | 2.05 | 0.56 |
| 1:A:23:PHE:HD1 | 1:A:23:PHE:H | 1.53 | 0.56 |
| 1:E:1238:VAL:CG2 | 1:E:1239:ASP:N | 2.68 | 0.56 |
| 1:B:377:ASP:OD1 | 1:B:406:HIS:HD2 | 1.88 | 0.56 |
| 1:G:1976:PRO:HA | 1:G:2012:SER:OG | 2.05 | 0.56 |
| 1:C:683:TYR:CE1 | 1:C:698:CYS:HB2 | 2.40 | 0.56 |
| 1:C:642:LEU:O | 1:C:644:HIS:N | 2.39 | 0.56 |
| 1:B:492:PHE:CD1 | 1:B:492:PHE:C | 2.79 | 0.56 |
| 1:A:59:LYS:HB2 | 1:A:89:LEU:CD2 | 2.33 | 0.56 |
| 1:D:1077:LYS:HB2 | 1:D:1111:THR:HB | 1.87 | 0.56 |
| 1:F:1582:GLU:HA | 1:F:1599:ILE:HG22 | 1.88 | 0.56 |
| 1:C:770:GLY:O | 1:C:786:PHE:HB2 | 2.06 | 0.56 |
| 1:F:1504:PRO:HB3 | 1:F:1683:TRP:CZ2 | 2.40 | 0.56 |
| 1:A:127:GLN:O | 1:A:127:GLN:HG2 | 2.06 | 0.56 |
| 1:C:704:THR:HG23 | 1:C:741:THR:HG22 | 1.88 | 0.56 |
| 1:C:745:LEU:O | 1:C:746:ASP:C | 2.43 | 0.56 |
| 1:E:1350:ARG:O | 1:E:1354:ILE:HG13 | 2.05 | 0.56 |
| 1:A:81:VAL:H | 1:A:143:GLN:HE21 | 1.52 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1270:LEU:O | 1:E:1270:LEU:HD23 | 2.06 | 0.56 |
| 1:G:1832:HIS:CE1 | 1:G:1850:VAL:HB | 2.40 | 0.56 |
| 1:G:2017:TYR:O | 1:G:2018:LEU:HD23 | 2.06 | 0.56 |
| 1:A:110:HIS:CD2 | 1:A:136:ASN:HB3 | 2.41 | 0.56 |
| 1:A:91:GLU:CB | 1:C:691:GLU:HB3 | 2.26 | 0.56 |
| 1:E:1295:ARG:HB3 | 1:E:1295:ARG:HH11 | 1.68 | 0.56 |
| 1:F:1560:THR:HG23 | 1:F:1560:THR:O | 2.05 | 0.56 |
| 1:E:1221:ILE:O | 1:E:1224:LEU:HB2 | 2.06 | 0.56 |
| 1:C:724:ASP:OD2 | 1:C:819:THR:HA | 2.06 | 0.56 |
| 1:H:2210:HIS:CD2 | 1:H:2236:ASN:HB3 | 2.41 | 0.56 |
| 1:C:616:LYS:HG3 | 1:C:617:ASN:H | 1.70 | 0.55 |
| 1:A:217:TYR:O | 1:A:218:LEU:HD23 | 2.06 | 0.55 |
| 1:E:1238:VAL:CG2 | 1:E:1239:ASP:H | 2.18 | 0.55 |
| 1:B:356:ASP:N | 1:B:395:ARG:HH12 | 2.04 | 0.55 |
| 1:C:796:LYS:HD3 | 1:C:797:TYR:N | 2.20 | 0.55 |
| 1:E:1216:LYS:HG3 | 1:E:1217:ASN:H | 1.71 | 0.55 |
| 1:E:1212:SER:HB3 | 1:E:1387:PHE:CE2 | 2.42 | 0.55 |
| 1:B:520:THR:O | 1:B:521:LYS:C | 2.43 | 0.55 |
| 1:B:302:GLN:H | 1:B:302:GLN:NE2 | 2.04 | 0.55 |
| 1:G:1929:LEU:C | 1:G:1929:LEU:HD12 | 2.27 | 0.55 |
| 1:H:2162:LEU:HD12 | 1:H:2168:ALA:HA | 1.88 | 0.55 |
| 1:C:679:TYR:CE2 | 1:C:744:GLU:HG3 | 2.42 | 0.55 |
| 1:D:1096:LYS:HD3 | 1:D:1096:LYS:C | 2.26 | 0.55 |
| 1:B:509:ASN:CG | 1:B:510:LYS:N | 2.60 | 0.55 |
| 1:E:1409:ASN:CG | 1:E:1410:LYS:H | 2.08 | 0.55 |
| 1:E:1291:GLU:H | 1:G:1891:GLU:CD | 2.06 | 0.55 |
| 1:G:1910:HIS:NE2 | 1:G:1936:ASN:HB3 | 2.21 | 0.55 |
| 1:B:429:LEU:HD12 | 1:B:429:LEU:C | 2.26 | 0.55 |
| 1:F:1512:SER:OG | 1:F:1668:GLU:HA | 2.06 | 0.55 |
| 1:F:1623:ILE:O | 1:F:1624:ASP:HB2 | 2.07 | 0.55 |
| 1:E:1274:LYS:N | 1:E:1274:LYS:HD2 | 2.22 | 0.55 |
| 1:C:682:GLU:OE1 | 1:C:682:GLU:N | 2.40 | 0.55 |
| 1:B:477:LYS:HD3 | 1:B:477:LYS:O | 2.07 | 0.55 |
| 1:B:322:TYR:O | 1:B:323:PHE:C | 2.45 | 0.55 |
| 1:B:323:PHE:O | 1:B:324:LEU:C | 2.45 | 0.55 |
| 1:A:47:ILE:HD13 | 1:A:89:LEU:HD22 | 1.89 | 0.55 |
| 1:F:1538:VAL:CG2 | 1:F:1539:ASP:N | 2.69 | 0.55 |
| 1:D:953:PRO:HG2 | 1:D:954:ASN:H | 1.71 | 0.55 |
| 1:E:1367:TYR:CD1 | 1:E:1367:TYR:N | 2.75 | 0.55 |
| 1:A:167:TYR:CD1 | 1:A:167:TYR:N | 2.73 | 0.55 |
| 1:B:331:THR:HG22 | 1:B:379:TYR:CD1 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1409:ASN:CG | 1:E:1410:LYS:N | 2.60 | 0.55 |
| 1:D:1067:TYR:CD1 | 1:D:1067:TYR:N | 2.74 | 0.54 |
| 1:H:2195:ARG:CZ | 1:H:2195:ARG:HB3 | 2.36 | 0.54 |
| 1:C:683:TYR:HB2 | 1:C:794:GLN:HE21 | 1.73 | 0.54 |
| 1:C:602:GLN:NE2 | 1:C:602:GLN:N | 2.54 | 0.54 |
| 1:H:2279:LYS:HG3 | 1:H:2280:GLU:N | 2.23 | 0.54 |
| 1:E:1240:GLN:HB2 | 1:E:1245:ASP:O | 2.07 | 0.54 |
| 1:F:1523:PHE:H | 1:F:1523:PHE:HD1 | 1.54 | 0.54 |
| 1:D:904:PRO:HD3 | 1:D:1083:TRP:NE1 | 2.23 | 0.54 |
| 1:E:1204:PRO:HB3 | 1:E:1383:TRP:CZ2 | 2.42 | 0.54 |
| 1:F:1651:LYS:HE2 | 1:F:1655:ASP:OD2 | 2.07 | 0.54 |
| 1:E:1379:LYS:HG3 | 1:E:1380:GLU:N | 2.22 | 0.54 |
| 1:A:85:HIS:CD2 | 1:B:394:GLU:HG2 | 2.43 | 0.54 |
| 1:B:304:PRO:HD3 | 1:B:483:TRP:CE2 | 2.42 | 0.54 |
| 1:F:1667:TYR:CD1 | 1:F:1667:TYR:N | 2.74 | 0.54 |
| 1:E:1350:ARG:O | 1:E:1351:LYS:C | 2.45 | 0.54 |
| 1:G:1873:ASP:C | 1:G:1874:LYS:HD2 | 2.28 | 0.54 |
| 1:A:4:PRO:HB3 | 1:A:183:TRP:CZ2 | 2.42 | 0.54 |
| 1:D:916:LYS:HE2 | 1:D:1091:GLU:HA | 1.89 | 0.54 |
| 1:F:1679:LYS:CG | 1:F:1680:GLU:H | 2.19 | 0.54 |
| 1:H:2138:VAL:CG2 | 1:H:2139:ASP:N | 2.71 | 0.54 |
| 1:C:631:THR:HG22 | 1:C:679:TYR:HD1 | 1.71 | 0.54 |
| 1:D:982:GLU:HA | 1:D:999:ILE:HG22 | 1.90 | 0.54 |
| 1:F:1588:TYR:CD1 | 1:F:1588:TYR:N | 2.76 | 0.54 |
| 1:F:1621:VAL:HG12 | 1:F:1622:SER:N | 2.23 | 0.54 |
| 1:A:161:THR:O | 1:A:163:GLY:N | 2.41 | 0.54 |
| 1:E:1216:LYS:HE2 | 1:E:1391:GLU:HA | 1.89 | 0.54 |
| 1:F:1531:THR:O | 1:F:1532:HIS:CG | 2.61 | 0.54 |
| 1:B:454:ILE:CG1 | 1:B:459:LEU:HB3 | 2.33 | 0.54 |
| 1:D:980:GLY:HA2 | 1:D:1043:GLN:NE2 | 2.22 | 0.54 |
| 1:H:2142:LEU:O | 1:H:2144:HIS:N | 2.40 | 0.54 |
| 1:G:1840:GLN:O | 1:G:1840:GLN:HG3 | 2.08 | 0.54 |
| 1:F:1562:LEU:CD1 | 1:F:1568:ALA:HA | 2.37 | 0.54 |
| 1:E:1223:PHE:CE2 | 1:F:1595:ARG:CZ | 2.90 | 0.53 |
| 1:H:2104:PRO:HD3 | 1:H:2283:TRP:NE1 | 2.23 | 0.53 |
| 1:B:479:LYS:CG | 1:B:480:GLU:H | 2.05 | 0.53 |
| 1:B:440:VAL:HG21 | 1:B:445:LEU:HD11 | 1.89 | 0.53 |
| 1:H:2195:ARG:NH1 | 1:H:2195:ARG:CB | 2.69 | 0.53 |
| 1:D:977:ASP:OD1 | 1:D:1006:HIS:HD2 | 1.91 | 0.53 |
| 1:A:98:CYS:O | 1:A:99:ILE:HG23 | 2.09 | 0.53 |
| 1:A:179:LYS:CG | 1:A:180:GLU:H | 2.17 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1262:LEU:CD2 | 1:E:1301:GLY:HA2 | 2.39 | 0.53 |
| 1:D:921:ILE:HG22 | 1:D:1060:TYR:CE1 | 2.44 | 0.53 |
| 1:E:1343:GLN:HG3 | 1:E:1401:TYR:CE1 | 2.44 | 0.53 |
| 1:C:685:HIS:O | 1:C:686:LEU:HB2 | 2.08 | 0.53 |
| 1:G:1894:GLU:O | 1:G:1895:ARG:HB2 | 2.08 | 0.53 |
| 1:H:2188:TYR:N | 1:H:2188:TYR:CD1 | 2.76 | 0.53 |
| 1:C:713:ILE:HD12 | 1:C:713:ILE:N | 2.23 | 0.53 |
| 1:H:2115:VAL:CG1 | 1:H:2292:PHE:HE2 | 2.22 | 0.53 |
| 1:G:1879:TYR:CD2 | 1:G:1944:GLU:HG3 | 2.44 | 0.53 |
| 1:A:115:LYS:HD3 | 1:A:210:LYS:HZ3 | 1.70 | 0.53 |
| 1:C:707:GLU:N | 1:C:707:GLU:OE1 | 2.38 | 0.53 |
| 1:D:1107:LEU:HD12 | 1:D:1107:LEU:O | 2.07 | 0.53 |
| 1:F:1654:ILE:CG1 | 1:F:1659:LEU:HB3 | 2.32 | 0.53 |
| 1:B:323:PHE:H | 1:B:323:PHE:HD1 | 1.57 | 0.53 |
| 1:H:2209:ASN:O | 1:H:2237:LYS:HA | 2.09 | 0.53 |
| 1:H:2110:HIS:ND1 | 1:H:2287:PHE:O | 2.42 | 0.53 |
| 1:G:1824:LEU:HD13 | 1:G:1998:LEU:HD21 | 1.91 | 0.53 |
