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

Jan 31, 2016 – 09:07 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1NIK |
| Title | : | Wild Type RNA Polymerase II |
| Authors | : | Bushnell, D.A.; Kornberg, R.D. |
| Deposited on | : | 2002-12-24 |
| Resolution | : | 4.10 Å(reported) |

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

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

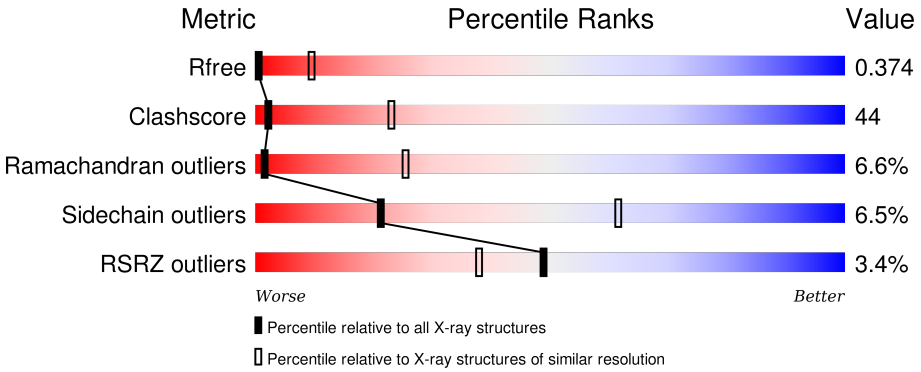
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 1018 (4.60-3.60) |
| Clashscore | 102246 | 1117 (4.60-3.60) |
| Ramachandran outliers | 100387 | 1063 (4.60-3.60) |
| Sidechain outliers | 100360 | 1049 (4.60-3.60) |
| RSRZ outliers | 91569 | 1022 (4.60-3.60) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1733 | 2% 32% 40% 7% • 20% |
| 2 | B | 1224 | 3% 32% 51% 7% 10% |
| 3 | C | 318 | 2% 37% 40% 7% 16% |
| 4 | D | 161 | 91% • 5% |
| 5 | E | 215 | 5% 42% 55% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | F | 155 | 2% 18% 32% 46% |
| 7 | G | 170 | 95% 5% |
| 8 | H | 146 | 4% 30% 52% 9% 9% |
| 9 | I | 122 | 11% 35% 51% 11% |
| 10 | J | 70 | 4% 31% 51% 9% 7% |
| 11 | K | 120 | % 41% 50% 5% |
| 12 | L | 70 | 7% 17% 33% 13% 34% |

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28295 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 RPB1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 1388 | 10864 | 6858 | 1899 | 2046 | 61 | 0 | 0 | 7 |

- Molecule 2 is a protein called ORF YOR151c.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | B | 1097 | 8721 | 5526 | 1523 | 1618 | 54 | 0 | 0 | 0 |

- Molecule 3 is a protein called DNA-directed RNA polymerase II, chain RPB3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | C | 266 | 2095 | 1317 | 348 | 417 | 13 | 0 | 0 | 0 |

- Molecule 4 is a protein called DNA-directed RNA polymerase II, chain RPB4.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|
| | | | Total | C | | | |
| 4 | D | 153 | 153 | 153 | 0 | 0 | 153 |

- Molecule 5 is a protein called DNA-directed RNA polymerase II, chain RPB5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | E | 214 | 1752 | 1111 | 309 | 321 | 11 | 0 | 0 | 0 |

- Molecule 6 is a protein called DNA-directed RNA polymerase I, II and III 23 kDa polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | F | 84 | 679 | 434 | 115 | 127 | 3 | 0 | 0 | 0 |

- Molecule 7 is a protein called DNA-directed RNA polymerase II, chain RPB7.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 7 | G | 170 | Total C<br>170 170 | 0 | 0 | 170 |

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit RPB8.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 8 | H | 133 | Total C N O S<br>1068 673 180 211 4 | 0 | 0 | 0 |

- Molecule 9 is a protein called DNA-directed RNA polymerase II, chain RPB9.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 9 | I | 119 | Total C N O S<br>971 596 179 186 10 | 0 | 0 | 0 |

- Molecule 10 is a protein called DNA-directed RNA polymerase II, chain RPB10.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 10 | J | 65 | Total C N O S<br>532 339 93 94 6 | 0 | 0 | 0 |

- Molecule 11 is a protein called DNA-directed RNA polymerase II, chain RPB11.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 11 | K | 114 | Total C N O S<br>919 590 156 171 2 | 0 | 0 | 0 |

- Molecule 12 is a protein called DNA-directed RNA polymerase II, chain RPB12.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 12 | L | 46 | Total C N O S<br>364 224 72 64 4 | 0 | 0 | 0 |

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 13 | B | 1 | Total Zn<br>1 1 | 0 | 0 |
| 13 | A | 2 | Total Zn<br>2 2 | 0 | 0 |

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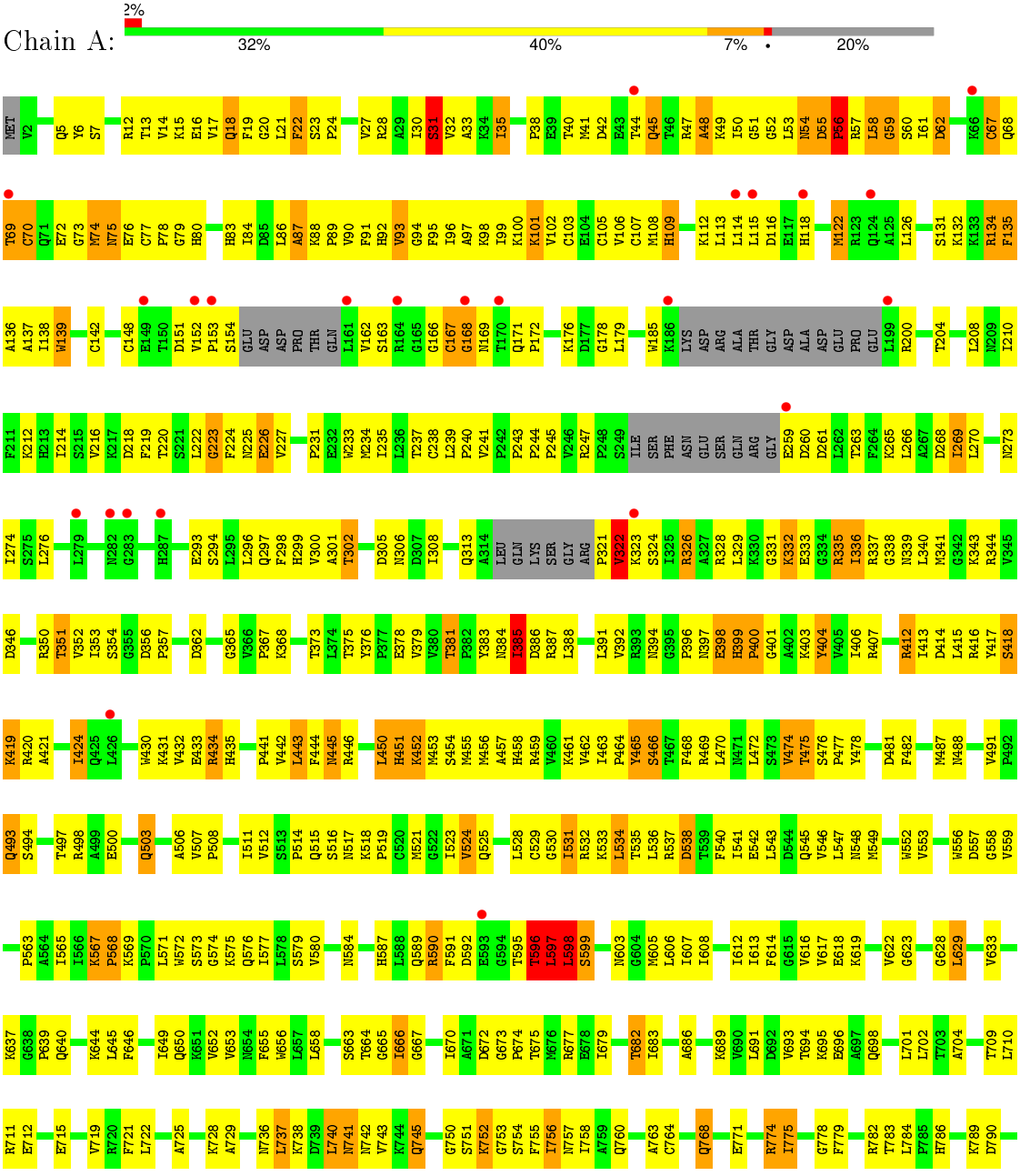
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 13 | C | 1 | Total Zn<br>1 1 | 0 | 0 |
| 13 | J | 1 | Total Zn<br>1 1 | 0 | 0 |
| 13 | I | 2 | Total Zn<br>2 2 | 0 | 0 |

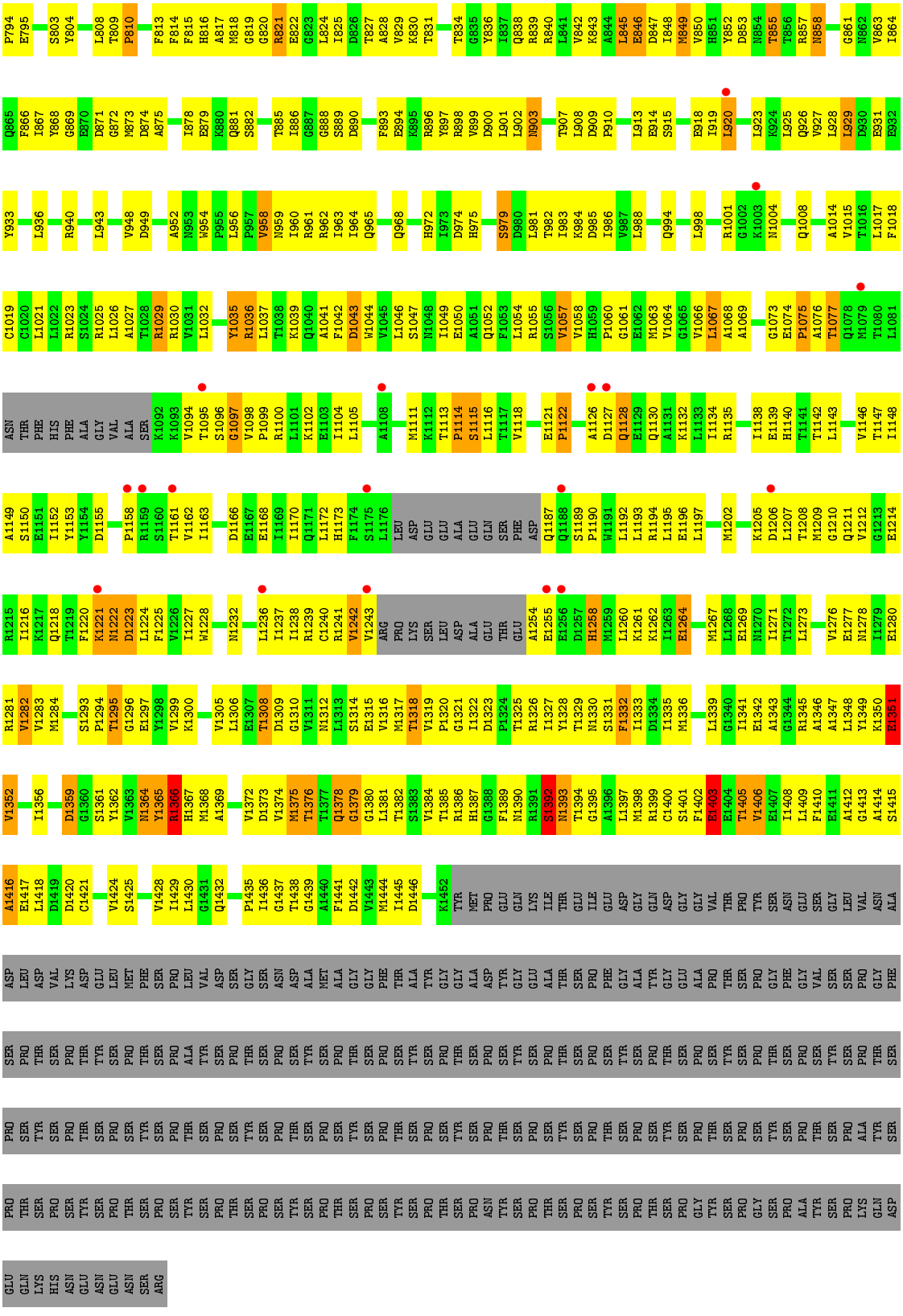
# 3 Residue-property plots (i)