| 1:C:767:TYR:CD1 | 1:C:767:TYR:N | 2.77 | 0.53 |
| 1:D:1109:ASN:CG | 1:D:1110:LYS:N | 2.62 | 0.53 |
| 1:A:25:TYR:CZ | 1:A:150:ARG:NH1 | 2.77 | 0.53 |
| 1:B:443:GLN:O | 1:B:444:GLU:C | 2.47 | 0.53 |
| 1:C:660:THR:HA | 1:C:699:ILE:O | 2.09 | 0.53 |
| 1:C:619:GLN:O | 1:C:622:TYR:HB3 | 2.09 | 0.52 |
| 1:H:2116:LYS:O | 1:H:2118:LEU:N | 2.42 | 0.52 |
| 1:D:1000:TYR:HE2 | 1:D:1099:MET:HG2 | 1.74 | 0.52 |
| 1:A:79:TYR:CD2 | 1:A:144:GLU:HA | 2.44 | 0.52 |
| 1:A:87:CYS:SG | 1:A:98:CYS:N | 2.82 | 0.52 |
| 1:A:159:LEU:HG | 1:A:160:TYR:CD2 | 2.44 | 0.52 |
| 1:C:694:GLU:O | 1:C:695:ARG:HB2 | 2.09 | 0.52 |
| 1:G:1842:LEU:O | 1:G:1844:HIS:N | 2.42 | 0.52 |
| 1:E:1309:ASN:O | 1:E:1337:LYS:HA | 2.09 | 0.52 |
| 1:G:1950:ARG:O | 1:G:1951:LYS:C | 2.45 | 0.52 |
| 1:C:754:ILE:HA | 1:C:759:LEU:H | 1.74 | 0.52 |
| 1:D:917:ASN:HB3 | 1:D:919:GLN:OE1 | 2.08 | 0.52 |
| 1:A:98:CYS:O | 1:A:99:ILE:CG2 | 2.58 | 0.52 |
| 1:H:2182:GLU:HA | 1:H:2198:CYS:O | 2.09 | 0.52 |
| 1:B:446:ASP:O | 1:B:450:ARG:HG3 | 2.10 | 0.52 |
| 1:G:1802:GLN:N | 1:G:1802:GLN:HE21 | 2.07 | 0.52 |
| 1:D:1077:LYS:O | 1:D:1077:LYS:HD3 | 2.08 | 0.52 |
| 1:H:2279:LYS:HG3 | 1:H:2280:GLU:H | 1.75 | 0.52 |
| 1:B:304:PRO:HB3 | 1:B:483:TRP:CZ2 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1388:PRO:HG3 | 1:E:1392:PHE:CE2 | 2.44 | 0.52 |
| 1:B:382:GLU:OE1 | 1:B:382:GLU:N | 2.40 | 0.52 |
| 1:A:200:ILE:HG13 | 1:A:201:TYR:CD2 | 2.45 | 0.52 |
| 1:C:667:MET:O | 1:C:670:LEU:HB3 | 2.10 | 0.52 |
| 1:E:1291:GLU:N | 1:G:1891:GLU:OE1 | 2.28 | 0.52 |
| 1:D:1047:TYR:O | 1:D:1050:ARG:N | 2.43 | 0.52 |
| 1:H:2134:ASN:OD1 | 1:H:2175:ASN:HB3 | 2.10 | 0.52 |
| 1:A:70:LEU:HD23 | 1:A:70:LEU:O | 2.09 | 0.52 |
| 1:D:1109:ASN:CG | 1:D:1110:LYS:H | 2.13 | 0.52 |
| 1:G:1883:TYR:CE1 | 1:G:1898:CYS:HB2 | 2.44 | 0.52 |
| 1:G:1802:GLN:NE2 | 1:G:1802:GLN:N | 2.56 | 0.52 |
| 1:G:1829:PRO:HD3 | 1:G:1947:TYR:OH | 2.10 | 0.52 |
| 1:E:1202:GLN:NE2 | 1:E:1202:GLN:H | 2.08 | 0.52 |
| 1:H:2115:VAL:O | 1:H:2116:LYS:O | 2.27 | 0.52 |
| 1:C:743:GLN:OE1 | 1:C:801:TYR:HB3 | 2.09 | 0.52 |
| 1:A:81:VAL:O | 1:A:99:ILE:HG22 | 2.09 | 0.52 |
| 1:D:994:GLU:O | 1:D:995:ARG:HB2 | 2.09 | 0.52 |
| 1:H:2129:PRO:HD3 | 1:H:2247:TYR:CZ | 2.44 | 0.52 |
| 1:A:56:ASP:N | 1:A:95:ARG:HH12 | 2.07 | 0.52 |
| 1:C:670:LEU:O | 1:C:674:LYS:HD3 | 2.09 | 0.52 |
| 1:E:1329:LEU:C | 1:E:1329:LEU:HD12 | 2.30 | 0.52 |
| 1:C:615:VAL:HG11 | 1:C:618:LEU:HD13 | 1.92 | 0.52 |
| 1:F:1583:TYR:CE2 | 1:F:1695:SER:HB3 | 2.45 | 0.52 |
| 1:H:2195:ARG:CB | 1:H:2195:ARG:HH11 | 2.23 | 0.52 |
| 1:F:1585:HIS:O | 1:F:1586:LEU:HB2 | 2.10 | 0.52 |
| 1:G:1959:LEU:HG | 1:G:1960:TYR:CD2 | 2.45 | 0.52 |
| 1:E:1247:ILE:HD13 | 1:E:1289:LEU:HD22 | 1.92 | 0.52 |
| 1:D:1007:GLU:N | 1:D:1007:GLU:OE1 | 2.43 | 0.52 |
| 1:B:412:GLU:HB3 | 1:B:413:ILE:HD12 | 1.92 | 0.52 |
| 1:D:982:GLU:OE1 | 1:D:982:GLU:N | 2.43 | 0.52 |
| 1:D:1043:GLN:O | 1:D:1044:GLU:C | 2.49 | 0.52 |
| 1:A:2:GLN:N | 1:A:2:GLN:HE21 | 2.07 | 0.52 |
| 1:D:938:VAL:HG23 | 1:D:939:ASP:N | 2.24 | 0.52 |
| 1:A:143:GLN:HG3 | 1:A:201:TYR:CE1 | 2.45 | 0.51 |
| 1:G:1830:VAL:HG21 | 1:G:1882:GLU:HB3 | 1.92 | 0.51 |
| 1:A:85:HIS:O | 1:A:86:LEU:HB2 | 2.10 | 0.51 |
| 1:E:1393:THR:O | 1:E:1394:GLN:C | 2.47 | 0.51 |
| 1:G:1907:GLU:N | 1:G:1907:GLU:OE1 | 2.43 | 0.51 |
| 1:F:1559:LYS:HB2 | 1:F:1589:LEU:CD2 | 2.36 | 0.51 |
| 1:G:1935:THR:OG1 | 1:G:1936:ASN:N | 2.40 | 0.51 |
| 1:B:404:THR:CG2 | 1:B:441:THR:HG22 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1571:PHE:O | 1:F:1572:LYS:C | 2.47 | 0.51 |
| 1:D:1050:ARG:O | 1:D:1051:LYS:C | 2.48 | 0.51 |
| 1:C:777:LYS:HD3 | 1:C:777:LYS:C | 2.31 | 0.51 |
| 1:C:740:VAL:HG21 | 1:C:745:LEU:HD11 | 1.93 | 0.51 |
| 1:B:304:PRO:HD3 | 1:B:483:TRP:NE1 | 2.24 | 0.51 |
| 1:F:1604:THR:HG23 | 1:F:1641:THR:HG22 | 1.93 | 0.51 |
| 1:D:930:VAL:HG13 | 1:D:955:TYR:OH | 2.10 | 0.51 |
| 1:E:1354:ILE:HA | 1:E:1359:LEU:H | 1.75 | 0.51 |
| 1:F:1707:LEU:HD12 | 1:F:1707:LEU:C | 2.31 | 0.51 |
| 1:C:645:ASP:O | 1:C:646:LEU:HD23 | 2.10 | 0.51 |
| 1:H:2294:GLN:O | 1:H:2295:SER:C | 2.49 | 0.51 |
| 1:H:2156:ASP:N | 1:H:2195:ARG:HH12 | 2.09 | 0.51 |
| 1:F:1615:LYS:HG2 | 1:F:1709:ASN:HD22 | 1.75 | 0.51 |
| 1:H:2177:ASP:OD2 | 1:H:2206:HIS:HA | 2.11 | 0.51 |
| 1:A:119:VAL:HG22 | 1:A:214:ILE:HB | 1.93 | 0.51 |
| 1:C:779:LYS:HG3 | 1:C:780:GLU:N | 2.26 | 0.51 |
| 1:A:113:ILE:HD12 | 1:A:113:ILE:N | 2.25 | 0.51 |
| 1:F:1502:GLN:NE2 | 1:F:1502:GLN:H | 2.09 | 0.51 |
| 1:D:983:TYR:CE1 | 1:D:998:CYS:HB2 | 2.45 | 0.51 |
| 1:E:1285:HIS:O | 1:E:1286:LEU:HB2 | 2.11 | 0.51 |
| 1:A:67:MET:O | 1:A:70:LEU:HB3 | 2.11 | 0.51 |
| 1:D:1120:THR:O | 1:D:1121:LYS:C | 2.49 | 0.51 |
| 1:A:10:HIS:CD2 | 1:A:10:HIS:N | 2.79 | 0.51 |
| 1:D:988:TYR:N | 1:D:988:TYR:CD1 | 2.79 | 0.51 |
| 1:B:380:GLY:HA2 | 1:B:443:GLN:HE21 | 1.76 | 0.51 |
| 1:G:1954:ILE:HG12 | 1:G:1959:LEU:HB3 | 1.91 | 0.51 |
| 1:G:1877:ASP:OD1 | 1:G:1906:HIS:CD2 | 2.64 | 0.51 |
| 1:F:1540:GLN:HB2 | 1:F:1545:ASP:O | 2.11 | 0.51 |
| 1:F:1579:TYR:CD2 | 1:F:1644:GLU:HG3 | 2.46 | 0.51 |
| 1:H:2296:LYS:HD3 | 1:H:2297:TYR:CA | 2.41 | 0.51 |
| 1:D:1004:THR:HG23 | 1:D:1041:THR:HG22 | 1.93 | 0.51 |
| 1:A:145:LEU:O | 1:A:147:TYR:N | 2.45 | 0.50 |
| 1:G:1996:LYS:HD3 | 1:G:1997:TYR:CA | 2.41 | 0.50 |
| 1:H:2125:TYR:CD2 | 1:H:2250:ARG:HD2 | 2.46 | 0.50 |
| 1:G:1950:ARG:O | 1:G:1954:ILE:HG13 | 2.09 | 0.50 |
| 1:E:1260:THR:O | 1:E:1260:THR:HG23 | 2.11 | 0.50 |
| 1:C:635:VAL:O | 1:C:675:ASN:HA | 2.10 | 0.50 |
| 1:F:1670:GLY:CA | 1:F:1718:LEU:HD23 | 2.40 | 0.50 |
| 1:F:1647:TYR:O | 1:F:1648:LYS:C | 2.50 | 0.50 |
| 1:D:902:GLN:H | 1:D:902:GLN:NE2 | 2.10 | 0.50 |
| 1:F:1629:LEU:C | 1:F:1629:LEU:HD12 | 2.31 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:983:TYR:CE1 | 1:D:1000:TYR:HE1 | 2.29 | 0.50 |
| 1:D:982:GLU:HA | 1:D:998:CYS:O | 2.12 | 0.50 |
| 1:A:30:VAL:CG2 | 1:A:82:GLU:HB3 | 2.40 | 0.50 |
| 1:F:1530:VAL:HG21 | 1:F:1582:GLU:HB3 | 1.93 | 0.50 |
| 1:C:685:HIS:O | 1:C:686:LEU:CB | 2.60 | 0.50 |
| 1:C:744:GLU:O | 1:C:747:TYR:HB3 | 2.12 | 0.50 |
| 1:G:1819:GLN:O | 1:G:1822:TYR:HB3 | 2.12 | 0.50 |
| 1:A:79:TYR:CE2 | 1:A:144:GLU:HA | 2.47 | 0.50 |
| 1:G:1823:PHE:HD1 | 1:G:1823:PHE:H | 1.59 | 0.50 |
| 1:A:196:LYS:HD3 | 1:A:197:TYR:CA | 2.41 | 0.50 |
| 1:C:642:LEU:C | 1:C:644:HIS:H | 2.15 | 0.50 |