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

- Molecule 1: RPB1

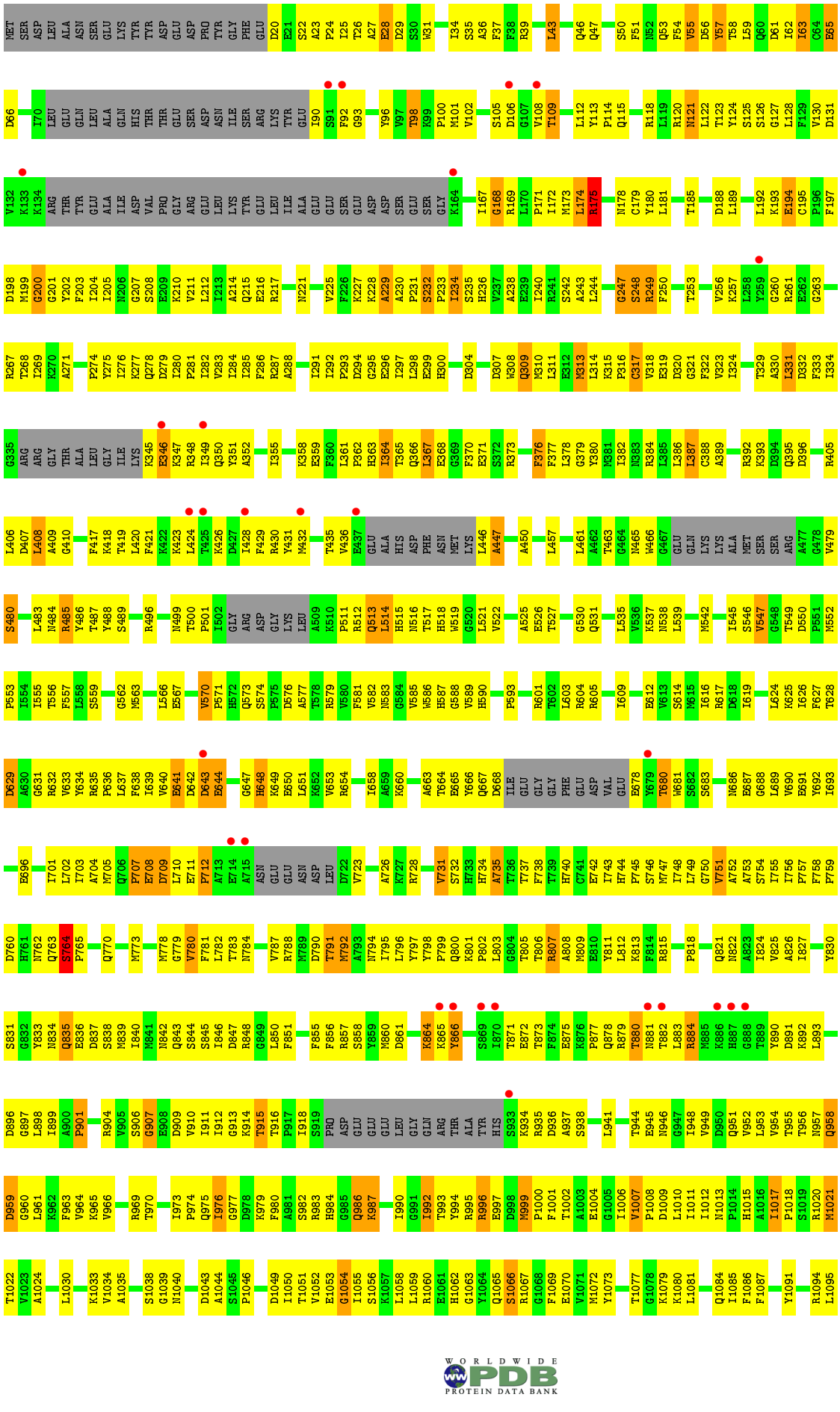
Chain A:

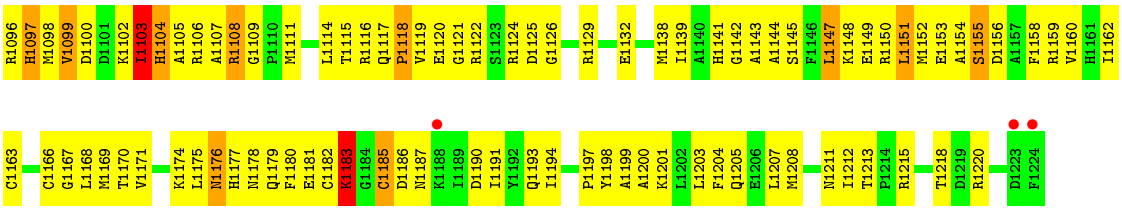




- Molecule 2: ORF YOR151c

Chain B:

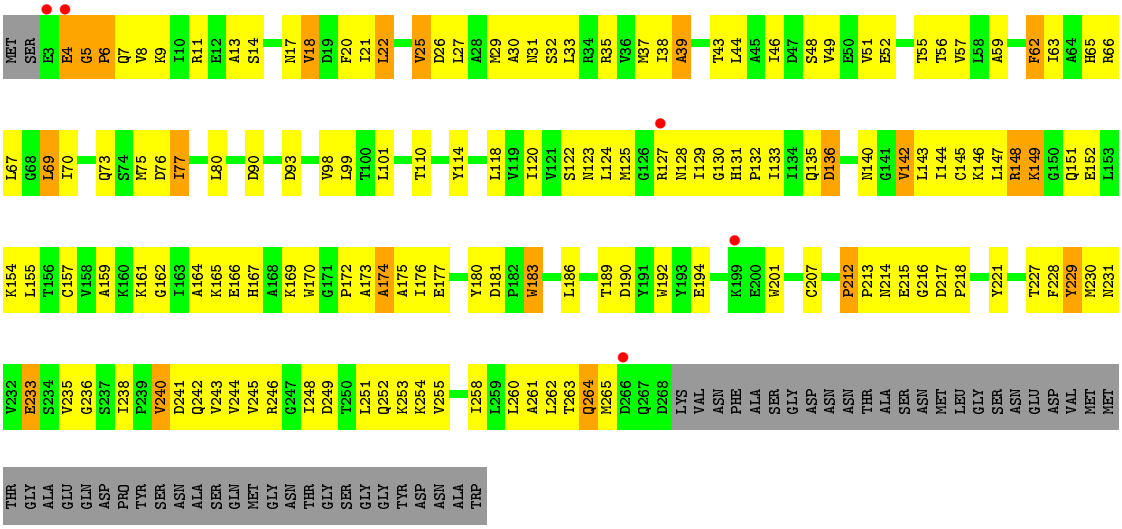






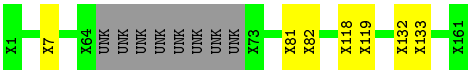
• Molecule 3: DNA-directed RNA polymerase II, chain RPB3

Chain C:

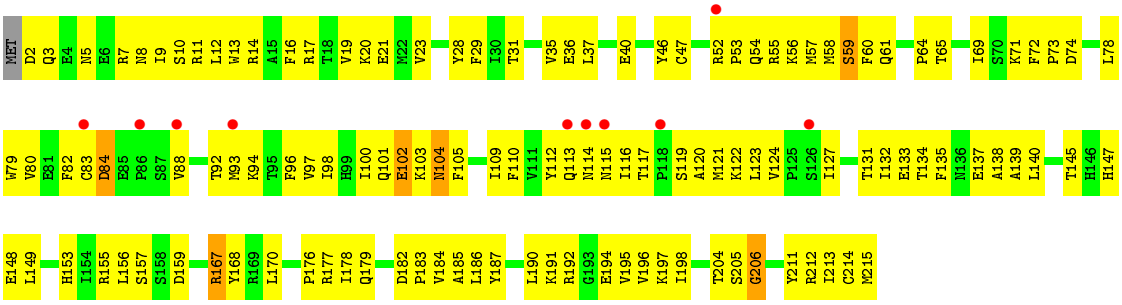
• Molecule 4: DNA-directed RNA polymerase II, chain RPB4

Chain D:

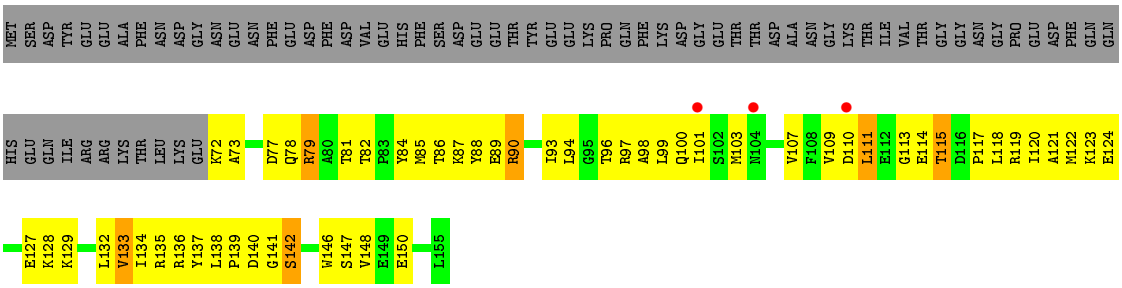
• Molecule 5: DNA-directed RNA polymerase II, chain RPB5

Chain E:

• Molecule 6: DNA-directed RNA polymerase I, II and III 23 kDa polypeptide

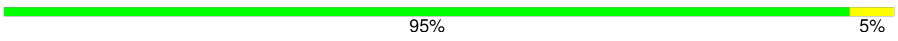
Chain F:

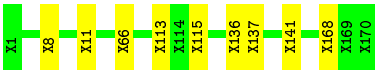




• Molecule 7: DNA-directed RNA polymerase II, chain RPB7

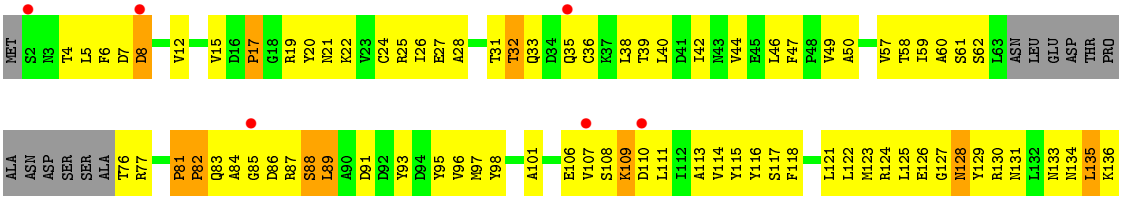
Chain G:



• Molecule 8: DNA-directed RNA polymerase subunit RPB8

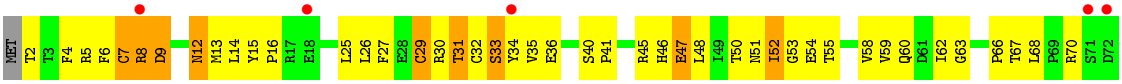
Chain H:

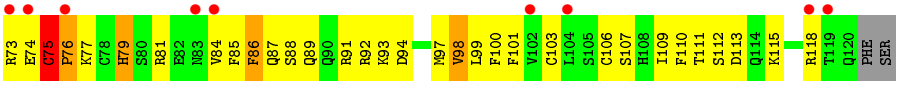





• Molecule 9: DNA-directed RNA polymerase II, chain RPB9

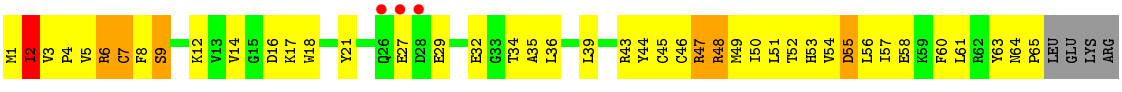
Chain I:



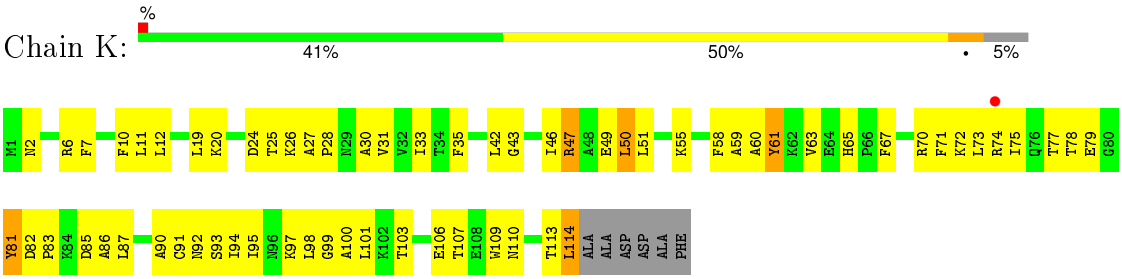
• Molecule 10: DNA-directed RNA polymerase II, chain RPB10

Chain J:

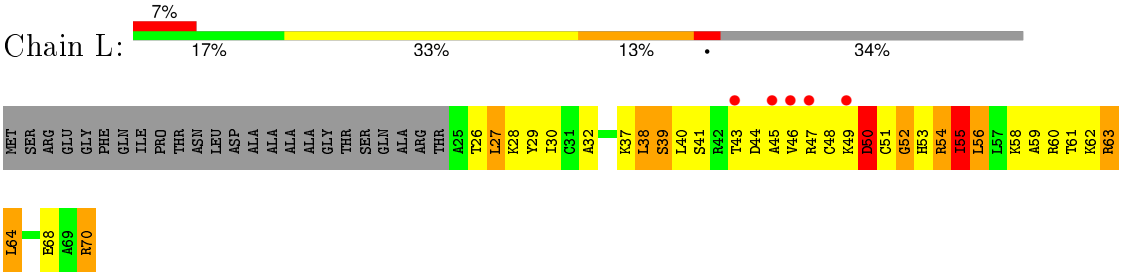
• Molecule 11: DNA-directed RNA polymerase II, chain RPB11

Chain K:




- Molecule 12: DNA-directed RNA polymerase II, chain RPB12

Chain L:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 224.10Å 394.46Å 284.34Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 4.10<br>39.97 – 4.11 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | (Not available) (40.00-4.10)<br>86.4 (39.97-4.11) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.58 (at 4.13Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.334 , 0.360<br>0.351 , 0.374 | Depositor<br>DCC |
| $R_{free}$ test set | 3272 reflections (4.02%) | DCC |
| Wilson B-factor (Å$^2$) | 114.0 | Xtriage |
| Anisotropy | 0.378 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.26 , 168.4 | EDS |
| Estimated twinning fraction | 0.044 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.047 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.44$, $< L^2 > = 0.27$ | Xtriage |
| Outliers | 0 of 96816 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.78 | EDS |
| Total number of atoms | 28295 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 194.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.41 | 0/11048 | 0.71 | 6/14936 (0.0%) |
| 2 | B | 0.46 | 0/8891 | 0.71 | 1/11990 (0.0%) |
| 3 | C | 0.48 | 0/2133 | 0.76 | 2/2891 (0.1%) |
| 5 | E | 0.37 | 0/1788 | 0.65 | 0/2406 |
| 6 | F | 0.40 | 0/691 | 0.64 | 0/933 |
| 8 | H | 0.40 | 0/1086 | 0.73 | 0/1470 |
| 9 | I | 0.48 | 0/989 | 0.76 | 1/1331 (0.1%) |
| 10 | J | 0.53 | 0/541 | 0.78 | 0/727 |
| 11 | K | 0.46 | 0/937 | 0.68 | 0/1265 |
| 12 | L | 0.49 | 0/366 | 0.78 | 0/485 |
| All | All | 0.44 | 0/28470 | 0.71 | 10/38434 (0.0%) |

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1392 | SER | N-CA-C | 6.34 | 128.13 | 111.00 |
| 3 | C | 39 | ALA | N-CA-C | 6.06 | 127.35 | 111.00 |
| 1 | A | 398 | GLU | N-CA-C | -5.77 | 95.43 | 111.00 |
| 3 | C | 183 | TRP | N-CA-C | -5.61 | 95.86 | 111.00 |
| 2 | B | 647 | GLY | N-CA-C | 5.22 | 126.15 | 113.10 |
| 1 | A | 1403 | GLU | N-CA-C | 5.22 | 125.08 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 750 | GLY | N-CA-C | -5.17 | 100.18 | 113.10 |
| 9 | I | 75 | CYS | N-CA-C | -5.13 | 97.14 | 111.00 |
| 1 | A | 452 | LYS | N-CA-C | -5.07 | 97.32 | 111.00 |
| 1 | A | 466 | SER | N-CA-C | 5.03 | 124.59 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 811 | TYR | Sidechain |