| 1:C:783:TRP:O | 1:C:784:PHE:HD2 | 1.95 | 0.50 |
| 1:C:709:ASN:O | 1:C:737:LYS:HA | 2.11 | 0.50 |
| 1:F:1720:THR:O | 1:F:1720:THR:HG22 | 2.10 | 0.50 |
| 1:E:1327:GLN:HG2 | 1:E:1327:GLN:O | 2.12 | 0.50 |
| 1:B:385:HIS:O | 1:B:386:LEU:HB2 | 2.11 | 0.50 |
| 1:B:379:TYR:CD2 | 1:B:444:GLU:HG3 | 2.47 | 0.50 |
| 1:A:16:LYS:O | 1:A:17:ASN:C | 2.49 | 0.50 |
| 1:A:16:LYS:HD3 | 1:A:191:GLU:HG2 | 1.93 | 0.50 |
| 1:D:1077:LYS:CB | 1:D:1111:THR:HB | 2.41 | 0.50 |
| 1:B:404:THR:HG23 | 1:B:441:THR:HG22 | 1.94 | 0.50 |
| 1:B:341:LEU:HG | 1:B:342:LEU:HG | 1.92 | 0.50 |
| 1:B:459:LEU:HG | 1:B:460:TYR:CD2 | 2.46 | 0.50 |
| 1:G:1870:LEU:C | 1:G:1870:LEU:HD23 | 2.31 | 0.50 |
| 1:A:19:GLN:O | 1:A:22:TYR:HB3 | 2.12 | 0.50 |
| 1:F:1530:VAL:HG13 | 1:F:1555:TYR:OH | 2.11 | 0.50 |
| 1:A:145:LEU:O | 1:A:146:ASP:C | 2.51 | 0.50 |
| 1:H:2182:GLU:HA | 1:H:2199:ILE:HG22 | 1.93 | 0.50 |
| 1:B:374:LYS:N | 1:B:374:LYS:HD2 | 2.26 | 0.50 |
| 1:G:1877:ASP:OD1 | 1:G:1906:HIS:HD2 | 1.95 | 0.50 |
| 1:B:343:SER:HB2 | 1:C:789:GLU:HB3 | 1.94 | 0.50 |
| 1:C:776:PRO:HB2 | 1:C:779:LYS:HB3 | 1.94 | 0.49 |
| 1:C:782:PHE:CE2 | 1:C:805:GLU:HG2 | 2.47 | 0.49 |
| 1:D:1050:ARG:O | 1:D:1054:ILE:HG13 | 2.12 | 0.49 |
| 1:E:1359:LEU:HG | 1:E:1360:TYR:CE2 | 2.47 | 0.49 |
| 1:A:16:LYS:HG3 | 1:A:17:ASN:N | 2.28 | 0.49 |
| 1:D:994:GLU:O | 1:D:995:ARG:CB | 2.60 | 0.49 |
| 1:E:1291:GLU:OE2 | 1:G:1890:CYS:HA | 2.12 | 0.49 |
| 1:H:2177:ASP:OD1 | 1:H:2206:HIS:CD2 | 2.66 | 0.49 |
| 1:A:115:LYS:HE3 | 1:A:210:LYS:HD3 | 1.93 | 0.49 |
| 1:D:1013:ILE:HD12 | 1:D:1013:ILE:N | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:143:GLN:OE1 | 1:A:201:TYR:HB3 | 2.13 | 0.49 |
| 1:A:146:ASP:O | 1:A:150:ARG:HG3 | 2.12 | 0.49 |
| 1:E:1231:THR:HG22 | 1:E:1279:TYR:CD1 | 2.47 | 0.49 |
| 1:C:695:ARG:NH1 | 1:C:695:ARG:HB3 | 2.28 | 0.49 |
| 1:F:1502:GLN:HE21 | 1:F:1502:GLN:H | 1.60 | 0.49 |
| 1:A:129:LEU:C | 1:A:129:LEU:HD12 | 2.31 | 0.49 |
| 1:B:319:GLN:O | 1:B:322:TYR:N | 2.45 | 0.49 |
| 1:E:1343:GLN:O | 1:E:1344:GLU:C | 2.51 | 0.49 |
| 1:E:1347:TYR:O | 1:E:1348:LYS:C | 2.49 | 0.49 |
| 1:D:1116:VAL:C | 1:D:1117:TYR:CD1 | 2.86 | 0.49 |
| 1:B:382:GLU:HA | 1:B:399:ILE:HG22 | 1.94 | 0.49 |
| 1:D:1045:LEU:HD12 | 1:D:1074:PHE:HE2 | 1.78 | 0.49 |
| 1:F:1651:LYS:O | 1:F:1654:ILE:HB | 2.11 | 0.49 |
| 1:C:670:LEU:C | 1:C:670:LEU:HD23 | 2.33 | 0.49 |
| 1:C:621:ILE:O | 1:C:624:LEU:HB2 | 2.13 | 0.49 |
| 1:H:2150:VAL:HG23 | 1:H:2155:TYR:HE1 | 1.77 | 0.49 |
| 1:H:2129:PRO:HD3 | 1:H:2247:TYR:CE2 | 2.48 | 0.49 |
| 1:H:2183:TYR:CE2 | 1:H:2295:SER:HB3 | 2.48 | 0.49 |
| 1:D:1043:GLN:OE1 | 1:D:1101:TYR:HB3 | 2.12 | 0.49 |
| 1:A:172:ILE:HB | 1:A:186:PHE:CE2 | 2.46 | 0.49 |
| 1:F:1672:ILE:HB | 1:F:1686:PHE:CE2 | 2.47 | 0.49 |
| 1:E:1391:GLU:N | 1:H:2143:SER:OG | 2.45 | 0.49 |
| 1:H:2200:TYR:CE2 | 1:H:2299:MET:HG2 | 2.48 | 0.49 |
| 1:C:630:VAL:CG2 | 1:C:682:GLU:HB3 | 2.43 | 0.49 |
| 1:H:2142:LEU:C | 1:H:2144:HIS:N | 2.66 | 0.49 |
| 1:C:688:TYR:N | 1:C:688:TYR:CD1 | 2.80 | 0.49 |
| 1:G:1817:ASN:HA | 1:G:1819:GLN:HE22 | 1.77 | 0.49 |
| 1:H:2194:GLU:O | 1:H:2195:ARG:HB2 | 2.13 | 0.49 |
| 1:B:302:GLN:N | 1:B:302:GLN:HE21 | 2.11 | 0.49 |
| 1:F:1702:LYS:C | 1:F:1704:ASN:H | 2.15 | 0.49 |
| 1:C:643:SER:O | 1:C:665:GLN:HA | 2.13 | 0.49 |
| 1:H:2180:GLY:CA | 1:H:2243:GLN:NE2 | 2.76 | 0.49 |
| 1:G:1888:TYR:CD1 | 1:G:1888:TYR:N | 2.80 | 0.49 |
| 1:D:940:GLN:HB2 | 1:D:945:ASP:O | 2.13 | 0.48 |
| 1:H:2115:VAL:HG11 | 1:H:2118:LEU:HD13 | 1.95 | 0.48 |
| 1:F:1525:TYR:CZ | 1:F:1650:ARG:NH1 | 2.81 | 0.48 |
| 1:H:2170:LEU:HD22 | 1:H:2171:PHE:CD1 | 2.48 | 0.48 |
| 1:B:413:ILE:N | 1:B:413:ILE:HD12 | 2.28 | 0.48 |
| 1:C:735:THR:OG1 | 1:C:736:ASN:N | 2.46 | 0.48 |
| 1:F:1591:GLU:OE1 | 1:H:2191:GLU:HG2 | 2.13 | 0.48 |
| 1:C:743:GLN:HG3 | 1:C:801:TYR:CE1 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2243:GLN:O | 1:H:2244:GLU:C | 2.50 | 0.48 |
| 1:D:1100:ILE:HG13 | 1:D:1101:TYR:CD2 | 2.48 | 0.48 |
| 1:G:1862:LEU:HD13 | 1:G:1867:MET:HG2 | 1.95 | 0.48 |
| 1:G:1879:TYR:CE2 | 1:G:1944:GLU:HA | 2.48 | 0.48 |
| 1:E:1260:THR:HA | 1:E:1299:ILE:O | 2.13 | 0.48 |
| 1:H:2117:ASN:HB3 | 1:H:2119:GLN:OE1 | 2.13 | 0.48 |
| 1:D:1096:LYS:HD3 | 1:D:1097:TYR:N | 2.28 | 0.48 |
| 1:G:1993:THR:HA | 1:H:2194:GLU:OE2 | 2.13 | 0.48 |
| 1:D:923:PHE:HD1 | 1:D:923:PHE:H | 1.62 | 0.48 |
| 1:H:2320:THR:HG22 | 1:H:2320:THR:O | 2.13 | 0.48 |
| 1:F:1589:LEU:HD12 | 1:F:1596:SER:HB3 | 1.95 | 0.48 |
| 1:C:716:LYS:HG2 | 1:C:734:GLU:HG2 | 1.95 | 0.48 |
| 1:D:916:LYS:CG | 1:D:917:ASN:H | 2.20 | 0.48 |
| 1:F:1531:THR:HG22 | 1:F:1579:TYR:CD1 | 2.49 | 0.48 |
| 1:C:634:ASN:OD1 | 1:C:675:ASN:HB3 | 2.13 | 0.48 |
| 1:C:685:HIS:CD2 | 1:C:686:LEU:HG | 2.49 | 0.48 |
| 1:D:1023:ILE:O | 1:D:1024:ASP:HB2 | 2.14 | 0.48 |
| 1:A:32:HIS:CE1 | 1:A:50:VAL:HB | 2.49 | 0.48 |
| 1:F:1674:PHE:HB2 | 1:F:1682:PHE:CE1 | 2.49 | 0.48 |
| 1:B:382:GLU:H | 1:B:382:GLU:CD | 2.17 | 0.48 |
| 1:B:496:LYS:O | 1:B:496:LYS:HD3 | 2.13 | 0.48 |
| 1:B:383:TYR:CZ | 1:B:398:CYS:HB2 | 2.48 | 0.48 |
| 1:F:1585:HIS:O | 1:F:1586:LEU:CB | 2.61 | 0.48 |
| 1:F:1643:GLN:O | 1:F:1644:GLU:C | 2.51 | 0.48 |
| 1:B:443:GLN:HG3 | 1:B:501:TYR:CD1 | 2.49 | 0.48 |
| 1:G:1840:GLN:HB2 | 1:G:1845:ASP:O | 2.13 | 0.48 |
| 1:B:447:TYR:O | 1:B:448:LYS:C | 2.52 | 0.48 |
| 1:D:1074:PHE:HB2 | 1:D:1082:PHE:CE1 | 2.49 | 0.47 |
| 1:H:2177:ASP:OD1 | 1:H:2206:HIS:HD2 | 1.97 | 0.47 |
| 1:B:315:VAL:HG13 | 1:B:492:PHE:HE2 | 1.78 | 0.47 |
| 1:A:121:VAL:O | 1:A:127:GLN:HA | 2.14 | 0.47 |
| 1:F:1502:GLN:HE21 | 1:F:1502:GLN:N | 2.12 | 0.47 |
| 1:F:1510:HIS:CD2 | 1:F:1510:HIS:N | 2.81 | 0.47 |
| 1:A:19:GLN:HG2 | 1:A:20:ASN:N | 2.29 | 0.47 |
| 1:H:2254:ILE:O | 1:H:2258:GLN:HA | 2.14 | 0.47 |
| 1:D:942:LEU:C | 1:D:944:HIS:H | 2.18 | 0.47 |
| 1:E:1313:ILE:HD12 | 1:E:1313:ILE:N | 2.29 | 0.47 |
| 1:A:56:ASP:O | 1:A:57:LYS:HD3 | 2.14 | 0.47 |
| 1:F:1570:LEU:C | 1:F:1570:LEU:HD23 | 2.33 | 0.47 |
| 1:F:1600:TYR:CE2 | 1:F:1699:MET:HG2 | 2.49 | 0.47 |
| 1:D:1108:ASP:OD2 | 1:D:1111:THR:HG23 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1324:ASP:OD2 | 1:E:1419:THR:HA | 2.14 | 0.47 |
| 1:F:1644:GLU:O | 1:F:1645:LEU:C | 2.52 | 0.47 |
| 1:A:199:MET:C | 1:A:201:TYR:H | 2.16 | 0.47 |
| 1:D:1038:LYS:O | 1:D:1109:ASN:OD1 | 2.33 | 0.47 |
| 1:E:1345:LEU:O | 1:E:1346:ASP:C | 2.53 | 0.47 |