## 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 | 10864 | 0 | 10959 | 1032 | 1 |
| 2 | B | 8721 | 0 | 8746 | 900 | 0 |
| 3 | C | 2095 | 0 | 2052 | 162 | 1 |
| 4 | D | 153 | 0 | 0 | 4 | 0 |
| 5 | E | 1752 | 0 | 1776 | 129 | 0 |
| 6 | F | 679 | 0 | 701 | 66 | 0 |
| 7 | G | 170 | 0 | 0 | 5 | 0 |
| 8 | H | 1068 | 0 | 1040 | 134 | 0 |
| 9 | I | 971 | 0 | 933 | 101 | 0 |
| 10 | J | 532 | 0 | 544 | 77 | 0 |
| 11 | K | 919 | 0 | 929 | 84 | 0 |
| 12 | L | 364 | 0 | 390 | 50 | 0 |
| 13 | A | 2 | 0 | 0 | 0 | 0 |
| 13 | B | 1 | 0 | 0 | 0 | 0 |
| 13 | C | 1 | 0 | 0 | 0 | 0 |
| 13 | I | 2 | 0 | 0 | 1 | 0 |
| 13 | J | 1 | 0 | 0 | 1 | 0 |
| All | All | 28295 | 0 | 28070 | 2499 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (2499) 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) |
|---|---|---|---|
| 4:D:132:UNK:CA | 4:D:133:UNK:CA | 2.01 | 1.36 |
| 12:L:60:ARG:HG3 | 12:L:61:THR:H | 1.05 | 1.17 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:HD2 | 1.18 | 1.15 |
| 9:I:111:THR:HG22 | 9:I:113:ASP:H | 1.05 | 1.14 |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:HG2 | 1.65 | 1.11 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:HE | 1.12 | 1.10 |
| 1:A:93:VAL:HG13 | 1:A:301:ALA:HB1 | 1.33 | 1.08 |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:H | 1.00 | 1.08 |
| 1:A:666:ILE:HD11 | 2:B:1030:LEU:HD13 | 1.27 | 1.08 |
| 5:E:124:VAL:HG13 | 5:E:132:ILE:HB | 1.33 | 1.07 |
| 1:A:704:ALA:HB2 | 1:A:710:LEU:HG | 1.34 | 1.07 |
| 2:B:512:ARG:HH21 | 2:B:535:LEU:HD11 | 1.17 | 1.06 |
| 2:B:708:GLU:HG3 | 2:B:709:ASP:H | 1.17 | 1.06 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H | 1.18 | 1.05 |
| 2:B:570:VAL:HB | 2:B:573:GLN:HB3 | 1.36 | 1.05 |
| 2:B:345:LYS:HA | 2:B:348:ARG:HE | 1.11 | 1.05 |
| 6:F:81:THR:HG21 | 6:F:136:ARG:HD3 | 1.38 | 1.04 |
| 2:B:120:ARG:HG2 | 2:B:955:THR:HG21 | 1.40 | 1.03 |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:H | 1.16 | 1.03 |
| 1:A:902:LEU:HG | 1:A:926:GLN:HG3 | 1.40 | 1.02 |
| 2:B:287:ARG:HG2 | 2:B:292:ILE:HA | 1.38 | 1.02 |
| 2:B:1159:ARG:HE | 2:B:1193:GLN:NE2 | 1.56 | 1.02 |
| 12:L:32:ALA:HB3 | 12:L:55:ILE:HD12 | 1.39 | 1.02 |
| 2:B:1159:ARG:NE | 2:B:1193:GLN:HE21 | 1.57 | 1.02 |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:H | 1.25 | 1.01 |
| 3:C:80:LEU:HD22 | 3:C:129:ILE:HD11 | 1.41 | 1.00 |
| 1:A:567:LYS:CB | 1:A:568:PRO:HD2 | 1.91 | 1.00 |
| 2:B:977:GLY:HA3 | 2:B:1099:VAL:HG21 | 1.41 | 0.99 |
| 3:C:57:VAL:HG11 | 10:J:60:PHE:HB3 | 1.44 | 0.99 |
| 1:A:567:LYS:HB3 | 8:H:96:VAL:H | 1.26 | 0.99 |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:H | 1.22 | 0.98 |
| 5:E:135:PHE:HB3 | 5:E:140:LEU:HD11 | 1.45 | 0.98 |
| 1:A:244:PRO:HG2 | 1:A:245:PRO:HD3 | 1.46 | 0.98 |
| 11:K:113:THR:O | 11:K:114:LEU:HB2 | 1.60 | 0.97 |
| 2:B:842:ASN:ND2 | 2:B:845:SER:H | 1.62 | 0.97 |
| 9:I:7:CYS:HB2 | 9:I:14:LEU:HD21 | 1.47 | 0.97 |
| 3:C:167:HIS:CD2 | 3:C:169:LYS:H | 1.83 | 0.96 |
| 2:B:1100:ASP:HA | 2:B:1103:ILE:HD11 | 1.46 | 0.96 |
| 2:B:955:THR:HG22 | 2:B:956:THR:H | 1.31 | 0.96 |
| 2:B:392:ARG:HH21 | 9:I:52:ILE:HD11 | 1.30 | 0.96 |
| 2:B:1159:ARG:HD3 | 2:B:1193:GLN:HG3 | 1.47 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:174:LEU:O | 2:B:175:ARG:HB2 | 1.64 | 0.95 |
| 2:B:200:GLY:HA2 | 2:B:202:TYR:CE2 | 2.01 | 0.95 |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:N | 1.81 | 0.95 |
| 3:C:56:THR:HG22 | 3:C:57:VAL:H | 1.28 | 0.94 |
| 2:B:737:THR:HG21 | 9:I:66:PRO:O | 1.68 | 0.94 |
| 2:B:639:ILE:HD11 | 2:B:691:GLU:HG3 | 1.47 | 0.94 |
| 1:A:1399:ARG:HB3 | 1:A:1408:ILE:HD13 | 1.50 | 0.94 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:H | 1.14 | 0.93 |
| 1:A:783:THR:HG22 | 1:A:784:LEU:HG | 1.49 | 0.93 |
| 1:A:1281:ARG:HD2 | 1:A:1309:ASP:OD2 | 1.68 | 0.93 |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:N | 1.84 | 0.92 |
| 2:B:1159:ARG:HE | 2:B:1193:GLN:HE21 | 0.93 | 0.92 |
| 1:A:1116:LEU:HD12 | 1:A:1329:THR:OG1 | 1.67 | 0.92 |
| 1:A:1445:ILE:O | 1:A:1446:ASP:CA | 2.16 | 0.92 |
| 2:B:824:ILE:HG12 | 10:J:48:ARG:HH12 | 1.32 | 0.92 |
| 5:E:5:ASN:HD21 | 5:E:52:ARG:HG2 | 1.35 | 0.92 |
| 12:L:60:ARG:HG3 | 12:L:61:THR:N | 1.85 | 0.92 |
| 1:A:338:GLY:HA2 | 2:B:1129:ARG:HH22 | 1.33 | 0.92 |
| 2:B:955:THR:HG22 | 2:B:956:THR:N | 1.86 | 0.91 |
| 9:I:75:CYS:HG | 13:I:204:ZN:ZN | 0.68 | 0.91 |
| 1:A:1435:PRO:HA | 1:A:1439:GLY:O | 1.69 | 0.91 |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:H | 1.35 | 0.90 |
| 1:A:590:ARG:NH1 | 1:A:590:ARG:HG3 | 1.86 | 0.90 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:CD | 2.01 | 0.90 |
| 1:A:1194:ARG:NH2 | 1:A:1237:ILE:HD13 | 1.87 | 0.90 |
| 2:B:842:ASN:HD22 | 2:B:845:SER:H | 1.17 | 0.90 |
| 1:A:15:LYS:HB3 | 2:B:1220:ARG:HG2 | 1.51 | 0.90 |
| 7:G:11:UNK:CA | 7:G:66:UNK:CA | 2.49 | 0.90 |
| 1:A:549:MET:SD | 1:A:577:ILE:HD12 | 2.12 | 0.90 |
| 3:C:167:HIS:HD2 | 3:C:169:LYS:H | 0.90 | 0.90 |
| 1:A:353:ILE:HD13 | 1:A:487:MET:HE3 | 1.53 | 0.89 |
| 9:I:111:THR:HG22 | 9:I:113:ASP:N | 1.86 | 0.89 |
| 1:A:381:THR:HG22 | 1:A:383:TYR:H | 1.35 | 0.89 |
| 3:C:22:LEU:HD22 | 3:C:25:VAL:HG21 | 1.53 | 0.89 |
| 1:A:567:LYS:NZ | 8:H:46:LEU:HB2 | 1.87 | 0.89 |
| 1:A:962:ARG:HA | 1:A:965:GLN:HE21 | 1.37 | 0.89 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:H | 1.37 | 0.89 |
| 3:C:44:LEU:HB2 | 3:C:77:ILE:HD11 | 1.55 | 0.88 |
| 1:A:868:TYR:HD2 | 1:A:1058:VAL:HG21 | 1.38 | 0.88 |
| 3:C:57:VAL:HG11 | 10:J:60:PHE:CB | 2.03 | 0.88 |
| 1:A:886:ILE:HD11 | 1:A:943:LEU:HB3 | 1.56 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:956:THR:HA | 2:B:961:LEU:O | 1.71 | 0.88 |
| 1:A:1410:PHE:CD2 | 2:B:1212:ILE:HD11 | 2.08 | 0.88 |
| 1:A:337:ARG:NH1 | 1:A:839:ARG:HH12 | 1.72 | 0.88 |
| 2:B:800:GLN:HB3 | 10:J:52:THR:HG21 | 1.54 | 0.88 |
| 6:F:93:ILE:HD11 | 6:F:134:ILE:HD11 | 1.54 | 0.88 |
| 1:A:1105:LEU:HD22 | 1:A:1384:VAL:HG21 | 1.53 | 0.88 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:N | 1.72 | 0.88 |
| 2:B:977:GLY:HA3 | 2:B:1099:VAL:CG2 | 2.04 | 0.87 |
| 2:B:955:THR:CG2 | 2:B:956:THR:H | 1.87 | 0.87 |
| 1:A:666:ILE:CD1 | 2:B:1030:LEU:HD13 | 2.04 | 0.87 |
| 1:A:590:ARG:HH11 | 1:A:590:ARG:HG3 | 1.37 | 0.87 |
| 2:B:228:LYS:HD3 | 2:B:234:ILE:HD13 | 1.57 | 0.86 |
| 1:A:351:THR:HG23 | 2:B:1103:ILE:HA | 1.53 | 0.86 |
| 1:A:269:ILE:HD11 | 1:A:300:VAL:HA | 1.57 | 0.86 |
| 2:B:130:VAL:HG21 | 2:B:167:ILE:HD12 | 1.56 | 0.86 |
| 1:A:1039:LYS:O | 1:A:1043:ASP:HB2 | 1.75 | 0.86 |
| 2:B:512:ARG:HH21 | 2:B:535:LEU:CD1 | 1.88 | 0.86 |
| 1:A:667:GLY:HA2 | 1:A:670:ILE:HD12 | 1.56 | 0.86 |
| 2:B:345:LYS:CA | 2:B:348:ARG:HE | 1.87 | 0.86 |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:H | 1.40 | 0.86 |
| 1:A:1192:LEU:HD11 | 1:A:1239:ARG:HB3 | 1.57 | 0.86 |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:HB | 1.58 | 0.85 |
| 1:A:417:TYR:O | 1:A:418:SER:HB2 | 1.75 | 0.85 |
| 8:H:125:LEU:HG | 8:H:130:ARG:NH1 | 1.92 | 0.85 |
| 2:B:744:HIS:HD2 | 2:B:746:SER:H | 1.23 | 0.85 |
| 1:A:605:MET:HE3 | 1:A:614:PHE:O | 1.75 | 0.85 |
| 11:K:10:PHE:CD1 | 11:K:11:LEU:HD13 | 2.11 | 0.85 |
| 2:B:801:LYS:O | 10:J:52:THR:HG23 | 1.76 | 0.85 |
| 5:E:177:ARG:HD3 | 5:E:215:MET:SD | 2.18 | 0.84 |
| 11:K:12:LEU:H | 11:K:12:LEU:HD12 | 1.42 | 0.84 |
| 2:B:108:VAL:HG12 | 2:B:109:THR:H | 1.42 | 0.84 |
| 2:B:345:LYS:HA | 2:B:348:ARG:NE | 1.91 | 0.84 |
| 2:B:1106:ARG:HH21 | 2:B:1109:GLY:H | 1.24 | 0.84 |
| 5:E:2:ASP:O | 5:E:3:GLN:HG2 | 1.78 | 0.83 |
| 2:B:1106:ARG:NH1 | 2:B:1118:PRO:HB3 | 1.91 | 0.83 |
| 2:B:912:ILE:O | 2:B:938:SER:HB2 | 1.76 | 0.83 |
| 1:A:709:THR:HG21 | 9:I:93:LYS:O | 1.77 | 0.83 |
| 1:A:1118:VAL:CG2 | 1:A:1306:LEU:HB2 | 2.08 | 0.83 |
| 3:C:11:ARG:NH2 | 3:C:229:TYR:HD2 | 1.77 | 0.83 |
| 6:F:147:SER:OG | 6:F:150:GLU:HG3 | 1.78 | 0.83 |