| 1:C:732:ASP:O | 1:C:733:ILE:HG23 | 2.14 | 0.47 |
| 1:H:2117:ASN:HA | 1:H:2119:GLN:HE22 | 1.79 | 0.47 |
| 1:B:509:ASN:CG | 1:B:510:LYS:H | 2.17 | 0.47 |
| 1:F:1640:VAL:HG21 | 1:F:1645:LEU:HD11 | 1.97 | 0.47 |
| 1:A:25:TYR:CD2 | 1:A:150:ARG:HD2 | 2.50 | 0.47 |
| 1:E:1343:GLN:OE1 | 1:E:1401:TYR:HB3 | 2.13 | 0.47 |
| 1:G:1831:THR:HG22 | 1:G:1879:TYR:CD1 | 2.50 | 0.47 |
| 1:E:1337:LYS:HB2 | 1:E:1340:VAL:HG12 | 1.96 | 0.47 |
| 1:B:332:HIS:CD2 | 1:B:350:VAL:HG21 | 2.50 | 0.47 |
| 1:H:2246:ASP:O | 1:H:2250:ARG:HG3 | 2.14 | 0.47 |
| 1:H:2131:THR:HG22 | 1:H:2179:TYR:CE1 | 2.50 | 0.47 |
| 1:G:1946:ASP:OD2 | 1:G:1950:ARG:NE | 2.48 | 0.47 |
| 1:H:2267:TYR:HD1 | 1:H:2267:TYR:H | 1.62 | 0.47 |
| 1:C:623:PHE:HD1 | 1:C:623:PHE:H | 1.63 | 0.47 |
| 1:C:729:LEU:HD12 | 1:C:729:LEU:C | 2.35 | 0.47 |
| 1:D:1058:GLN:N | 1:D:1058:GLN:CD | 2.68 | 0.47 |
| 1:D:919:GLN:NE2 | 1:D:919:GLN:N | 2.50 | 0.47 |
| 1:F:1654:ILE:HA | 1:F:1659:LEU:H | 1.80 | 0.47 |
| 1:G:1909:ASN:O | 1:G:1937:LYS:HA | 2.14 | 0.47 |
| 1:E:1216:LYS:O | 1:E:1218:LEU:N | 2.48 | 0.47 |
| 1:A:95:ARG:NE | 1:B:323:PHE:CE2 | 2.83 | 0.47 |
| 1:H:2183:TYR:CE1 | 1:H:2198:CYS:HB2 | 2.50 | 0.47 |
| 1:A:196:LYS:HD3 | 1:A:197:TYR:HA | 1.96 | 0.47 |
| 1:G:1874:LYS:N | 1:G:1874:LYS:HD2 | 2.29 | 0.47 |
| 1:A:170:GLY:O | 1:A:186:PHE:HB2 | 2.15 | 0.47 |
| 1:F:1512:SER:HG | 1:F:1668:GLU:HA | 1.78 | 0.47 |
| 1:H:2272:ILE:HG22 | 1:H:2284:PHE:HB2 | 1.98 | 0.47 |
| 1:H:2150:VAL:HG23 | 1:H:2155:TYR:CE1 | 2.50 | 0.47 |
| 1:B:467:TYR:CD2 | 1:B:518:LEU:HB3 | 2.50 | 0.47 |
| 1:B:358:LEU:HD12 | 1:B:397:ALA:O | 2.14 | 0.47 |
| 1:C:759:LEU:HG | 1:C:760:TYR:CD2 | 2.50 | 0.46 |
| 1:D:919:GLN:O | 1:D:922:TYR:HB3 | 2.15 | 0.46 |
| 1:B:385:HIS:CD2 | 1:B:386:LEU:HG | 2.49 | 0.46 |
| 1:A:143:GLN:HG3 | 1:A:201:TYR:CD1 | 2.51 | 0.46 |
| 1:G:1972:ILE:HG12 | 1:G:1974:PHE:CE1 | 2.51 | 0.46 |
| 1:H:2155:TYR:CD1 | 1:H:2155:TYR:O | 2.68 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1312:GLU:C | 1:E:1313:ILE:HD12 | 2.35 | 0.46 |
| 1:H:2160:THR:HA | 1:H:2199:ILE:O | 2.14 | 0.46 |
| 1:B:325:TYR:CZ | 1:B:450:ARG:NH1 | 2.83 | 0.46 |
| 1:E:1295:ARG:CB | 1:E:1295:ARG:HH11 | 2.28 | 0.46 |
| 1:E:1304:THR:CG2 | 1:E:1341:THR:HG22 | 2.45 | 0.46 |
| 1:F:1702:LYS:C | 1:F:1704:ASN:N | 2.69 | 0.46 |
| 1:E:1402:LYS:C | 1:E:1404:ASN:N | 2.68 | 0.46 |
| 1:F:1659:LEU:HG | 1:F:1660:TYR:CD2 | 2.50 | 0.46 |
| 1:G:1885:HIS:O | 1:G:1886:LEU:HB2 | 2.15 | 0.46 |
| 1:A:70:LEU:HD23 | 1:A:70:LEU:C | 2.35 | 0.46 |
| 1:H:2104:PRO:HB3 | 1:H:2283:TRP:CZ2 | 2.50 | 0.46 |
| 1:G:1885:HIS:O | 1:G:1886:LEU:CB | 2.64 | 0.46 |
| 1:G:2000:ILE:HG13 | 1:G:2001:TYR:CD2 | 2.51 | 0.46 |
| 1:F:1540:GLN:HG3 | 1:F:1540:GLN:O | 2.14 | 0.46 |
| 1:H:2213:ILE:HD12 | 1:H:2213:ILE:N | 2.31 | 0.46 |
| 1:B:394:GLU:O | 1:B:395:ARG:HB2 | 2.15 | 0.46 |
| 1:G:1972:ILE:HB | 1:G:1986:PHE:CE2 | 2.51 | 0.46 |
| 1:G:1852:GLY:HA3 | 1:G:1855:TYR:CZ | 2.51 | 0.46 |
| 1:E:1323:ILE:O | 1:E:1324:ASP:HB2 | 2.16 | 0.46 |
| 1:B:419:VAL:HG22 | 1:B:514:ILE:HB | 1.98 | 0.46 |
| 1:E:1216:LYS:CG | 1:E:1217:ASN:H | 2.26 | 0.46 |
| 1:G:1816:LYS:O | 1:G:1818:LEU:N | 2.49 | 0.46 |
| 1:H:2252:TYR:O | 1:H:2254:ILE:N | 2.49 | 0.46 |
| 1:B:319:GLN:O | 1:B:322:TYR:HB3 | 2.16 | 0.46 |
| 1:G:1943:GLN:O | 1:G:1944:GLU:C | 2.54 | 0.46 |
| 1:G:1917:ILE:O | 1:G:1932:ASP:HA | 2.16 | 0.46 |
| 1:H:2211:LEU:HD23 | 1:H:2238:LYS:HE2 | 1.97 | 0.46 |
| 1:A:140:VAL:HG21 | 1:A:145:LEU:HD11 | 1.97 | 0.46 |
| 1:B:445:LEU:O | 1:B:446:ASP:C | 2.54 | 0.46 |
| 1:D:970:LEU:O | 1:D:974:LYS:HD3 | 2.15 | 0.46 |
| 1:E:1247:ILE:HD13 | 1:E:1289:LEU:CD2 | 2.46 | 0.46 |
| 1:G:1879:TYR:CD2 | 1:G:1944:GLU:HA | 2.51 | 0.46 |
| 1:E:1321:VAL:HG12 | 1:E:1322:SER:N | 2.31 | 0.46 |
| 1:E:1390:PRO:HD3 | 1:H:2165:GLN:OE1 | 2.15 | 0.46 |
| 1:H:2250:ARG:O | 1:H:2251:LYS:C | 2.53 | 0.46 |
| 1:F:1516:LYS:HE2 | 1:F:1692:PHE:H | 1.81 | 0.46 |
| 1:H:2167:MET:O | 1:H:2170:LEU:HB3 | 2.16 | 0.46 |
| 1:G:1912:GLU:C | 1:G:1913:ILE:HD12 | 2.37 | 0.46 |
| 1:A:117:ILE:HD11 | 1:A:209:ASN:HB2 | 1.97 | 0.46 |
| 1:H:2146:LEU:O | 1:H:2159:LYS:HA | 2.16 | 0.45 |
| 1:E:1252:GLY:HA3 | 1:E:1255:TYR:CE2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2277:LYS:CB | 1:H:2311:THR:HB | 2.46 | 0.45 |
| 1:G:1804:PRO:HA | 1:G:1808:GLN:NE2 | 2.31 | 0.45 |
| 1:C:677:ASP:OD1 | 1:C:706:HIS:CD2 | 2.66 | 0.45 |
| 1:G:1879:TYR:HH | 1:G:1947:TYR:HD2 | 1.58 | 0.45 |
| 1:C:623:PHE:CE2 | 1:D:995:ARG:NH2 | 2.84 | 0.45 |
| 1:C:783:TRP:O | 1:C:784:PHE:CD2 | 2.69 | 0.45 |
| 1:D:1010:HIS:CD2 | 1:D:1036:ASN:HB3 | 2.51 | 0.45 |
| 1:A:124:ASP:OD2 | 1:A:219:THR:HA | 2.16 | 0.45 |
| 1:H:2314:ILE:HG22 | 1:H:2315:GLU:N | 2.31 | 0.45 |
| 1:E:1217:ASN:CA | 1:E:1219:GLN:HE22 | 2.29 | 0.45 |
| 1:C:679:TYR:CD2 | 1:C:744:GLU:HA | 2.51 | 0.45 |
| 1:F:1643:GLN:HG3 | 1:F:1701:TYR:CD1 | 2.51 | 0.45 |
| 1:A:80:GLY:HA2 | 1:A:143:GLN:NE2 | 2.32 | 0.45 |
| 1:H:2183:TYR:CE1 | 1:H:2198:CYS:CB | 3.00 | 0.45 |
| 1:E:1259:LYS:HG2 | 1:E:1260:THR:N | 2.31 | 0.45 |
| 1:G:1900:TYR:CE2 | 1:G:1999:MET:HG2 | 2.51 | 0.45 |
| 1:B:467:TYR:CD1 | 1:B:467:TYR:N | 2.85 | 0.45 |
| 1:E:1402:LYS:O | 1:E:1404:ASN:N | 2.49 | 0.45 |
| 1:A:88:TYR:CD1 | 1:A:88:TYR:N | 2.84 | 0.45 |
| 1:H:2123:PHE:H | 1:H:2123:PHE:HD1 | 1.64 | 0.45 |
| 1:B:388:TYR:N | 1:B:388:TYR:CD1 | 2.83 | 0.45 |
| 1:A:144:GLU:O | 1:A:147:TYR:HB3 | 2.16 | 0.45 |
| 1:H:2104:PRO:HD3 | 1:H:2283:TRP:CD1 | 2.51 | 0.45 |
| 1:G:1932:ASP:N | 1:G:1932:ASP:OD2 | 2.50 | 0.45 |
| 1:G:1810:HIS:ND1 | 1:G:1987:PHE:O | 2.50 | 0.45 |
| 1:F:1614:PRO:HB3 | 1:F:1634:GLU:HB3 | 1.98 | 0.45 |
| 1:H:2254:ILE:CG1 | 1:H:2259:LEU:HB3 | 2.31 | 0.45 |
| 1:B:459:LEU:HG | 1:B:460:TYR:CE2 | 2.51 | 0.45 |
| 1:F:1541:LEU:HG | 1:F:1542:LEU:N | 2.32 | 0.45 |
| 1:C:677:ASP:OD2 | 1:C:706:HIS:HA | 2.16 | 0.45 |
| 1:A:77:ASP:OD1 | 1:A:106:HIS:CD2 | 2.68 | 0.45 |
| 1:D:1077:LYS:C | 1:D:1077:LYS:HD3 | 2.37 | 0.45 |
| 1:H:2185:HIS:O | 1:H:2186:LEU:HB2 | 2.17 | 0.45 |
| 1:A:151:LYS:HE2 | 1:A:155:ASP:OD2 | 2.16 | 0.45 |
| 1:F:1524:LEU:HD11 | 1:F:1694:GLN:HG2 | 1.99 | 0.45 |
| 1:B:380:GLY:CA | 1:B:443:GLN:NE2 | 2.79 | 0.45 |
| 1:A:74:LYS:N | 1:A:74:LYS:HD2 | 2.32 | 0.45 |
| 1:G:1904:THR:HG23 | 1:G:1941:THR:HG22 | 1.99 | 0.45 |
| 1:B:355:TYR:C | 1:B:395:ARG:HH12 | 2.20 | 0.45 |
| 1:G:1976:PRO:HD2 | 1:G:1980:GLU:O | 2.16 | 0.45 |
| 1:G:1843:SER:HB3 | 1:G:1865:GLN:HG3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1646:ASP:O | 1:F:1650:ARG:HG3 | 2.16 | 0.45 |
| 1:H:2183:TYR:CE1 | 1:H:2200:TYR:HE1 | 2.35 | 0.45 |
| 1:A:15:VAL:HG12 | 1:A:16:LYS:O | 2.17 | 0.45 |
| 1:G:2003:ASP:O | 1:G:2004:ASN:C | 2.55 | 0.45 |
| 1:H:2215:LYS:HE3 | 1:H:2310:LYS:HD3 | 1.98 | 0.45 |
| 1:B:305:ASP:O | 1:B:307:SER:N | 2.49 | 0.45 |
| 1:G:1815:VAL:HG13 | 1:G:1992:PHE:HE2 | 1.80 | 0.45 |
| 1:G:1859:LYS:HB2 | 1:G:1889:LEU:CD2 | 2.40 | 0.45 |
| 1:C:694:GLU:O | 1:C:695:ARG:CB | 2.65 | 0.45 |
| 1:G:1941:THR:C | 1:G:1943:GLN:N | 2.68 | 0.45 |
| 1:E:1256:ASP:O | 1:E:1257:LYS:HD3 | 2.17 | 0.45 |
| 1:B:303:ASP:OD2 | 1:B:473:LYS:NZ | 2.47 | 0.45 |
| 1:B:440:VAL:CG2 | 1:B:445:LEU:HD11 | 2.47 | 0.45 |
| 1:D:956:ASP:O | 1:D:957:LYS:CD | 2.64 | 0.45 |
| 1:C:694:GLU:HG2 | 1:D:985:HIS:CD2 | 2.51 | 0.45 |
| 1:D:938:VAL:CG2 | 1:D:939:ASP:N | 2.79 | 0.45 |
| 1:H:2245:LEU:O | 1:H:2246:ASP:C | 2.55 | 0.45 |
| 1:D:1059:LEU:HG | 1:D:1060:TYR:CD2 | 2.52 | 0.45 |
| 1:H:2145:ASP:OD1 | 1:H:2145:ASP:C | 2.55 | 0.45 |
| 1:E:1294:GLU:O | 1:E:1295:ARG:HB2 | 2.17 | 0.45 |
| 1:C:659:LYS:HG2 | 1:C:660:THR:N | 2.32 | 0.45 |
| 1:G:1913:ILE:HA | 1:G:1914:PRO:HD3 | 1.86 | 0.45 |
| 1:D:910:HIS:N | 1:D:910:HIS:CD2 | 2.84 | 0.45 |
| 1:A:19:GLN:O | 1:A:22:TYR:N | 2.51 | 0.44 |
| 1:F:1583:TYR:HB2 | 1:F:1694:GLN:NE2 | 2.32 | 0.44 |
| 1:E:1407:LEU:C | 1:E:1407:LEU:HD12 | 2.36 | 0.44 |
| 1:C:642:LEU:C | 1:C:644:HIS:N | 2.71 | 0.44 |
| 1:B:415:LYS:HG2 | 1:B:509:ASN:HD22 | 1.82 | 0.44 |
| 1:F:1624:ASP:OD2 | 1:F:1719:THR:HA | 2.16 | 0.44 |
| 1:H:2185:HIS:CD2 | 1:H:2186:LEU:HG | 2.51 | 0.44 |
| 1:H:2143:SER:O | 1:H:2165:GLN:HA | 2.16 | 0.44 |
| 1:F:1697:TYR:O | 1:F:1700:ILE:HG23 | 2.17 | 0.44 |
| 1:B:454:ILE:HG12 | 1:B:460:TYR:H | 1.81 | 0.44 |
| 1:C:623:PHE:CE2 | 1:D:995:ARG:CZ | 3.01 | 0.44 |
| 1:E:1242:LEU:C | 1:E:1244:HIS:H | 2.20 | 0.44 |
| 1:C:772:ILE:HB | 1:C:786:PHE:CZ | 2.53 | 0.44 |
| 1:A:52:GLY:HA3 | 1:A:55:TYR:CZ | 2.52 | 0.44 |
| 1:D:919:GLN:N | 1:D:919:GLN:HE21 | 2.05 | 0.44 |
| 1:F:1585:HIS:C | 1:F:1586:LEU:HG | 2.38 | 0.44 |
| 1:A:15:VAL:HA | 1:A:190:PRO:HA | 1.97 | 0.44 |
| 1:B:310:HIS:CD2 | 1:B:310:HIS:N | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:777:LYS:HB2 | 1:C:811:THR:HB | 2.00 | 0.44 |
| 1:D:1000:TYR:N | 1:D:1000:TYR:CD1 | 2.85 | 0.44 |
| 1:D:946:LEU:O | 1:D:959:LYS:HA | 2.18 | 0.44 |
| 1:D:904:PRO:HB3 | 1:D:1083:TRP:CH2 | 2.52 | 0.44 |
| 1:E:1402:LYS:C | 1:E:1404:ASN:H | 2.21 | 0.44 |
| 1:E:1255:TYR:C | 1:E:1295:ARG:HH12 | 2.21 | 0.44 |
| 1:F:1567:MET:O | 1:F:1570:LEU:HB3 | 2.17 | 0.44 |
| 1:A:85:HIS:CD2 | 1:A:86:LEU:HG | 2.52 | 0.44 |
| 1:D:1067:TYR:CD2 | 1:D:1118:LEU:HD13 | 2.52 | 0.44 |
| 1:D:1066:LYS:HB3 | 1:D:1067:TYR:CE1 | 2.53 | 0.44 |
| 1:G:1870:LEU:HD23 | 1:G:1870:LEU:O | 2.17 | 0.44 |
| 1:G:1895:ARG:NH1 | 1:G:1895:ARG:HB3 | 2.33 | 0.44 |
| 1:E:1317:ILE:HD11 | 1:E:1409:ASN:HB2 | 1.99 | 0.44 |
| 1:D:945:ASP:C | 1:D:945:ASP:OD1 | 2.56 | 0.44 |
| 1:G:2020:THR:O | 1:G:2021:LYS:C | 2.55 | 0.44 |
| 1:G:1923:ILE:O | 1:G:1926:ILE:HG12 | 2.17 | 0.44 |
| 1:D:987:CYS:SG | 1:D:997:ALA:C | 2.96 | 0.44 |
| 1:B:427:GLN:O | 1:B:427:GLN:HG2 | 2.16 | 0.44 |
| 1:D:929:PRO:HD3 | 1:D:1047:TYR:OH | 2.17 | 0.44 |
| 1:H:2297:TYR:O | 1:H:2299:MET:N | 2.51 | 0.44 |
| 1:F:1547:ILE:HD13 | 1:F:1589:LEU:CD2 | 2.45 | 0.44 |
| 1:A:16:LYS:HE2 | 1:A:192:PHE:N | 2.28 | 0.44 |
| 1:F:1594:GLU:O | 1:F:1595:ARG:CB | 2.66 | 0.44 |
| 1:B:334:ASN:HB2 | 1:B:406:HIS:NE2 | 2.32 | 0.44 |
| 1:G:1966:LYS:HB3 | 1:G:1967:TYR:CD1 | 2.53 | 0.44 |
| 1:D:929:PRO:HD3 | 1:D:1047:TYR:CE2 | 2.52 | 0.44 |
| 1:D:1072:ILE:HB | 1:D:1086:PHE:CZ | 2.53 | 0.44 |
| 1:A:58:LEU:HD12 | 1:A:97:ALA:O | 2.17 | 0.44 |
| 1:B:499:MET:C | 1:B:501:TYR:N | 2.71 | 0.44 |
| 1:D:970:LEU:C | 1:D:970:LEU:HD23 | 2.38 | 0.44 |
| 1:D:942:LEU:C | 1:D:944:HIS:N | 2.71 | 0.44 |
| 1:E:1219:GLN:O | 1:E:1222:TYR:HB3 | 2.18 | 0.44 |
| 1:C:750:ARG:O | 1:C:751:LYS:C | 2.55 | 0.44 |
| 1:H:2221:VAL:HB | 1:H:2229:LEU:CD1 | 2.46 | 0.44 |
| 1:G:1883:TYR:CE1 | 1:G:1900:TYR:HE1 | 2.35 | 0.44 |
| 1:C:601:GLN:OE1 | 1:C:783:TRP:NE1 | 2.51 | 0.44 |
| 1:H:2105:ASP:O | 1:H:2107:SER:N | 2.50 | 0.44 |
| 1:B:368:ALA:O | 1:B:369:THR:C | 2.57 | 0.44 |
| 1:D:1054:ILE:HA | 1:D:1059:LEU:H | 1.82 | 0.44 |
| 1:F:1580:GLY:CA | 1:F:1643:GLN:NE2 | 2.81 | 0.44 |
| 1:A:192:PHE:C | 1:A:192:PHE:CD1 | 2.90 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:334:ASN:OD1 | 1:B:375:ASN:HB3 | 2.18 | 0.44 |
| 1:C:674:LYS:CD | 1:C:674:LYS:N | 2.81 | 0.44 |
| 1:F:1717:TYR:N | 1:F:1717:TYR:CD1 | 2.86 | 0.44 |
| 1:E:1210:HIS:CD2 | 1:E:1210:HIS:N | 2.85 | 0.44 |
| 1:D:912:SER:HB3 | 1:D:1087:PHE:CE2 | 2.53 | 0.44 |
| 1:B:360:THR:O | 1:B:360:THR:HG23 | 2.18 | 0.43 |
| 1:C:774:PHE:HB2 | 1:C:782:PHE:CE1 | 2.53 | 0.43 |
| 1:D:1097:TYR:O | 1:D:1100:ILE:HG23 | 2.17 | 0.43 |
| 1:C:776:PRO:HD2 | 1:C:780:GLU:O | 2.18 | 0.43 |
| 1:D:1029:LEU:CD1 | 1:D:1029:LEU:C | 2.86 | 0.43 |
| 1:C:807:LEU:HD12 | 1:C:807:LEU:O | 2.17 | 0.43 |
| 1:A:152:TYR:CE1 | 1:A:156:ASN:ND2 | 2.86 | 0.43 |
| 1:D:1000:TYR:O | 1:D:1001:GLY:C | 2.57 | 0.43 |
| 1:D:1092:PHE:CD1 | 1:D:1092:PHE:C | 2.92 | 0.43 |
| 1:B:385:HIS:O | 1:B:386:LEU:CB | 2.65 | 0.43 |
| 1:A:87:CYS:SG | 1:A:97:ALA:C | 2.96 | 0.43 |
| 1:H:2297:TYR:C | 1:H:2299:MET:H | 2.20 | 0.43 |
| 1:H:2266:LYS:HB3 | 1:H:2267:TYR:CE1 | 2.54 | 0.43 |
| 1:G:1881:VAL:H | 1:G:1943:GLN:NE2 | 2.15 | 0.43 |
| 1:H:2168:ALA:C | 1:H:2170:LEU:H | 2.22 | 0.43 |
| 1:D:990:CYS:C | 1:D:992:ASN:N | 2.71 | 0.43 |
| 1:D:919:GLN:C | 1:D:921:ILE:H | 2.21 | 0.43 |
| 1:F:1645:LEU:O | 1:F:1646:ASP:C | 2.56 | 0.43 |
| 1:A:94:GLU:OE1 | 1:B:385:HIS:HB3 | 2.18 | 0.43 |
| 1:H:2145:ASP:CG | 1:H:2159:LYS:HD2 | 2.38 | 0.43 |
| 1:G:1823:PHE:CE2 | 1:H:2195:ARG:NE | 2.86 | 0.43 |
| 1:E:1285:HIS:O | 1:E:1286:LEU:CB | 2.65 | 0.43 |
| 1:A:67:MET:O | 1:A:68:ALA:C | 2.57 | 0.43 |
| 1:F:1672:ILE:HB | 1:F:1686:PHE:CZ | 2.53 | 0.43 |
| 1:H:2274:PHE:HB2 | 1:H:2282:PHE:CE1 | 2.54 | 0.43 |
| 1:C:752:TYR:CD1 | 1:C:756:ASN:ND2 | 2.86 | 0.43 |
| 1:G:1815:VAL:HA | 1:G:1990:PRO:HA | 2.01 | 0.43 |
| 1:F:1516:LYS:HG2 | 1:F:1690:PRO:O | 2.19 | 0.43 |
| 1:F:1615:LYS:HG2 | 1:F:1709:ASN:ND2 | 2.34 | 0.43 |