| 1:A:683:ILE:HD11 | 1:A:764:CYS:HB2 | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1002:THR:CG2 | 2:B:1006:ILE:H | 1.91 | 0.83 |
| 1:A:535:THR:HG21 | 1:A:617:VAL:H | 1.43 | 0.83 |
| 2:B:200:GLY:HA2 | 2:B:202:TYR:HE2 | 1.42 | 0.82 |
| 1:A:1390:ASN:ND2 | 1:A:1399:ARG:HA | 1.93 | 0.82 |
| 2:B:763:GLN:HG2 | 2:B:765:PRO:HD2 | 1.61 | 0.82 |
| 1:A:1348:LEU:HD23 | 1:A:1372:VAL:HG13 | 1.59 | 0.82 |
| 1:A:565:ILE:HG23 | 1:A:567:LYS:HG2 | 1.62 | 0.82 |
| 2:B:637:LEU:HD12 | 2:B:693:ILE:HD12 | 1.60 | 0.82 |
| 2:B:1106:ARG:HH21 | 2:B:1109:GLY:N | 1.78 | 0.81 |
| 8:H:93:TYR:HB3 | 8:H:144:ILE:O | 1.80 | 0.81 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:H | 1.29 | 0.81 |
| 2:B:1106:ARG:HE | 2:B:1109:GLY:N | 1.79 | 0.81 |
| 2:B:313:MET:HE3 | 2:B:386:LEU:HD22 | 1.62 | 0.81 |
| 1:A:208:LEU:HD22 | 1:A:212:LYS:HE3 | 1.62 | 0.81 |
| 1:A:1017:LEU:HB2 | 5:E:206:GLY:H | 1.44 | 0.81 |
| 1:A:885:THR:HG23 | 1:A:893:PHE:HE1 | 1.44 | 0.81 |
| 1:A:406:ILE:HB | 1:A:431:LYS:HB2 | 1.61 | 0.81 |
| 10:J:48:ARG:HH21 | 10:J:49:MET:HE1 | 1.45 | 0.81 |
| 2:B:121:ASN:HD22 | 2:B:121:ASN:N | 1.79 | 0.81 |
| 10:J:3:VAL:HG21 | 10:J:18:TRP:HB2 | 1.61 | 0.81 |
| 3:C:148:ARG:NH1 | 10:J:64:ASN:HA | 1.96 | 0.81 |
| 1:A:742:ASN:HA | 1:A:745:GLN:HB2 | 1.63 | 0.81 |
| 2:B:244:LEU:O | 2:B:249:ARG:HG2 | 1.81 | 0.81 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CZ2 | 2.15 | 0.80 |
| 8:H:5:LEU:HD11 | 8:H:135:LEU:HG | 1.63 | 0.80 |
| 2:B:1106:ARG:NH2 | 2:B:1109:GLY:H | 1.79 | 0.80 |
| 2:B:899:ILE:HD11 | 2:B:911:ILE:HA | 1.63 | 0.80 |
| 2:B:999:MET:HG3 | 2:B:1000:PRO:HD2 | 1.61 | 0.80 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:NE | 1.95 | 0.80 |
| 2:B:796:LEU:HB3 | 2:B:799:PRO:HG3 | 1.63 | 0.80 |
| 8:H:81:PRO:HB2 | 8:H:82:PRO:CD | 2.11 | 0.80 |
| 2:B:800:GLN:HB3 | 10:J:52:THR:CG2 | 2.11 | 0.80 |
| 2:B:834:ASN:HB3 | 2:B:840:ILE:HG13 | 1.63 | 0.80 |
| 2:B:293:PRO:HG2 | 2:B:296:GLU:CB | 2.12 | 0.80 |
| 1:A:868:TYR:CE1 | 1:A:1064:VAL:HG11 | 2.17 | 0.80 |
| 3:C:167:HIS:HD2 | 3:C:169:LYS:N | 1.76 | 0.80 |
| 9:I:50:THR:CG2 | 9:I:52:ILE:HG23 | 2.11 | 0.80 |
| 10:J:46:CYS:HG | 13:J:101:ZN:ZN | 0.92 | 0.80 |
| 1:A:40:THR:HG22 | 1:A:41:MET:HG3 | 1.64 | 0.80 |
| 10:J:3:VAL:HG21 | 10:J:18:TRP:CB | 2.12 | 0.79 |
| 8:H:123:MET:HE3 | 8:H:142:LEU:HD22 | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:H | 1.47 | 0.79 |
| 3:C:37:MET:HG2 | 3:C:243:VAL:HG12 | 1.62 | 0.79 |
| 8:H:81:PRO:HB2 | 8:H:82:PRO:HD3 | 1.62 | 0.79 |
| 1:A:523:ILE:HD12 | 1:A:622:VAL:CG2 | 2.12 | 0.79 |
| 1:A:32:VAL:HG21 | 1:A:68:GLN:NE2 | 1.97 | 0.79 |
| 2:B:1100:ASP:HA | 2:B:1103:ILE:CD1 | 2.12 | 0.79 |
| 2:B:269:ILE:HD11 | 2:B:386:LEU:HD21 | 1.62 | 0.79 |
| 1:A:93:VAL:CG1 | 1:A:301:ALA:HB1 | 2.11 | 0.79 |
| 1:A:666:ILE:HD13 | 2:B:1030:LEU:HD22 | 1.65 | 0.79 |
| 1:A:337:ARG:NH1 | 1:A:839:ARG:NH1 | 2.29 | 0.79 |
| 1:A:298:PHE:O | 1:A:302:THR:HB | 1.83 | 0.79 |
| 1:A:679:ILE:HG23 | 1:A:729:ALA:HB1 | 1.63 | 0.79 |
| 1:A:768:GLN:CG | 1:A:816:HIS:HA | 2.13 | 0.78 |
| 2:B:487:THR:HG22 | 2:B:489:SER:H | 1.48 | 0.78 |
| 2:B:855:PHE:HZ | 2:B:857:ARG:NH1 | 1.81 | 0.78 |
| 1:A:783:THR:HG21 | 1:A:815:PHE:CZ | 2.19 | 0.78 |
| 1:A:472:LEU:O | 1:A:475:THR:HB | 1.81 | 0.78 |
| 10:J:64:ASN:HB3 | 10:J:65:PRO:HD3 | 1.63 | 0.78 |
| 2:B:842:ASN:ND2 | 2:B:845:SER:N | 2.31 | 0.78 |
| 1:A:1438:THR:HB | 2:B:1144:ALA:HB3 | 1.66 | 0.78 |
| 1:A:313:GLN:HB2 | 1:A:322:VAL:CG2 | 2.14 | 0.78 |
| 1:A:313:GLN:HB2 | 1:A:322:VAL:HG23 | 1.64 | 0.78 |
| 2:B:583:ASN:HD21 | 2:B:628:THR:HB | 1.49 | 0.78 |
| 1:A:399:HIS:O | 1:A:401:GLY:N | 2.17 | 0.78 |
| 1:A:58:LEU:HD22 | 1:A:80:HIS:O | 1.83 | 0.78 |
| 2:B:1106:ARG:HE | 2:B:1109:GLY:H | 1.29 | 0.78 |
| 1:A:23:SER:HB3 | 1:A:233:TRP:CZ2 | 2.19 | 0.78 |
| 3:C:56:THR:HG22 | 3:C:57:VAL:N | 1.97 | 0.78 |
| 1:A:353:ILE:HD13 | 1:A:487:MET:CE | 2.14 | 0.77 |
| 2:B:102:VAL:CG2 | 2:B:112:LEU:HB2 | 2.13 | 0.77 |
| 2:B:392:ARG:NH2 | 9:I:52:ILE:HD11 | 1.98 | 0.77 |
| 2:B:707:PRO:HG2 | 2:B:708:GLU:H | 1.49 | 0.77 |
| 2:B:1100:ASP:OD1 | 2:B:1103:ILE:HD11 | 1.84 | 0.77 |
| 1:A:326:ARG:HG2 | 1:A:1406:VAL:HG21 | 1.66 | 0.77 |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:N | 1.98 | 0.77 |
| 1:A:1281:ARG:O | 1:A:1282:VAL:HG23 | 1.83 | 0.77 |
| 3:C:165:LYS:O | 11:K:6:ARG:NH1 | 2.17 | 0.77 |
| 1:A:901:LEU:H | 1:A:926:GLN:NE2 | 1.82 | 0.77 |
| 2:B:708:GLU:HG3 | 2:B:709:ASP:N | 1.98 | 0.77 |
| 3:C:124:LEU:O | 3:C:127:ARG:HG2 | 1.85 | 0.77 |
| 1:A:31:SER:CB | 1:A:83:HIS:HB2 | 2.15 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:549:MET:HE1 | 1:A:656:TRP:HD1 | 1.49 | 0.77 |
| 2:B:102:VAL:HG23 | 2:B:112:LEU:HB2 | 1.65 | 0.77 |
| 1:A:1118:VAL:HG22 | 1:A:1306:LEU:HB2 | 1.64 | 0.77 |
| 4:D:81:UNK:CA | 4:D:82:UNK:CA | 2.63 | 0.77 |
| 1:A:70:CYS:O | 1:A:72:GLU:HG2 | 1.84 | 0.77 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:HB2 | 1.84 | 0.77 |
| 3:C:57:VAL:CG1 | 10:J:60:PHE:HB3 | 2.15 | 0.76 |
| 1:A:1345:ARG:HD2 | 1:A:1373:ASP:OD1 | 1.84 | 0.76 |
| 11:K:47:ARG:HH11 | 11:K:47:ARG:HB3 | 1.49 | 0.76 |
| 8:H:40:LEU:HD23 | 8:H:42:ILE:HD11 | 1.65 | 0.76 |
| 1:A:541:ILE:HG21 | 1:A:549:MET:HE3 | 1.67 | 0.76 |
| 3:C:166:GLU:HG3 | 11:K:10:PHE:HZ | 1.51 | 0.76 |
| 1:A:896:ARG:HD3 | 1:A:897:TYR:CE1 | 2.21 | 0.76 |
| 2:B:232:SER:OG | 2:B:234:ILE:HD12 | 1.84 | 0.76 |
| 8:H:93:TYR:HA | 8:H:145:ARG:HB3 | 1.68 | 0.76 |
| 5:E:61:GLN:HE21 | 5:E:105:PHE:HE2 | 1.34 | 0.76 |
| 11:K:55:LYS:HB3 | 11:K:81:TYR:HD1 | 1.50 | 0.76 |
| 2:B:899:ILE:CD1 | 2:B:911:ILE:HA | 2.16 | 0.76 |
| 2:B:496:ARG:NH1 | 2:B:539:LEU:HB2 | 1.99 | 0.76 |
| 2:B:770:GLN:HG2 | 2:B:983:ARG:O | 1.86 | 0.76 |
| 1:A:24:PRO:HB3 | 1:A:237:THR:HB | 1.67 | 0.76 |
| 2:B:708:GLU:CG | 2:B:709:ASP:H | 1.97 | 0.76 |
| 2:B:996:ARG:NH2 | 3:C:174:ALA:O | 2.19 | 0.76 |
| 1:A:1323:ASP:OD1 | 1:A:1325:THR:HB | 1.86 | 0.76 |
| 2:B:542:MET:HE3 | 2:B:747:MET:HG3 | 1.67 | 0.76 |
| 2:B:842:ASN:HD22 | 2:B:845:SER:N | 1.83 | 0.75 |
| 2:B:118:ARG:HG3 | 2:B:204:ILE:HD13 | 1.67 | 0.75 |
| 1:A:1094:VAL:HG13 | 1:A:1113:THR:HG21 | 1.66 | 0.75 |
| 1:A:95:PHE:O | 1:A:99:ILE:HG13 | 1.85 | 0.75 |
| 2:B:211:VAL:HG21 | 2:B:483:LEU:HD13 | 1.67 | 0.75 |
| 8:H:89:LEU:C | 8:H:91:ASP:H | 1.90 | 0.75 |
| 12:L:38:LEU:O | 12:L:39:SER:HB3 | 1.85 | 0.75 |
| 1:A:41:MET:HA | 1:A:49:LYS:HA | 1.68 | 0.75 |
| 2:B:1166:CYS:O | 2:B:1168:LEU:N | 2.18 | 0.75 |
| 10:J:12:LYS:O | 10:J:14:VAL:HG23 | 1.85 | 0.75 |
| 2:B:651:LEU:HD11 | 2:B:707:PRO:HB3 | 1.69 | 0.75 |
| 2:B:118:ARG:HH22 | 2:B:194:GLU:CD | 1.90 | 0.75 |
| 2:B:423:LYS:HA | 2:B:426:LYS:HE2 | 1.68 | 0.75 |
| 1:A:265:LYS:NZ | 1:A:323:LYS:H | 1.84 | 0.75 |
| 1:A:223:GLY:O | 1:A:1415:SER:HA | 1.86 | 0.75 |
| 1:A:469:ARG:HH21 | 2:B:976:ILE:HD13 | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:69:ILE:HG23 | 5:E:73:PRO:HA | 1.67 | 0.75 |
| 1:A:336:ILE:HD12 | 1:A:1405:THR:HG21 | 1.68 | 0.74 |
| 1:A:458:HIS:CE1 | 1:A:507:VAL:HG21 | 2.23 | 0.74 |
| 2:B:521:LEU:HD22 | 2:B:633:VAL:HG12 | 1.69 | 0.74 |
| 2:B:711:GLU:N | 2:B:712:PRO:HD3 | 2.01 | 0.74 |
| 1:A:535:THR:CG2 | 1:A:616:VAL:HA | 2.18 | 0.74 |
| 1:A:1436:ILE:HG22 | 1:A:1437:GLY:N | 2.02 | 0.74 |
| 1:A:1436:ILE:CG2 | 2:B:1142:GLY:HA2 | 2.17 | 0.74 |
| 2:B:542:MET:HE1 | 2:B:743:ILE:HG21 | 1.70 | 0.74 |
| 1:A:1146:VAL:HG11 | 1:A:1202:MET:SD | 2.27 | 0.74 |
| 6:F:111:LEU:N | 6:F:111:LEU:HD12 | 2.02 | 0.74 |
| 2:B:62:ILE:HG23 | 2:B:418:LYS:HG2 | 1.69 | 0.74 |
| 1:A:1399:ARG:HB2 | 1:A:1408:ILE:HG21 | 1.70 | 0.74 |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:HE1 | 1.51 | 0.74 |
| 2:B:570:VAL:HB | 2:B:573:GLN:CB | 2.18 | 0.74 |
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:N | 2.02 | 0.74 |
| 1:A:443:LEU:HD21 | 1:A:455:MET:HB3 | 1.70 | 0.74 |
| 2:B:46:GLN:HG3 | 2:B:47:GLN:N | 2.03 | 0.74 |