| 1:G:1850:VAL:HG23 | 1:G:1850:VAL:O | 2.18 | 0.43 |
| 1:E:1262:LEU:HD23 | 1:E:1301:GLY:HA2 | 2.01 | 0.43 |
| 1:C:733:ILE:HD13 | 1:C:749:VAL:HG22 | 1.99 | 0.43 |
| 1:C:656:ASP:O | 1:C:657:LYS:HD3 | 2.19 | 0.43 |
| 1:E:1361:THR:O | 1:E:1363:GLY:N | 2.51 | 0.43 |
| 1:A:146:ASP:OD2 | 1:A:150:ARG:NE | 2.51 | 0.43 |
| 1:E:1270:LEU:C | 1:E:1270:LEU:HD23 | 2.38 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1390:PRO:HD2 | 1:H:2143:SER:CB | 2.49 | 0.43 |
| 1:A:194:GLN:O | 1:A:195:SER:C | 2.57 | 0.43 |
| 1:A:100:TYR:HE2 | 1:A:199:MET:HG2 | 1.82 | 0.43 |
| 1:H:2181:VAL:H | 1:H:2243:GLN:NE2 | 2.10 | 0.43 |
| 1:B:507:LEU:HD12 | 1:B:507:LEU:C | 2.38 | 0.43 |
| 1:G:2015:GLU:HB3 | 1:G:2017:TYR:HE1 | 1.84 | 0.43 |
| 1:H:2170:LEU:C | 1:H:2170:LEU:HD23 | 2.39 | 0.43 |
| 1:G:1913:ILE:N | 1:G:1913:ILE:HD12 | 2.34 | 0.43 |
| 1:A:94:GLU:O | 1:A:95:ARG:HB2 | 2.19 | 0.43 |
| 1:B:446:ASP:OD2 | 1:B:450:ARG:HG3 | 2.18 | 0.43 |
| 1:E:1343:GLN:HG3 | 1:E:1401:TYR:CD1 | 2.53 | 0.43 |
| 1:B:315:VAL:HA | 1:B:490:PRO:HA | 2.00 | 0.43 |
| 1:F:1570:LEU:O | 1:F:1574:LYS:HD3 | 2.18 | 0.43 |
| 1:D:977:ASP:OD1 | 1:D:1006:HIS:CD2 | 2.71 | 0.43 |
| 1:C:641:LEU:HG | 1:C:642:LEU:HG | 1.99 | 0.43 |
| 1:D:940:GLN:HG3 | 1:D:940:GLN:O | 2.17 | 0.43 |
| 1:B:421:VAL:HG12 | 1:B:422:SER:N | 2.34 | 0.43 |
| 1:E:1232:HIS:CE1 | 1:E:1250:VAL:HB | 2.53 | 0.43 |
| 1:D:981:VAL:N | 1:D:1043:GLN:NE2 | 2.59 | 0.43 |
| 1:E:1417:TYR:O | 1:E:1418:LEU:HD23 | 2.18 | 0.43 |
| 1:B:520:THR:O | 1:B:521:LYS:OXT | 2.37 | 0.43 |
| 1:A:82:GLU:N | 1:A:82:GLU:OE1 | 2.49 | 0.43 |
| 1:B:499:MET:C | 1:B:501:TYR:H | 2.22 | 0.43 |
| 1:E:1396:LYS:HD3 | 1:E:1397:TYR:CA | 2.48 | 0.43 |
| 1:E:1223:PHE:HE2 | 1:F:1595:ARG:NH2 | 2.13 | 0.43 |
| 1:E:1279:TYR:CD2 | 1:E:1344:GLU:HA | 2.54 | 0.43 |
| 1:E:1270:LEU:O | 1:E:1274:LYS:HD3 | 2.19 | 0.43 |
| 1:H:2104:PRO:HD3 | 1:H:2283:TRP:CE2 | 2.54 | 0.43 |
| 1:A:112:GLU:C | 1:A:113:ILE:HD12 | 2.39 | 0.43 |
| 1:E:1243:SER:HB2 | 1:H:2289:GLU:HB3 | 2.01 | 0.43 |
| 1:E:1311:LEU:HG | 1:E:1338:LYS:HG2 | 2.01 | 0.43 |
| 1:F:1658:GLN:CD | 1:F:1658:GLN:N | 2.72 | 0.43 |
| 1:C:632:HIS:CE1 | 1:C:650:VAL:HB | 2.55 | 0.42 |
| 1:H:2179:TYR:CD2 | 1:H:2244:GLU:CG | 3.01 | 0.42 |
| 1:C:683:TYR:CE1 | 1:C:698:CYS:CB | 3.01 | 0.42 |
| 1:A:70:LEU:O | 1:A:74:LYS:HD3 | 2.19 | 0.42 |
| 1:D:995:ARG:NH1 | 1:D:995:ARG:HB3 | 2.34 | 0.42 |
| 1:C:741:THR:O | 1:C:742:ALA:C | 2.56 | 0.42 |
| 1:A:71:PHE:CD1 | 1:A:71:PHE:N | 2.87 | 0.42 |
| 1:D:971:PHE:CD1 | 1:D:971:PHE:N | 2.86 | 0.42 |
| 1:C:615:VAL:HA | 1:C:790:PRO:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:615:VAL:HG13 | 1:C:792:PHE:HE2 | 1.84 | 0.42 |
| 1:C:745:LEU:O | 1:C:747:TYR:N | 2.52 | 0.42 |
| 1:H:2125:TYR:O | 1:H:2247:TYR:HE1 | 2.01 | 0.42 |
| 1:D:1059:LEU:HG | 1:D:1060:TYR:CE2 | 2.54 | 0.42 |
| 1:G:1974:PHE:N | 1:G:1974:PHE:CD1 | 2.87 | 0.42 |
| 1:H:2170:LEU:O | 1:H:2174:LYS:HD3 | 2.19 | 0.42 |
| 1:A:113:ILE:HA | 1:A:114:PRO:HD3 | 1.90 | 0.42 |
| 1:D:1027:GLN:HG2 | 1:D:1027:GLN:O | 2.19 | 0.42 |
| 1:F:1700:ILE:HG13 | 1:F:1701:TYR:CD2 | 2.54 | 0.42 |
| 1:A:59:LYS:HG2 | 1:A:60:THR:N | 2.35 | 0.42 |
| 1:G:1951:LYS:O | 1:G:1954:ILE:HB | 2.20 | 0.42 |
| 1:E:1285:HIS:CD2 | 1:E:1286:LEU:HG | 2.54 | 0.42 |
| 1:B:377:ASP:OD2 | 1:B:406:HIS:HA | 2.19 | 0.42 |
| 1:E:1229:PRO:HD3 | 1:E:1347:TYR:OH | 2.19 | 0.42 |
| 1:G:1874:LYS:O | 1:G:1876:VAL:HG13 | 2.19 | 0.42 |
| 1:E:1406:THR:HG22 | 1:E:1407:LEU:N | 2.35 | 0.42 |
| 1:H:2168:ALA:O | 1:H:2170:LEU:N | 2.52 | 0.42 |
| 1:B:332:HIS:CE1 | 1:B:350:VAL:HB | 2.53 | 0.42 |
| 1:D:1050:ARG:NH2 | 1:D:1086:PHE:HD2 | 2.17 | 0.42 |
| 1:B:380:GLY:HA2 | 1:B:443:GLN:NE2 | 2.35 | 0.42 |
| 1:C:698:CYS:O | 1:C:699:ILE:CG2 | 2.66 | 0.42 |
| 1:G:1856:ASP:O | 1:G:1857:LYS:HD3 | 2.18 | 0.42 |
| 1:C:655:TYR:C | 1:C:655:TYR:CD1 | 2.92 | 0.42 |
| 1:E:1215:VAL:HA | 1:E:1390:PRO:HA | 2.01 | 0.42 |
| 1:C:680:GLY:HA2 | 1:C:743:GLN:NE2 | 2.34 | 0.42 |
| 1:A:108:GLY:O | 1:A:109:ASN:HB2 | 2.18 | 0.42 |
| 1:A:159:LEU:HG | 1:A:160:TYR:CE2 | 2.55 | 0.42 |
| 1:B:508:ASP:OD2 | 1:B:510:LYS:HB3 | 2.19 | 0.42 |
| 1:D:1047:TYR:O | 1:D:1049:VAL:N | 2.52 | 0.42 |
| 1:F:1515:VAL:O | 1:F:1516:LYS:O | 2.38 | 0.42 |
| 1:C:695:ARG:NH2 | 1:D:923:PHE:CE2 | 2.87 | 0.42 |
| 1:F:1706:THR:HG22 | 1:F:1707:LEU:N | 2.34 | 0.42 |
| 1:B:411:LEU:HB3 | 1:B:412:GLU:H | 1.76 | 0.42 |
| 1:A:175:ILE:HA | 1:A:176:PRO:HD3 | 1.79 | 0.42 |
| 1:E:1288:TYR:N | 1:E:1288:TYR:CD1 | 2.88 | 0.42 |
| 1:H:2137:SER:OG | 1:H:2172:LYS:O | 2.33 | 0.42 |
| 1:F:1518:LEU:O | 1:F:1519:GLN:C | 2.56 | 0.42 |
| 1:G:1862:LEU:HD12 | 1:G:1868:ALA:CA | 2.46 | 0.42 |
| 1:A:85:HIS:O | 1:A:86:LEU:CB | 2.67 | 0.42 |
| 1:G:1940:VAL:HG21 | 1:G:1945:LEU:HD21 | 2.01 | 0.42 |
| 1:E:1210:HIS:CD2 | 1:E:1210:HIS:H | 2.36 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1702:LYS:O | 1:F:1704:ASN:N | 2.52 | 0.42 |
| 1:E:1219:GLN:HG2 | 1:E:1220:ASN:N | 2.35 | 0.42 |
| 1:G:1829:PRO:HG3 | 1:G:1879:TYR:OH | 2.20 | 0.42 |
| 1:H:2223:ILE:O | 1:H:2224:ASP:HB2 | 2.19 | 0.42 |
| 1:H:2246:ASP:OD2 | 1:H:2250:ARG:NE | 2.53 | 0.42 |
| 1:H:2131:THR:O | 1:H:2132:HIS:CG | 2.72 | 0.42 |
| 1:B:443:GLN:OE1 | 1:B:501:TYR:HB3 | 2.19 | 0.42 |
| 1:F:1679:LYS:CG | 1:F:1680:GLU:N | 2.81 | 0.42 |
| 1:D:974:LYS:O | 1:D:976:VAL:HG13 | 2.20 | 0.42 |
| 1:B:410:HIS:NE2 | 1:B:436:ASN:HB3 | 2.35 | 0.42 |
| 1:B:329:PRO:HD3 | 1:B:447:TYR:CZ | 2.55 | 0.42 |
| 1:A:174:PHE:HB2 | 1:A:182:PHE:CE1 | 2.55 | 0.42 |
| 1:F:1637:LYS:HB2 | 1:F:1640:VAL:HG12 | 2.02 | 0.42 |
| 1:H:2130:VAL:O | 1:H:2179:TYR:HA | 2.20 | 0.42 |
| 1:B:310:HIS:ND1 | 1:B:487:PHE:O | 2.53 | 0.42 |
| 1:F:1715:GLU:HB3 | 1:F:1717:TYR:CE1 | 2.55 | 0.42 |
| 1:B:329:PRO:HD3 | 1:B:447:TYR:CE2 | 2.55 | 0.42 |
| 1:G:1923:ILE:O | 1:G:1924:ASP:HB2 | 2.20 | 0.42 |
| 1:B:391:GLU:CD | 1:D:991:GLU:H | 2.20 | 0.41 |
| 1:C:751:LYS:CE | 1:C:755:ASP:OD2 | 2.63 | 0.41 |
| 1:D:959:LYS:HG2 | 1:D:960:THR:N | 2.35 | 0.41 |
| 1:B:359:LYS:HG2 | 1:B:360:THR:N | 2.35 | 0.41 |
| 1:E:1379:LYS:CG | 1:E:1380:GLU:H | 2.31 | 0.41 |
| 1:D:985:HIS:O | 1:D:986:LEU:HB2 | 2.19 | 0.41 |
| 1:A:170:GLY:HA2 | 1:A:217:TYR:O | 2.20 | 0.41 |
| 1:B:508:ASP:OD2 | 1:B:511:THR:HG23 | 2.20 | 0.41 |
| 1:A:31:THR:O | 1:A:32:HIS:CG | 2.73 | 0.41 |
| 1:A:207:LEU:HD12 | 1:A:207:LEU:O | 2.19 | 0.41 |