| 2:B:879:ARG:HB3 | 2:B:883:LEU:HD23 | 1.70 | 0.74 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:H | 1.50 | 0.74 |
| 1:A:575:LYS:HB3 | 1:A:612:ILE:CG2 | 2.17 | 0.74 |
| 1:A:268:ASP:HB3 | 1:A:299:HIS:CE1 | 2.23 | 0.74 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:HB | 1.88 | 0.74 |
| 1:A:534:LEU:O | 1:A:574:GLY:HA3 | 1.88 | 0.74 |
| 1:A:567:LYS:HB3 | 8:H:96:VAL:N | 2.02 | 0.73 |
| 5:E:61:GLN:NE2 | 5:E:105:PHE:HE2 | 1.86 | 0.73 |
| 8:H:89:LEU:HB3 | 8:H:91:ASP:OD1 | 1.88 | 0.73 |
| 1:A:925:LEU:O | 1:A:929:LEU:HD23 | 1.88 | 0.73 |
| 1:A:710:LEU:H | 1:A:710:LEU:HD12 | 1.52 | 0.73 |
| 2:B:980:PHE:CE2 | 2:B:1094:ARG:HG3 | 2.23 | 0.73 |
| 1:A:154:SER:HB3 | 1:A:162:VAL:CG2 | 2.17 | 0.73 |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:HB3 | 1.70 | 0.73 |
| 1:A:445:ASN:HB2 | 1:A:455:MET:HG2 | 1.70 | 0.73 |
| 5:E:124:VAL:HA | 5:E:132:ILE:HD12 | 1.70 | 0.73 |
| 1:A:899:VAL:HB | 1:A:929:LEU:HD12 | 1.71 | 0.73 |
| 2:B:193:LYS:HD3 | 2:B:787:VAL:HG11 | 1.70 | 0.73 |
| 8:H:35:GLN:HB3 | 8:H:111:LEU:HD21 | 1.70 | 0.73 |
| 2:B:1106:ARG:NE | 2:B:1109:GLY:H | 1.85 | 0.73 |
| 1:A:1258:HIS:ND1 | 1:A:1262:LYS:HE3 | 2.04 | 0.73 |
| 2:B:363:HIS:O | 2:B:364:ILE:HB | 1.88 | 0.73 |
| 1:A:500:GLU:OE2 | 2:B:1145:SER:HB2 | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1441:PHE:CZ | 6:F:89:GLU:HA | 2.23 | 0.73 |
| 1:A:321:PRO:O | 1:A:322:VAL:HB | 1.87 | 0.73 |
| 1:A:445:ASN:CB | 1:A:455:MET:HG2 | 2.19 | 0.73 |
| 1:A:901:LEU:HG | 1:A:926:GLN:HE21 | 1.54 | 0.72 |
| 2:B:839:MET:HE3 | 2:B:1010:LEU:HD11 | 1.71 | 0.72 |
| 1:A:868:TYR:CD2 | 1:A:1058:VAL:HG21 | 2.23 | 0.72 |
| 1:A:1436:ILE:HG22 | 1:A:1437:GLY:H | 1.52 | 0.72 |
| 1:A:337:ARG:NE | 1:A:839:ARG:HH22 | 1.88 | 0.72 |
| 2:B:542:MET:HG3 | 2:B:747:MET:HE3 | 1.69 | 0.72 |
| 2:B:58:THR:O | 2:B:62:ILE:HG13 | 1.89 | 0.72 |
| 2:B:708:GLU:O | 2:B:710:LEU:N | 2.22 | 0.72 |
| 2:B:570:VAL:HG21 | 2:B:573:GLN:NE2 | 2.04 | 0.72 |
| 1:A:32:VAL:HB | 1:A:57:ARG:HD2 | 1.71 | 0.72 |
| 2:B:745:PRO:O | 2:B:748:ILE:HG12 | 1.89 | 0.72 |
| 1:A:855:THR:HG23 | 1:A:857:ARG:HG3 | 1.72 | 0.72 |
| 1:A:399:HIS:HB3 | 1:A:400:PRO:HD3 | 1.69 | 0.72 |
| 1:A:1209:MET:SD | 1:A:1236:LEU:HB3 | 2.30 | 0.72 |
| 1:A:567:LYS:HZ1 | 8:H:46:LEU:HB2 | 1.55 | 0.72 |
| 1:A:857:ARG:HD3 | 1:A:861:GLY:O | 1.88 | 0.72 |
| 11:K:65:HIS:CD2 | 11:K:67:PHE:H | 2.06 | 0.72 |
| 1:A:351:THR:HG21 | 2:B:1103:ILE:HG23 | 1.71 | 0.72 |
| 1:A:575:LYS:HB3 | 1:A:612:ILE:HG23 | 1.71 | 0.72 |
| 9:I:74:GLU:HB3 | 9:I:79:HIS:HA | 1.70 | 0.72 |
| 1:A:567:LYS:HD3 | 8:H:95:TYR:CD1 | 2.25 | 0.72 |
| 1:A:341:MET:HE1 | 1:A:1401:SER:HB2 | 1.72 | 0.72 |
| 8:H:5:LEU:HB3 | 8:H:133:ASN:O | 1.88 | 0.72 |
| 2:B:313:MET:CE | 2:B:386:LEU:HD22 | 2.19 | 0.72 |
| 1:A:994:GLN:HE22 | 1:A:1023:ARG:HE | 1.38 | 0.72 |
| 1:A:900:ASP:OD2 | 1:A:903:ASN:HB2 | 1.90 | 0.72 |
| 1:A:828:ALA:HB2 | 2:B:530:GLY:HA2 | 1.70 | 0.72 |
| 2:B:955:THR:CG2 | 2:B:956:THR:N | 2.49 | 0.71 |
| 1:A:567:LYS:HE3 | 8:H:46:LEU:HD12 | 1.71 | 0.71 |
| 1:A:1397:LEU:O | 1:A:1400:CYS:HB2 | 1.89 | 0.71 |
| 2:B:309:GLN:HG3 | 9:I:52:ILE:HD13 | 1.72 | 0.71 |
| 2:B:108:VAL:HG12 | 2:B:109:THR:N | 2.06 | 0.71 |
| 1:A:503:GLN:HE21 | 6:F:90:ARG:NH2 | 1.88 | 0.71 |
| 2:B:555:ILE:HD13 | 2:B:587:HIS:CE1 | 2.26 | 0.71 |
| 11:K:7:PHE:HB2 | 11:K:11:LEU:HD22 | 1.72 | 0.71 |
| 1:A:598:LEU:HD22 | 8:H:25:ARG:NH1 | 2.05 | 0.71 |
| 2:B:234:ILE:H | 2:B:234:ILE:HD12 | 1.53 | 0.71 |
| 5:E:168:TYR:HB3 | 5:E:170:LEU:HD21 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:417:TYR:O | 1:A:418:SER:CB | 2.36 | 0.71 |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:HD2 | 1.71 | 0.71 |
| 1:A:1152:ILE:HG23 | 1:A:1260:LEU:HD23 | 1.71 | 0.71 |
| 1:A:75:ASN:O | 1:A:76:GLU:HB3 | 1.88 | 0.71 |
| 1:A:383:TYR:HB3 | 6:F:115:THR:HG22 | 1.73 | 0.71 |
| 1:A:340:LEU:HD21 | 2:B:1200:ALA:HB2 | 1.72 | 0.71 |
| 1:A:672:ASP:HB2 | 1:A:736:ASN:OD1 | 1.90 | 0.71 |
| 1:A:44:THR:O | 1:A:45:GLN:HB2 | 1.91 | 0.71 |
| 1:A:1332:PHE:H | 1:A:1332:PHE:HD2 | 1.38 | 0.71 |
| 1:A:225:ASN:O | 1:A:227:VAL:N | 2.21 | 0.71 |
| 2:B:637:LEU:CD1 | 2:B:693:ILE:HD12 | 2.20 | 0.70 |
| 1:A:451:HIS:NE2 | 1:A:1074:GLU:HG3 | 2.07 | 0.70 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:H | 1.35 | 0.70 |
| 1:A:1015:VAL:HG12 | 1:A:1019:CYS:SG | 2.32 | 0.70 |
| 1:A:675:THR:HG21 | 1:A:736:ASN:ND2 | 2.06 | 0.70 |
| 1:A:367:PRO:HB3 | 1:A:466:SER:HA | 1.73 | 0.70 |
| 1:A:48:ALA:O | 1:A:49:LYS:HG3 | 1.89 | 0.70 |
| 2:B:737:THR:HG23 | 9:I:66:PRO:CB | 2.20 | 0.70 |
| 2:B:636:PRO:O | 2:B:637:LEU:HG | 1.90 | 0.70 |
| 1:A:691:LEU:HD11 | 1:A:695:LYS:HE3 | 1.71 | 0.70 |
| 2:B:792:MET:HA | 2:B:856:PHE:O | 1.91 | 0.70 |
| 1:A:463:ILE:HB | 1:A:464:PRO:HD2 | 1.74 | 0.70 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:HG11 | 1.72 | 0.70 |
| 2:B:130:VAL:HG12 | 2:B:131:ASP:N | 2.07 | 0.70 |
| 11:K:55:LYS:HD3 | 11:K:78:THR:CB | 2.20 | 0.70 |
| 2:B:542:MET:CE | 2:B:747:MET:HG3 | 2.22 | 0.70 |
| 2:B:463:THR:CG2 | 2:B:465:ASN:HD22 | 2.05 | 0.70 |
| 2:B:957:ASN:HD22 | 2:B:961:LEU:HD12 | 1.57 | 0.70 |
| 12:L:47:ARG:HG2 | 12:L:52:GLY:HA2 | 1.72 | 0.70 |
| 2:B:281:PRO:HG2 | 2:B:284:ILE:HD12 | 1.73 | 0.70 |
| 1:A:1208:THR:HB | 1:A:1211:GLN:HG3 | 1.74 | 0.70 |
| 1:A:335:ARG:HA | 1:A:339:ASN:HD22 | 1.57 | 0.70 |
| 5:E:56:LYS:HG3 | 5:E:84:ASP:HB2 | 1.73 | 0.70 |
| 2:B:65:GLU:HG3 | 2:B:66:ASP:H | 1.56 | 0.70 |
| 1:A:567:LYS:HE3 | 8:H:46:LEU:CD1 | 2.22 | 0.70 |
| 2:B:519:TRP:HZ2 | 2:B:705:MET:HE1 | 1.57 | 0.70 |
| 11:K:55:LYS:HD3 | 11:K:78:THR:HB | 1.72 | 0.70 |
| 2:B:1066:SER:O | 2:B:1067:ARG:HD3 | 1.90 | 0.69 |
| 8:H:36:CYS:SG | 8:H:130:ARG:NH2 | 2.65 | 0.69 |
| 2:B:293:PRO:HG2 | 2:B:296:GLU:HB3 | 1.74 | 0.69 |
| 1:A:72:GLU:OE2 | 2:B:1175:LEU:HD12 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:675:THR:CB | 1:A:736:ASN:HD21 | 2.04 | 0.69 |
| 8:H:49:VAL:HG12 | 8:H:50:ALA:N | 2.07 | 0.69 |
| 1:A:763:ALA:O | 1:A:803:SER:HB3 | 1.92 | 0.69 |
| 2:B:955:THR:HG23 | 12:L:54:ARG:O | 1.91 | 0.69 |
| 1:A:472:LEU:HD11 | 2:B:835:GLN:NE2 | 2.08 | 0.69 |
| 1:A:858:ASN:HD22 | 1:A:858:ASN:C | 1.96 | 0.69 |
| 1:A:584:ASN:O | 1:A:637:LYS:HE3 | 1.92 | 0.69 |
| 1:A:768:GLN:HG2 | 1:A:816:HIS:HA | 1.75 | 0.69 |
| 5:E:83:CYS:SG | 5:E:88:VAL:HG22 | 2.32 | 0.69 |
| 3:C:80:LEU:HD22 | 3:C:129:ILE:CD1 | 2.21 | 0.69 |
| 1:A:343:LYS:HE3 | 2:B:1151:LEU:O | 1.92 | 0.69 |
| 2:B:280:ILE:CD1 | 2:B:334:ILE:HG12 | 2.23 | 0.69 |
| 1:A:414:ASP:OD1 | 1:A:416:ARG:HG2 | 1.93 | 0.69 |
| 2:B:638:PHE:CE1 | 2:B:743:ILE:HA | 2.26 | 0.69 |
| 1:A:340:LEU:HD13 | 1:A:1429:ILE:HG23 | 1.74 | 0.69 |
| 2:B:378:LEU:O | 2:B:382:ILE:HG13 | 1.92 | 0.69 |
| 2:B:1056:SER:HB3 | 2:B:1066:SER:HB2 | 1.73 | 0.68 |
| 1:A:392:VAL:HG13 | 1:A:415:LEU:HD11 | 1.74 | 0.68 |
| 1:A:694:THR:O | 1:A:698:GLN:HG3 | 1.94 | 0.68 |
| 8:H:7:ASP:O | 8:H:8:ASP:HB2 | 1.92 | 0.68 |
| 1:A:599:SER:HB2 | 1:A:603:ASN:H | 1.58 | 0.68 |
| 3:C:39:ALA:HA | 3:C:164:ALA:HB3 | 1.74 | 0.68 |
| 1:A:391:LEU:HD22 | 1:A:400:PRO:O | 1.93 | 0.68 |
| 3:C:93:ASP:O | 3:C:127:ARG:NH2 | 2.27 | 0.68 |
| 2:B:54:PHE:HA | 2:B:58:THR:HB | 1.74 | 0.68 |
| 2:B:22:SER:O | 2:B:654:ARG:HD2 | 1.94 | 0.68 |
| 6:F:81:THR:HG21 | 6:F:136:ARG:CD | 2.20 | 0.68 |
| 2:B:976:ILE:O | 2:B:990:ILE:HB | 1.94 | 0.68 |
| 2:B:884:ARG:O | 2:B:936:ASP:HB3 | 1.93 | 0.68 |
| 1:A:381:THR:HG22 | 1:A:383:TYR:N | 2.09 | 0.68 |
| 2:B:314:LEU:O | 2:B:317:CYS:HB2 | 1.92 | 0.68 |
| 12:L:46:VAL:HG13 | 12:L:56:LEU:HD12 | 1.76 | 0.68 |
| 9:I:53:GLY:O | 9:I:89:GLN:HB2 | 1.94 | 0.68 |
| 3:C:51:VAL:HG22 | 3:C:155:LEU:HD22 | 1.76 | 0.68 |
| 2:B:709:ASP:O | 2:B:710:LEU:HD23 | 1.94 | 0.68 |
| 1:A:1095:THR:HG22 | 1:A:1100:ARG:HB2 | 1.74 | 0.68 |
| 3:C:166:GLU:HG3 | 11:K:10:PHE:CZ | 2.29 | 0.68 |