| 1:C:662:LEU:HD12 | 1:C:668:ALA:HA | 2.02 | 0.41 |
| 1:C:747:TYR:O | 1:C:750:ARG:N | 2.53 | 0.41 |
| 1:D:981:VAL:N | 1:D:1043:GLN:HE21 | 2.16 | 0.41 |
| 1:G:1972:ILE:HG22 | 1:G:1984:PHE:HB2 | 2.01 | 0.41 |
| 1:F:1604:THR:CG2 | 1:F:1641:THR:HG22 | 2.49 | 0.41 |
| 1:H:2252:TYR:C | 1:H:2254:ILE:N | 2.73 | 0.41 |
| 1:H:2250:ARG:O | 1:H:2252:TYR:N | 2.53 | 0.41 |
| 1:A:79:TYR:CD2 | 1:A:144:GLU:HG3 | 2.54 | 0.41 |
| 1:A:192:PHE:CD1 | 1:A:193:THR:N | 2.88 | 0.41 |
| 1:G:1959:LEU:HG | 1:G:1960:TYR:CE2 | 2.55 | 0.41 |
| 1:G:1943:GLN:HG3 | 1:G:2001:TYR:CD1 | 2.55 | 0.41 |
| 1:E:1210:HIS:ND1 | 1:E:1387:PHE:O | 2.54 | 0.41 |
| 1:H:2168:ALA:C | 1:H:2170:LEU:N | 2.72 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:429:LEU:CD1 | 1:B:429:LEU:C | 2.89 | 0.41 |
| 1:D:1013:ILE:HA | 1:D:1014:PRO:HD3 | 1.87 | 0.41 |
| 1:H:2153:PRO:HG2 | 1:H:2154:ASN:H | 1.84 | 0.41 |
| 1:G:1816:LYS:HG2 | 1:G:1990:PRO:O | 2.20 | 0.41 |
| 1:A:199:MET:C | 1:A:201:TYR:N | 2.74 | 0.41 |
| 1:E:1223:PHE:HD1 | 1:E:1223:PHE:H | 1.66 | 0.41 |
| 1:C:670:LEU:HD23 | 1:C:670:LEU:O | 2.20 | 0.41 |
| 1:D:1087:PHE:CD1 | 1:D:1087:PHE:N | 2.88 | 0.41 |
| 1:H:2317:TYR:CD1 | 1:H:2317:TYR:N | 2.89 | 0.41 |
| 1:H:2116:LYS:HE2 | 1:H:2291:GLU:HA | 2.02 | 0.41 |
| 1:F:1559:LYS:HE2 | 1:F:1598:CYS:SG | 2.60 | 0.41 |
| 1:G:1885:HIS:CD2 | 1:G:1886:LEU:HG | 2.55 | 0.41 |
| 1:G:1821:ILE:HG22 | 1:G:1960:TYR:CE1 | 2.55 | 0.41 |
| 1:G:1966:LYS:HB3 | 1:G:1967:TYR:CE1 | 2.55 | 0.41 |
| 1:B:302:GLN:H | 1:B:302:GLN:HE21 | 1.66 | 0.41 |
| 1:C:739:MET:HB3 | 1:C:806:THR:CG2 | 2.50 | 0.41 |
| 1:H:2194:GLU:O | 1:H:2195:ARG:CB | 2.68 | 0.41 |
| 1:G:1825:TYR:CZ | 1:G:1950:ARG:NH1 | 2.88 | 0.41 |
| 1:G:1831:THR:O | 1:G:1832:HIS:CG | 2.73 | 0.41 |
| 1:G:1894:GLU:O | 1:G:1895:ARG:CB | 2.67 | 0.41 |
| 1:D:1068:GLU:HB2 | 1:D:1121:LYS:OXT | 2.21 | 0.41 |
| 1:C:782:PHE:CZ | 1:C:805:GLU:HG2 | 2.55 | 0.41 |
| 1:B:474:PHE:HB2 | 1:B:482:PHE:CE1 | 2.56 | 0.41 |
| 1:C:802:LYS:C | 1:C:804:ASN:N | 2.74 | 0.41 |
| 1:B:475:ILE:HG22 | 1:B:475:ILE:O | 2.20 | 0.41 |
| 1:B:500:ILE:HG13 | 1:B:501:TYR:CE2 | 2.55 | 0.41 |
| 1:E:1242:LEU:C | 1:E:1244:HIS:N | 2.74 | 0.41 |
| 1:C:767:TYR:CD2 | 1:C:818:LEU:HB3 | 2.56 | 0.41 |
| 1:E:1309:ASN:CG | 1:E:1309:ASN:O | 2.59 | 0.41 |
| 1:H:2105:ASP:C | 1:H:2107:SER:H | 2.23 | 0.41 |
| 1:D:1057:LYS:HD3 | 1:D:1057:LYS:HA | 1.92 | 0.41 |
| 1:C:761:THR:O | 1:C:763:GLY:N | 2.52 | 0.41 |
| 1:A:90:CYS:HA | 1:C:691:GLU:OE2 | 2.21 | 0.41 |
| 1:F:1580:GLY:HA2 | 1:F:1643:GLN:NE2 | 2.35 | 0.41 |
| 1:F:1637:LYS:HG3 | 1:F:1637:LYS:H | 1.70 | 0.41 |
| 1:G:1804:PRO:HD3 | 1:G:1983:TRP:CE2 | 2.56 | 0.41 |
| 1:G:1941:THR:O | 1:G:1942:ALA:C | 2.59 | 0.41 |
| 1:G:1940:VAL:O | 1:G:2006:THR:HA | 2.20 | 0.41 |
| 1:H:2272:ILE:O | 1:H:2272:ILE:HG23 | 2.21 | 0.41 |
| 1:E:1202:GLN:HE21 | 1:E:1202:GLN:N | 2.18 | 0.41 |
| 1:C:621:ILE:HA | 1:C:624:LEU:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:220:THR:O | 1:A:221:LYS:C | 2.58 | 0.41 |
| 1:C:679:TYR:CE2 | 1:C:744:GLU:HA | 2.55 | 0.41 |
| 1:D:1070:GLY:O | 1:D:1086:PHE:HB2 | 2.21 | 0.41 |
| 1:D:917:ASN:HB3 | 1:D:920:ASN:ND2 | 2.36 | 0.41 |
| 1:F:1709:ASN:ND2 | 1:F:1710:LYS:N | 2.68 | 0.41 |
| 1:F:1558:LEU:HA | 1:F:1597:ALA:O | 2.21 | 0.41 |
| 1:F:1627:GLN:O | 1:F:1627:GLN:HG2 | 2.21 | 0.41 |
| 1:B:423:ILE:O | 1:B:424:ASP:HB2 | 2.21 | 0.41 |
| 1:C:617:ASN:HB3 | 1:C:619:GLN:OE1 | 2.21 | 0.40 |
| 1:C:631:THR:O | 1:C:632:HIS:CG | 2.73 | 0.40 |
| 1:C:679:TYR:CD2 | 1:C:744:GLU:HG3 | 2.57 | 0.40 |
| 1:B:381:VAL:H | 1:B:443:GLN:NE2 | 2.18 | 0.40 |
| 1:B:383:TYR:HB2 | 1:B:494:GLN:HE21 | 1.86 | 0.40 |
| 1:G:1823:PHE:CD1 | 1:G:1823:PHE:N | 2.89 | 0.40 |
| 1:H:2308:ASP:OD2 | 1:H:2311:THR:HG23 | 2.21 | 0.40 |
| 1:H:2229:LEU:HD12 | 1:H:2229:LEU:C | 2.42 | 0.40 |
| 1:F:1621:VAL:O | 1:F:1627:GLN:HG3 | 2.20 | 0.40 |
| 1:B:413:ILE:HA | 1:B:414:PRO:HD3 | 1.96 | 0.40 |
| 1:C:752:TYR:CE1 | 1:C:756:ASN:ND2 | 2.89 | 0.40 |
| 1:E:1265:GLN:O | 1:E:1268:ALA:HB3 | 2.21 | 0.40 |
| 1:H:2292:PHE:C | 1:H:2292:PHE:CD1 | 2.94 | 0.40 |
| 1:B:318:LEU:O | 1:B:319:GLN:C | 2.59 | 0.40 |
| 1:G:1882:GLU:CA | 1:G:1899:ILE:HG22 | 2.45 | 0.40 |
| 1:E:1234:ASN:OD1 | 1:E:1275:ASN:HB3 | 2.21 | 0.40 |
| 1:F:1534:ASN:OD1 | 1:F:1575:ASN:HB3 | 2.21 | 0.40 |
| 1:A:12:SER:O | 1:A:13:SER:C | 2.57 | 0.40 |
| 1:A:23:PHE:N | 1:A:23:PHE:CD1 | 2.88 | 0.40 |
| 1:E:1394:GLN:O | 1:E:1395:SER:C | 2.59 | 0.40 |
| 1:G:1952:TYR:CE1 | 1:G:1956:ASN:ND2 | 2.90 | 0.40 |
| 1:H:2115:VAL:HA | 1:H:2290:PRO:HA | 2.03 | 0.40 |
| 1:D:919:GLN:C | 1:D:921:ILE:N | 2.74 | 0.40 |
| 1:B:370:LEU:C | 1:B:370:LEU:HD23 | 2.42 | 0.40 |
| 1:B:316:LYS:HE2 | 1:B:492:PHE:N | 2.33 | 0.40 |
| 1:F:1708:ASP:OD2 | 1:F:1711:THR:HG23 | 2.21 | 0.40 |
| 1:G:1900:TYR:N | 1:G:1900:TYR:CD1 | 2.90 | 0.40 |
| 1:D:1102:LYS:C | 1:D:1104:ASN:N | 2.74 | 0.40 |
| 1:C:616:LYS:O | 1:C:618:LEU:N | 2.55 | 0.40 |
| 1:C:747:TYR:O | 1:C:748:LYS:C | 2.60 | 0.40 |
| 1:H:2146:LEU:HA | 1:H:2146:LEU:HD23 | 1.84 | 0.40 |
| 1:H:2307:LEU:HD12 | 1:H:2307:LEU:C | 2.41 | 0.40 |
| 1:F:1687:PHE:CD1 | 1:F:1687:PHE:N | 2.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2129:PRO:HD3 | 1:H:2247:TYR:OH | 2.21 | 0.40 |
| 1:A:95:ARG:NH1 | 1:A:95:ARG:CB | 2.84 | 0.40 |
| 1:A:109:ASN:O | 1:A:137:LYS:HA | 2.22 | 0.40 |
| 1:H:2228:SER:O | 1:H:2229:LEU:HB3 | 2.22 | 0.40 |
| 1:H:2171:PHE:N | 1:H:2171:PHE:CD1 | 2.90 | 0.40 |
| 1:H:2283:TRP:O | 1:H:2284:PHE:HD2 | 2.05 | 0.40 |
| 1:B:441:THR:O | 1:B:442:ALA:C | 2.58 | 0.40 |
| 1:A:174:PHE:N | 1:A:174:PHE:CD1 | 2.90 | 0.40 |
| 1:C:802:LYS:C | 1:C:804:ASN:H | 2.24 | 0.40 |
| 1:A:126:ILE:HG12 | 1:A:126:ILE:H | 1.74 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 219/221 (99%) | 164 (75%) | 40 (18%) | 15 (7%) | 1 | 24 |
| 1 | B | 219/221 (99%) | 168 (77%) | 35 (16%) | 16 (7%) | 1 | 22 |
| 1 | C | 219/221 (99%) | 172 (78%) | 34 (16%) | 13 (6%) | 2 | 28 |
| 1 | D | 219/221 (99%) | 171 (78%) | 37 (17%) | 11 (5%) | 3 | 31 |
| 1 | E | 219/221 (99%) | 163 (74%) | 46 (21%) | 10 (5%) | 3 | 33 |
| 1 | F | 219/221 (99%) | 160 (73%) | 50 (23%) | 9 (4%) | 3 | 36 |
| 1 | G | 219/221 (99%) | 178 (81%) | 31 (14%) | 10 (5%) | 3 | 33 |
| 1 | H | 219/221 (99%) | 173 (79%) | 34 (16%) | 12 (6%) | 2 | 30 |
| All | All | 1752/1768 (99%) | 1349 (77%) | 307 (18%) | 96 (6%) | 2 | 30 |