| 3:C:254:LYS:HB3 | 11:K:42:LEU:HD11 | 1.75 | 0.68 |
| 1:A:446:ARG:HH11 | 1:A:446:ARG:HG2 | 1.59 | 0.68 |
| 2:B:986:GLN:OE1 | 2:B:986:GLN:HA | 1.92 | 0.68 |
| 2:B:954:VAL:O | 12:L:55:ILE:O | 2.11 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:280:ILE:HG22 | 2:B:285:ILE:HG13 | 1.76 | 0.68 |
| 2:B:842:ASN:ND2 | 2:B:844:SER:HB2 | 2.09 | 0.68 |
| 5:E:93:MET:HE2 | 5:E:120:ALA:HB1 | 1.75 | 0.68 |
| 1:A:535:THR:HG21 | 1:A:616:VAL:HA | 1.76 | 0.67 |
| 2:B:711:GLU:N | 2:B:712:PRO:CD | 2.57 | 0.67 |
| 2:B:562:GLY:HA3 | 2:B:590:HIS:CE1 | 2.29 | 0.67 |
| 1:A:693:VAL:CG2 | 1:A:721:PHE:HE1 | 2.07 | 0.67 |
| 2:B:288:ALA:HB1 | 2:B:331:LEU:HD12 | 1.75 | 0.67 |
| 1:A:786:HIS:HE1 | 2:B:742:GLU:OE1 | 1.76 | 0.67 |
| 2:B:1002:THR:HG23 | 2:B:1004:GLU:N | 2.10 | 0.67 |
| 1:A:351:THR:CG2 | 2:B:1103:ILE:HG23 | 2.24 | 0.67 |
| 2:B:882:THR:HG21 | 2:B:935:ARG:HA | 1.75 | 0.67 |
| 2:B:1106:ARG:CZ | 2:B:1109:GLY:H | 2.07 | 0.67 |
| 1:A:994:GLN:HE21 | 1:A:1019:CYS:HB3 | 1.59 | 0.67 |
| 2:B:603:LEU:HB3 | 2:B:609:ILE:HG13 | 1.76 | 0.67 |
| 2:B:287:ARG:NH2 | 2:B:294:ASP:OD2 | 2.28 | 0.67 |
| 1:A:1390:ASN:HD22 | 1:A:1399:ARG:HA | 1.57 | 0.67 |
| 8:H:115:TYR:CE2 | 8:H:124:ARG:HG3 | 2.30 | 0.67 |
| 1:A:16:GLU:HB3 | 1:A:1418:LEU:HD11 | 1.77 | 0.67 |
| 5:E:127:ILE:O | 5:E:127:ILE:HG13 | 1.93 | 0.67 |
| 11:K:47:ARG:NH1 | 11:K:47:ARG:HB3 | 2.09 | 0.67 |
| 1:A:453:MET:HB3 | 1:A:477:PRO:HB3 | 1.76 | 0.67 |
| 3:C:260:LEU:O | 3:C:264:GLN:HG3 | 1.95 | 0.67 |
| 10:J:58:GLU:HA | 10:J:61:LEU:HD12 | 1.76 | 0.67 |
| 1:A:306:ASN:HD21 | 1:A:324:SER:H | 1.43 | 0.67 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:N | 2.09 | 0.67 |
| 8:H:26:ILE:HD12 | 8:H:42:ILE:HD12 | 1.76 | 0.67 |
| 1:A:897:TYR:CD2 | 1:A:936:LEU:HD13 | 2.30 | 0.67 |
| 1:A:443:LEU:HD22 | 1:A:455:MET:HE2 | 1.74 | 0.67 |
| 3:C:5:GLY:O | 3:C:7:GLN:HG3 | 1.94 | 0.67 |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:HD13 | 1.77 | 0.67 |
| 12:L:45:ALA:O | 12:L:46:VAL:HG23 | 1.95 | 0.67 |
| 10:J:1:MET:H2 | 10:J:56:LEU:HB2 | 1.59 | 0.67 |
| 1:A:816:HIS:CE1 | 2:B:764:SER:HB2 | 2.30 | 0.67 |
| 1:A:76:GLU:OE2 | 2:B:1159:ARG:NH1 | 2.28 | 0.66 |
| 1:A:1348:LEU:HD21 | 1:A:1375:MET:SD | 2.35 | 0.66 |
| 2:B:311:LEU:HB3 | 9:I:4:PHE:CZ | 2.31 | 0.66 |
| 2:B:864:LYS:HB3 | 2:B:872:GLU:H | 1.59 | 0.66 |
| 1:A:914:GLU:HB2 | 1:A:979:SER:O | 1.95 | 0.66 |
| 3:C:56:THR:HG21 | 3:C:145:CYS:SG | 2.35 | 0.66 |
| 1:A:814:PHE:O | 1:A:817:ALA:HB3 | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:22:LEU:HD22 | 3:C:25:VAL:CG2 | 2.25 | 0.66 |
| 2:B:514:LEU:HD12 | 2:B:515:HIS:N | 2.09 | 0.66 |
| 1:A:563:PRO:HB2 | 1:A:565:ILE:O | 1.94 | 0.66 |
| 1:A:1364:ASN:ND2 | 1:A:1365:TYR:N | 2.43 | 0.66 |
| 1:A:381:THR:CG2 | 1:A:383:TYR:H | 2.09 | 0.66 |
| 1:A:828:ALA:CB | 2:B:530:GLY:HA2 | 2.25 | 0.66 |
| 2:B:1147:LEU:HD22 | 2:B:1151:LEU:HD22 | 1.77 | 0.66 |
| 1:A:1333:ILE:O | 1:A:1336:MET:HB3 | 1.96 | 0.66 |
| 1:A:1342:GLU:OE2 | 5:E:212:ARG:NH1 | 2.28 | 0.66 |
| 1:A:1267:MET:HA | 1:A:1271:ILE:HD12 | 1.77 | 0.66 |
| 9:I:55:THR:HG23 | 9:I:58:VAL:HG21 | 1.76 | 0.66 |
| 3:C:98:VAL:C | 3:C:99:LEU:HD23 | 2.16 | 0.66 |
| 9:I:32:CYS:SG | 9:I:33:SER:N | 2.69 | 0.66 |
| 2:B:121:ASN:HA | 2:B:207:GLY:HA3 | 1.77 | 0.66 |
| 2:B:363:HIS:O | 2:B:364:ILE:CB | 2.44 | 0.66 |
| 1:A:590:ARG:HB3 | 1:A:605:MET:N | 2.10 | 0.66 |
| 8:H:95:TYR:CE2 | 8:H:97:MET:HG3 | 2.31 | 0.66 |
| 2:B:128:LEU:HB3 | 2:B:167:ILE:O | 1.95 | 0.66 |
| 2:B:566:LEU:HD13 | 2:B:588:GLY:HA2 | 1.78 | 0.66 |
| 2:B:649:LYS:HE2 | 2:B:738:PHE:O | 1.96 | 0.66 |
| 1:A:525:GLN:CB | 2:B:835:GLN:HG2 | 2.25 | 0.66 |
| 1:A:741:ASN:HD22 | 1:A:741:ASN:C | 1.99 | 0.66 |
| 6:F:109:VAL:HG12 | 6:F:110:ASP:N | 2.10 | 0.66 |
| 1:A:535:THR:HG21 | 1:A:617:VAL:N | 2.08 | 0.66 |
| 2:B:986:GLN:HE22 | 2:B:1020:ARG:CZ | 2.08 | 0.66 |
| 7:G:113:UNK:CA | 7:G:115:UNK:CA | 2.74 | 0.66 |
| 2:B:957:ASN:O | 2:B:959:ASP:N | 2.28 | 0.66 |
| 2:B:46:GLN:HE22 | 2:B:496:ARG:HA | 1.61 | 0.66 |
| 8:H:38:LEU:HD13 | 8:H:125:LEU:HD13 | 1.77 | 0.65 |
| 1:A:95:PHE:HE2 | 1:A:1414:ALA:HB2 | 1.62 | 0.65 |
| 1:A:90:VAL:CG1 | 1:A:297:GLN:HA | 2.26 | 0.65 |
| 1:A:305:ASP:HB3 | 1:A:308:ILE:HD11 | 1.77 | 0.65 |
| 2:B:293:PRO:HG2 | 2:B:296:GLU:HB2 | 1.79 | 0.65 |
| 1:A:381:THR:HG21 | 1:A:383:TYR:CD1 | 2.31 | 0.65 |
| 1:A:751:SER:O | 1:A:752:LYS:HG2 | 1.96 | 0.65 |
| 2:B:1001:PHE:CZ | 2:B:1073:TYR:HB2 | 2.30 | 0.65 |
| 2:B:120:ARG:CG | 2:B:955:THR:HG21 | 2.23 | 0.65 |
| 1:A:1115:SER:HA | 1:A:1308:THR:HG22 | 1.77 | 0.65 |
| 1:A:590:ARG:HH11 | 1:A:590:ARG:CG | 2.06 | 0.65 |
| 2:B:1039:GLY:HA2 | 10:J:51:LEU:HD21 | 1.77 | 0.65 |
| 3:C:11:ARG:HH21 | 3:C:229:TYR:HD2 | 1.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:523:ILE:HD12 | 1:A:622:VAL:HG22 | 1.79 | 0.65 |
| 2:B:46:GLN:HG3 | 2:B:47:GLN:H | 1.59 | 0.65 |
| 2:B:211:VAL:HG23 | 2:B:483:LEU:HB2 | 1.79 | 0.65 |
| 5:E:176:PRO:O | 5:E:212:ARG:HA | 1.95 | 0.65 |
| 2:B:751:VAL:O | 2:B:754:SER:HB2 | 1.95 | 0.65 |
| 1:A:1319:VAL:HG13 | 1:A:1320:PRO:HD2 | 1.79 | 0.65 |
| 5:E:124:VAL:HG22 | 5:E:132:ILE:HG21 | 1.78 | 0.65 |
| 1:A:1111:MET:HE1 | 1:A:1330:ASN:OD1 | 1.97 | 0.65 |
| 2:B:114:PRO:HG3 | 2:B:181:LEU:HD11 | 1.79 | 0.65 |
| 2:B:911:ILE:CG2 | 2:B:966:VAL:HG11 | 2.26 | 0.65 |
| 12:L:51:CYS:O | 12:L:53:HIS:N | 2.28 | 0.65 |
| 1:A:512:VAL:HA | 1:A:519:PRO:HA | 1.79 | 0.65 |
| 8:H:24:CYS:HB2 | 8:H:44:VAL:CG2 | 2.27 | 0.65 |
| 9:I:111:THR:HG21 | 9:I:113:ASP:HB2 | 1.78 | 0.65 |
| 2:B:349:ILE:O | 2:B:352:ALA:HB3 | 1.96 | 0.65 |
| 8:H:107:VAL:HG21 | 8:H:126:GLU:HG3 | 1.79 | 0.65 |
| 1:A:450:LEU:HD13 | 1:A:1074:GLU:HG2 | 1.77 | 0.65 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:H | 1.60 | 0.65 |
| 1:A:1111:MET:HE1 | 1:A:1114:PRO:HA | 1.79 | 0.65 |
| 1:A:1042:PHE:CE2 | 1:A:1046:LEU:HD11 | 2.31 | 0.65 |
| 1:A:87:ALA:HB3 | 1:A:276:LEU:HD23 | 1.79 | 0.65 |
| 1:A:1224:LEU:HD12 | 1:A:1241:ARG:O | 1.97 | 0.65 |
| 2:B:577:ALA:HB1 | 2:B:589:VAL:CG1 | 2.27 | 0.64 |
| 2:B:805:THR:HG21 | 2:B:815:ARG:HE | 1.62 | 0.64 |
| 1:A:579:SER:OG | 1:A:612:ILE:HG22 | 1.98 | 0.64 |
| 1:A:1035:TYR:O | 1:A:1037:LEU:N | 2.30 | 0.64 |
| 1:A:329:LEU:HD23 | 1:A:335:ARG:HG3 | 1.78 | 0.64 |
| 2:B:1170:THR:O | 2:B:1170:THR:HG22 | 1.97 | 0.64 |
| 2:B:25:ILE:HG22 | 2:B:29:ASP:HB2 | 1.79 | 0.64 |
| 1:A:1445:ILE:C | 1:A:1446:ASP:CA | 2.65 | 0.64 |
| 2:B:879:ARG:HB3 | 2:B:883:LEU:CD2 | 2.26 | 0.64 |
| 3:C:241:ASP:HB3 | 11:K:109:TRP:CE2 | 2.32 | 0.64 |
| 2:B:515:HIS:HD2 | 2:B:517:THR:OG1 | 1.81 | 0.64 |
| 1:A:715:GLU:O | 1:A:719:VAL:HG23 | 1.96 | 0.64 |
| 1:A:901:LEU:HA | 1:A:907:THR:HG23 | 1.80 | 0.64 |
| 6:F:96:THR:O | 6:F:100:GLN:HG3 | 1.97 | 0.64 |
| 2:B:604:ARG:HG2 | 2:B:604:ARG:O | 1.98 | 0.64 |
| 6:F:86:THR:OG1 | 6:F:89:GLU:HG3 | 1.98 | 0.64 |
| 2:B:519:TRP:CZ2 | 2:B:705:MET:HE1 | 2.32 | 0.64 |
| 1:A:1193:LEU:HB2 | 1:A:1260:LEU:HD11 | 1.78 | 0.64 |
| 1:A:629:LEU:HD13 | 1:A:645:LEU:HD21 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1394:THR:CG2 | 1:A:1395:GLY:N | 2.60 | 0.64 |
| 2:B:711:GLU:H | 2:B:712:PRO:HD3 | 1.61 | 0.64 |
| 8:H:106:GLU:C | 8:H:108:SER:H | 2.02 | 0.64 |
| 2:B:824:ILE:CG1 | 10:J:48:ARG:HH12 | 2.08 | 0.63 |
| 1:A:523:ILE:HD12 | 1:A:622:VAL:HG21 | 1.80 | 0.63 |
| 2:B:1197:PRO:HG2 | 2:B:1200:ALA:HB2 | 1.79 | 0.63 |
| 8:H:49:VAL:HG12 | 8:H:50:ALA:H | 1.62 | 0.63 |
| 1:A:709:THR:HB | 1:A:712:GLU:H | 1.64 | 0.63 |
| 1:A:225:ASN:O | 1:A:226:GLU:HG2 | 1.99 | 0.63 |
| 2:B:1001:PHE:CE1 | 2:B:1073:TYR:HB2 | 2.33 | 0.63 |
| 2:B:780:VAL:HG21 | 10:J:56:LEU:CD1 | 2.29 | 0.63 |
| 2:B:842:ASN:HD21 | 2:B:844:SER:HB2 | 1.63 | 0.63 |
| 10:J:9:SER:OG | 10:J:48:ARG:NH2 | 2.30 | 0.63 |
| 2:B:1104:HIS:HB2 | 2:B:1122:ARG:HD2 | 1.80 | 0.63 |
| 1:A:994:GLN:HE22 | 1:A:1023:ARG:NE | 1.95 | 0.63 |
| 8:H:101:ALA:HB2 | 8:H:116:TYR:CE2 | 2.33 | 0.63 |