All (96) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 109 | ASN |
| 1 | B | 316 | LYS |
| 1 | B | 334 | ASN |
| 1 | D | 916 | LYS |
| 1 | E | 1216 | LYS |
| 1 | F | 1516 | LYS |
| 1 | G | 1816 | LYS |
| 1 | H | 2116 | LYS |
| 1 | A | 16 | LYS |
| 1 | A | 17 | ASN |
| 1 | A | 86 | LEU |
| 1 | B | 322 | TYR |
| 1 | B | 386 | LEU |
| 1 | B | 443 | GLN |
| 1 | C | 616 | LYS |
| 1 | C | 634 | ASN |
| 1 | C | 643 | SER |
| 1 | C | 686 | LEU |
| 1 | C | 744 | GLU |
| 1 | D | 934 | ASN |
| 1 | D | 943 | SER |
| 1 | D | 1047 | TYR |
| 1 | D | 1098 | LEU |
| 1 | E | 1234 | ASN |
| 1 | E | 1286 | LEU |
| 1 | F | 1534 | ASN |
| 1 | F | 1543 | SER |
| 1 | F | 1586 | LEU |
| 1 | F | 1609 | ASN |
| 1 | F | 1644 | GLU |
| 1 | F | 1710 | LYS |
| 1 | G | 1843 | SER |
| 1 | G | 1886 | LEU |
| 1 | H | 2117 | ASN |
| 1 | H | 2143 | SER |
| 1 | H | 2186 | LEU |
| 1 | H | 2298 | LEU |
| 1 | A | 34 | ASN |
| 1 | A | 144 | GLU |
| 1 | A | 145 | LEU |
| 1 | A | 146 | ASP |
| 1 | B | 368 | ALA |
| 1 | B | 405 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 409 | ASN |
| 1 | B | 444 | GLU |
| 1 | B | 453 | THR |
| 1 | C | 695 | ARG |
| 1 | C | 743 | GLN |
| 1 | C | 745 | LEU |
| 1 | D | 995 | ARG |
| 1 | D | 1009 | ASN |
| 1 | D | 1048 | LYS |
| 1 | E | 1217 | ASN |
| 1 | E | 1309 | ASN |
| 1 | E | 1410 | LYS |
| 1 | F | 1541 | LEU |
| 1 | F | 1652 | TYR |
| 1 | G | 1895 | ARG |
| 1 | G | 1952 | TYR |
| 1 | H | 2106 | PRO |
| 1 | H | 2251 | LYS |
| 1 | H | 2253 | THR |
| 1 | A | 143 | GLN |
| 1 | A | 152 | TYR |
| 1 | A | 159 | LEU |
| 1 | B | 306 | PRO |
| 1 | B | 452 | TYR |
| 1 | B | 498 | LEU |
| 1 | C | 705 | ASN |
| 1 | C | 752 | TYR |
| 1 | C | 759 | LEU |
| 1 | D | 1043 | GLN |
| 1 | D | 1044 | GLU |
| 1 | E | 1206 | PRO |
| 1 | E | 1222 | TYR |
| 1 | E | 1297 | ALA |
| 1 | E | 1352 | TYR |
| 1 | G | 1909 | ASN |
| 1 | G | 1953 | THR |
| 1 | H | 2134 | ASN |
| 1 | H | 2205 | ASN |
| 1 | H | 2209 | ASN |
| 1 | A | 68 | ALA |
| 1 | A | 198 | LEU |
| 1 | A | 210 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 445 | LEU |
| 1 | C | 637 | SER |
| 1 | C | 746 | ASP |
| 1 | H | 2169 | THR |
| 1 | A | 15 | VAL |
| 1 | B | 323 | PHE |
| 1 | B | 451 | LYS |
| 1 | D | 986 | LEU |
| 1 | G | 1817 | ASN |
| 1 | G | 1834 | ASN |
| 1 | G | 1943 | GLN |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 208/208 (100%) | 200 (96%) | 8 (4%) | 40 | 74 |
| 1 | B | 208/208 (100%) | 204 (98%) | 4 (2%) | 65 | 86 |
| 1 | C | 208/208 (100%) | 203 (98%) | 5 (2%) | 57 | 82 |
| 1 | D | 208/208 (100%) | 200 (96%) | 8 (4%) | 40 | 74 |
| 1 | E | 208/208 (100%) | 204 (98%) | 4 (2%) | 65 | 86 |
| 1 | F | 208/208 (100%) | 203 (98%) | 5 (2%) | 57 | 82 |
| 1 | G | 208/208 (100%) | 203 (98%) | 5 (2%) | 57 | 82 |
| 1 | H | 208/208 (100%) | 201 (97%) | 7 (3%) | 44 | 77 |
| All | All | 1664/1664 (100%) | 1618 (97%) | 46 (3%) | 51 | 79 |

All (46) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | GLN |
| 1 | A | 19 | GLN |
| 1 | A | 36 | LYS |
| 1 | A | 82 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 107 | GLU |
| 1 | A | 129 | LEU |
| 1 | A | 167 | TYR |
| 1 | A | 177 | LYS |
| 1 | B | 302 | GLN |
| 1 | B | 319 | GLN |
| 1 | B | 382 | GLU |
| 1 | B | 507 | LEU |
| 1 | C | 602 | GLN |
| 1 | C | 619 | GLN |
| 1 | C | 682 | GLU |
| 1 | C | 777 | LYS |
| 1 | C | 807 | LEU |
| 1 | D | 902 | GLN |
| 1 | D | 919 | GLN |
| 1 | D | 982 | GLU |
| 1 | D | 988 | TYR |
| 1 | D | 1000 | TYR |
| 1 | D | 1007 | GLU |
| 1 | D | 1090 | PRO |
| 1 | D | 1107 | LEU |
| 1 | E | 1202 | GLN |
| 1 | E | 1219 | GLN |
| 1 | E | 1282 | GLU |
| 1 | E | 1307 | GLU |
| 1 | F | 1502 | GLN |
| 1 | F | 1519 | GLN |
| 1 | F | 1582 | GLU |
| 1 | F | 1588 | TYR |
| 1 | F | 1607 | GLU |
| 1 | G | 1802 | GLN |
| 1 | G | 1819 | GLN |
| 1 | G | 1882 | GLU |
| 1 | G | 1888 | TYR |
| 1 | G | 2017 | TYR |
| 1 | H | 2102 | GLN |
| 1 | H | 2119 | GLN |
| 1 | H | 2182 | GLU |
| 1 | H | 2188 | TYR |
| 1 | H | 2207 | GLU |
| 1 | H | 2229 | LEU |
| 1 | H | 2267 | TYR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1 | GLN |
| 1 | A | 2 | GLN |
| 1 | A | 8 | GLN |
| 1 | A | 19 | GLN |
| 1 | A | 20 | ASN |
| 1 | A | 85 | HIS |
| 1 | A | 106 | HIS |
| 1 | A | 110 | HIS |
| 1 | A | 143 | GLN |
| 1 | A | 156 | ASN |
| 1 | A | 162 | ASN |
| 1 | A | 194 | GLN |
| 1 | B | 301 | GLN |
| 1 | B | 302 | GLN |
| 1 | B | 308 | GLN |
| 1 | B | 319 | GLN |
| 1 | B | 344 | HIS |
| 1 | B | 385 | HIS |
| 1 | B | 406 | HIS |
| 1 | B | 443 | GLN |
| 1 | B | 456 | ASN |
| 1 | B | 462 | ASN |
| 1 | B | 494 | GLN |
| 1 | B | 509 | ASN |
| 1 | C | 601 | GLN |
| 1 | C | 602 | GLN |
| 1 | C | 608 | GLN |
| 1 | C | 619 | GLN |
| 1 | C | 685 | HIS |
| 1 | C | 706 | HIS |
| 1 | C | 743 | GLN |
| 1 | C | 756 | ASN |
| 1 | C | 794 | GLN |
| 1 | C | 809 | ASN |
| 1 | D | 901 | GLN |
| 1 | D | 902 | GLN |
| 1 | D | 908 | GLN |
| 1 | D | 919 | GLN |
| 1 | D | 920 | ASN |
| 1 | D | 985 | HIS |
| 1 | D | 1006 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 1010 | HIS |
| 1 | D | 1043 | GLN |
| 1 | D | 1094 | GLN |
| 1 | E | 1201 | GLN |
| 1 | E | 1202 | GLN |
| 1 | E | 1208 | GLN |
| 1 | E | 1219 | GLN |
| 1 | E | 1220 | ASN |
| 1 | E | 1285 | HIS |
| 1 | E | 1343 | GLN |
| 1 | E | 1394 | GLN |
| 1 | F | 1501 | GLN |
| 1 | F | 1502 | GLN |
| 1 | F | 1508 | GLN |
| 1 | F | 1519 | GLN |
| 1 | F | 1585 | HIS |
| 1 | F | 1610 | HIS |
| 1 | F | 1643 | GLN |
| 1 | F | 1656 | ASN |
| 1 | F | 1662 | ASN |
| 1 | F | 1694 | GLN |
| 1 | F | 1709 | ASN |
| 1 | G | 1801 | GLN |
| 1 | G | 1802 | GLN |
| 1 | G | 1808 | GLN |
| 1 | G | 1819 | GLN |
| 1 | G | 1885 | HIS |
| 1 | G | 1906 | HIS |
| 1 | G | 1943 | GLN |
| 1 | G | 1956 | ASN |
| 1 | G | 1994 | GLN |
| 1 | G | 2009 | ASN |
| 1 | H | 2101 | GLN |
| 1 | H | 2102 | GLN |
| 1 | H | 2108 | GLN |
| 1 | H | 2119 | GLN |
| 1 | H | 2185 | HIS |
| 1 | H | 2206 | HIS |
| 1 | H | 2243 | GLN |
| 1 | H | 2294 | GLN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

## 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

## 6.4 Ligands

EDS was not executed - this section will therefore be empty.

## 6.5 Other polymers

EDS was not executed - this section will therefore be empty.