| 1:A:84:ILE:HG23 | 1:A:239:LEU:HB3 | 1.80 | 0.63 |
| 2:B:221:ASN:OD1 | 2:B:242:SER:HA | 1.98 | 0.63 |
| 1:A:475:THR:HG22 | 1:A:476:SER:N | 2.12 | 0.63 |
| 6:F:109:VAL:HG21 | 6:F:124:GLU:HA | 1.80 | 0.63 |
| 2:B:525:ALA:O | 2:B:527:THR:HG22 | 1.99 | 0.63 |
| 8:H:31:THR:O | 8:H:32:THR:CB | 2.47 | 0.63 |
| 1:A:108:MET:O | 1:A:109:HIS:HB2 | 1.99 | 0.63 |
| 1:A:354:SER:HA | 1:A:482:PHE:CD2 | 2.34 | 0.63 |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:N | 2.12 | 0.63 |
| 5:E:96:PHE:CZ | 5:E:100:ILE:HD11 | 2.32 | 0.63 |
| 1:A:268:ASP:HB3 | 1:A:299:HIS:ND1 | 2.14 | 0.63 |
| 3:C:114:TYR:CD2 | 3:C:140:ASN:HB3 | 2.32 | 0.63 |
| 2:B:373:ARG:NE | 2:B:567:GLU:OE2 | 2.29 | 0.63 |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:CD | 2.29 | 0.63 |
| 6:F:135:ARG:HG2 | 6:F:137:TYR:CE1 | 2.34 | 0.63 |
| 1:A:1317:MET:HA | 1:A:1322:ILE:HD11 | 1.81 | 0.63 |
| 1:A:418:SER:O | 1:A:420:ARG:N | 2.32 | 0.63 |
| 2:B:1201:LYS:O | 2:B:1205:GLN:HG3 | 1.97 | 0.63 |
| 1:A:982:THR:HG22 | 1:A:984:LYS:H | 1.64 | 0.63 |
| 2:B:788:ARG:NH1 | 2:B:790:ASP:OD1 | 2.31 | 0.63 |
| 12:L:40:LEU:HD13 | 12:L:44:ASP:CG | 2.19 | 0.63 |
| 1:A:1402:PHE:CD2 | 1:A:1403:GLU:HG3 | 2.33 | 0.63 |
| 6:F:111:LEU:H | 6:F:111:LEU:HD12 | 1.61 | 0.62 |
| 4:D:7:UNK:CA | 7:G:8:UNK:CA | 2.76 | 0.62 |
| 8:H:12:VAL:HA | 8:H:28:ALA:CB | 2.28 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1106:ARG:HD2 | 2:B:1126:GLY:O | 1.99 | 0.62 |
| 1:A:33:ALA:O | 1:A:83:HIS:HB3 | 1.99 | 0.62 |
| 6:F:97:ARG:O | 6:F:101:ILE:HG13 | 1.99 | 0.62 |
| 1:A:821:ARG:HG3 | 1:A:825:ILE:HD11 | 1.81 | 0.62 |
| 1:A:73:GLY:O | 1:A:75:ASN:N | 2.32 | 0.62 |
| 2:B:914:LYS:HB3 | 2:B:937:ALA:O | 1.98 | 0.62 |
| 2:B:616:ILE:N | 2:B:616:ILE:HD12 | 2.14 | 0.62 |
| 2:B:446:LEU:O | 2:B:447:ALA:HB3 | 1.97 | 0.62 |
| 2:B:208:SER:OG | 2:B:210:LYS:HD3 | 1.99 | 0.62 |
| 2:B:25:ILE:HG22 | 2:B:26:THR:H | 1.65 | 0.62 |
| 1:A:871:ASP:HB3 | 5:E:204:THR:HG22 | 1.82 | 0.62 |
| 1:A:1054:LEU:O | 1:A:1057:VAL:HG23 | 1.99 | 0.62 |
| 12:L:55:ILE:HG13 | 12:L:56:LEU:H | 1.63 | 0.62 |
| 3:C:173:ALA:O | 3:C:174:ALA:HB3 | 2.00 | 0.62 |
| 1:A:915:SER:O | 1:A:919:ILE:HG13 | 2.00 | 0.62 |
| 9:I:7:CYS:HB2 | 9:I:29:CYS:HB2 | 1.81 | 0.62 |
| 1:A:1436:ILE:HB | 2:B:1144:ALA:HB2 | 1.80 | 0.62 |
| 5:E:96:PHE:O | 5:E:100:ILE:HG13 | 1.98 | 0.62 |
| 1:A:445:ASN:HB2 | 1:A:454:SER:O | 2.00 | 0.62 |
| 2:B:195:CYS:HB3 | 2:B:782:LEU:HD22 | 1.81 | 0.62 |
| 8:H:123:MET:HE3 | 8:H:142:LEU:CD2 | 2.29 | 0.62 |
| 2:B:1072:MET:CE | 2:B:1085:ILE:HB | 2.28 | 0.62 |
| 1:A:689:LYS:O | 1:A:693:VAL:HG23 | 2.00 | 0.62 |
| 1:A:898:ARG:HB2 | 1:A:933:TYR:CE1 | 2.35 | 0.62 |
| 1:A:328:ARG:O | 1:A:335:ARG:HG2 | 1.99 | 0.62 |
| 1:A:672:ASP:OD1 | 1:A:674:PRO:HD2 | 2.00 | 0.62 |
| 1:A:1212:VAL:O | 1:A:1216:ILE:HG13 | 1.99 | 0.62 |
| 1:A:88:LYS:HD2 | 1:A:293:GLU:CD | 2.20 | 0.62 |
| 2:B:1051:THR:CG2 | 2:B:1053:GLU:H | 1.93 | 0.62 |
| 1:A:871:ASP:HB3 | 5:E:204:THR:CG2 | 2.30 | 0.62 |
| 5:E:100:ILE:HG23 | 5:E:105:PHE:HB2 | 1.80 | 0.62 |
| 2:B:787:VAL:O | 2:B:787:VAL:HG12 | 2.00 | 0.62 |
| 2:B:446:LEU:O | 2:B:447:ALA:CB | 2.48 | 0.62 |
| 2:B:1034:VAL:HG23 | 2:B:1059:LEU:HB2 | 1.80 | 0.62 |
| 2:B:39:ARG:HE | 2:B:665:GLU:HG2 | 1.65 | 0.62 |
| 10:J:3:VAL:HG21 | 10:J:18:TRP:CG | 2.34 | 0.62 |
| 1:A:590:ARG:HB3 | 1:A:605:MET:H | 1.63 | 0.62 |
| 6:F:101:ILE:HD12 | 6:F:121:ALA:HB2 | 1.82 | 0.62 |
| 1:A:871:ASP:OD2 | 5:E:204:THR:HG23 | 1.99 | 0.61 |
| 2:B:496:ARG:HH11 | 2:B:539:LEU:HB2 | 1.62 | 0.61 |
| 1:A:778:GLY:HA3 | 2:B:516:ASN:HB2 | 1.80 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:L:51:CYS:HB2 | 12:L:53:HIS:CD2 | 2.35 | 0.61 |
| 1:A:1444:MET:HE1 | 6:F:135:ARG:NE | 2.15 | 0.61 |
| 1:A:148:CYS:O | 1:A:168:GLY:HA2 | 1.99 | 0.61 |
| 5:E:178:ILE:HG23 | 5:E:214:CYS:HA | 1.81 | 0.61 |
| 2:B:1187:ASN:OD1 | 2:B:1190:ASP:HB3 | 1.99 | 0.61 |
| 1:A:1021:LEU:O | 1:A:1025:ARG:HG2 | 2.00 | 0.61 |
| 2:B:211:VAL:O | 2:B:480:SER:HA | 2.00 | 0.61 |
| 6:F:111:LEU:H | 6:F:111:LEU:CD1 | 2.12 | 0.61 |
| 1:A:503:GLN:HE21 | 6:F:90:ARG:HH21 | 1.47 | 0.61 |
| 1:A:736:ASN:O | 1:A:737:LEU:C | 2.38 | 0.61 |
| 5:E:93:MET:O | 5:E:97:VAL:HG23 | 2.00 | 0.61 |
| 2:B:913:GLY:HA2 | 2:B:938:SER:HB3 | 1.81 | 0.61 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:HG12 | 1.81 | 0.61 |
| 1:A:567:LYS:HZ2 | 8:H:46:LEU:HB2 | 1.64 | 0.61 |
| 3:C:166:GLU:HA | 11:K:6:ARG:HB3 | 1.82 | 0.61 |
| 5:E:78:LEU:C | 5:E:78:LEU:HD23 | 2.20 | 0.61 |
| 6:F:109:VAL:HG23 | 6:F:124:GLU:HG2 | 1.82 | 0.61 |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:N | 2.01 | 0.61 |
| 1:A:961:ARG:O | 1:A:965:GLN:HG3 | 2.00 | 0.61 |
| 3:C:235:VAL:HG21 | 10:J:6:ARG:HH21 | 1.65 | 0.61 |
| 3:C:123:ASN:HD22 | 3:C:125:MET:HG2 | 1.66 | 0.61 |
| 2:B:512:ARG:NH2 | 2:B:535:LEU:CD1 | 2.62 | 0.61 |
| 2:B:1002:THR:HG23 | 2:B:1004:GLU:H | 1.64 | 0.61 |
| 1:A:549:MET:SD | 1:A:577:ILE:CD1 | 2.87 | 0.61 |
| 1:A:1364:ASN:HD22 | 1:A:1364:ASN:C | 2.04 | 0.61 |
| 10:J:64:ASN:HB3 | 10:J:65:PRO:CD | 2.29 | 0.61 |
| 2:B:582:VAL:HG22 | 2:B:626:ILE:HB | 1.82 | 0.61 |
| 1:A:567:LYS:CG | 1:A:568:PRO:HD2 | 2.31 | 0.61 |
| 1:A:1437:GLY:HA3 | 6:F:88:TYR:CD2 | 2.36 | 0.61 |
| 2:B:198:ASP:OD1 | 2:B:485:ARG:NH2 | 2.33 | 0.61 |
| 2:B:185:THR:HG23 | 2:B:188:ASP:OD2 | 2.01 | 0.61 |
| 1:A:1192:LEU:HD22 | 1:A:1239:ARG:NH2 | 2.16 | 0.61 |
| 1:A:528:LEU:O | 1:A:531:ILE:HG22 | 2.01 | 0.61 |
| 1:A:506:ALA:HB1 | 1:A:508:PRO:HD2 | 1.83 | 0.61 |
| 6:F:138:LEU:HB3 | 6:F:139:PRO:HD2 | 1.83 | 0.61 |
| 12:L:70:ARG:HG2 | 12:L:70:ARG:HH11 | 1.66 | 0.61 |
| 1:A:1132:LYS:O | 1:A:1135:ARG:HB3 | 2.01 | 0.61 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:CD1 | 2.30 | 0.61 |
| 2:B:57:TYR:CD1 | 2:B:57:TYR:N | 2.68 | 0.61 |
| 1:A:789:LYS:HG3 | 9:I:67:THR:HB | 1.83 | 0.61 |
| 12:L:26:THR:O | 12:L:27:LEU:HB3 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:L:48:CYS:SG | 12:L:49:LYS:N | 2.70 | 0.61 |
| 2:B:1169:MET:HE1 | 2:B:1201:LYS:O | 2.00 | 0.60 |
| 3:C:49:VAL:HG21 | 3:C:67:LEU:HD12 | 1.83 | 0.60 |
| 5:E:29:PHE:HB2 | 5:E:65:THR:HG22 | 1.83 | 0.60 |
| 3:C:46:ILE:HA | 3:C:159:ALA:HA | 1.82 | 0.60 |
| 1:A:244:PRO:CG | 1:A:245:PRO:HD3 | 2.27 | 0.60 |
| 2:B:778:MET:CE | 2:B:1094:ARG:HD3 | 2.32 | 0.60 |
| 5:E:78:LEU:HD23 | 5:E:79:TRP:N | 2.16 | 0.60 |
| 1:A:1293:SER:OG | 1:A:1294:PRO:HD2 | 2.01 | 0.60 |
| 11:K:63:VAL:O | 11:K:63:VAL:CG2 | 2.49 | 0.60 |
| 2:B:114:PRO:HB3 | 2:B:174:LEU:HD11 | 1.82 | 0.60 |
| 2:B:463:THR:HG22 | 2:B:465:ASN:HD22 | 1.66 | 0.60 |
| 1:A:565:ILE:CG2 | 1:A:567:LYS:HG2 | 2.31 | 0.60 |
| 1:A:855:THR:CG2 | 1:A:857:ARG:HG3 | 2.30 | 0.60 |
| 2:B:839:MET:HE3 | 2:B:1010:LEU:CD1 | 2.31 | 0.60 |
| 2:B:686:ASN:C | 2:B:688:GLY:H | 2.04 | 0.60 |
| 11:K:90:ALA:O | 11:K:94:ILE:HG13 | 2.01 | 0.60 |
| 9:I:5:ARG:HD3 | 9:I:36:GLU:OE2 | 2.01 | 0.60 |
| 2:B:1051:THR:HG22 | 2:B:1052:VAL:N | 2.17 | 0.60 |
| 2:B:1039:GLY:HA2 | 10:J:51:LEU:CD2 | 2.31 | 0.60 |
| 2:B:744:HIS:CD2 | 2:B:746:SER:H | 2.14 | 0.60 |
| 2:B:549:THR:HB | 2:B:628:THR:CG2 | 2.30 | 0.60 |
| 1:A:1208:THR:O | 1:A:1212:VAL:HG23 | 2.01 | 0.60 |
| 1:A:779:PHE:CZ | 2:B:517:THR:HA | 2.37 | 0.60 |
| 2:B:299:GLU:OE1 | 2:B:571:PRO:HG2 | 2.01 | 0.60 |
| 1:A:663:SER:OG | 1:A:664:THR:N | 2.34 | 0.60 |
| 8:H:15:VAL:HG22 | 8:H:26:ILE:HG12 | 1.83 | 0.60 |
| 2:B:975:GLN:HG2 | 2:B:976:ILE:H | 1.67 | 0.60 |
| 1:A:322:VAL:O | 1:A:323:LYS:HG3 | 2.01 | 0.60 |
| 1:A:306:ASN:OD1 | 1:A:324:SER:HB3 | 2.01 | 0.60 |
| 11:K:49:GLU:HG3 | 11:K:94:ILE:HG12 | 1.83 | 0.60 |
| 1:A:709:THR:OG1 | 1:A:712:GLU:HG3 | 2.00 | 0.60 |
| 2:B:479:VAL:HG12 | 2:B:480:SER:N | 2.17 | 0.60 |
| 5:E:47:CYS:HA | 5:E:53:PRO:HA | 1.83 | 0.60 |
| 10:J:1:MET:N | 10:J:56:LEU:HB2 | 2.17 | 0.60 |
| 1:A:338:GLY:HA2 | 2:B:1129:ARG:NH2 | 2.10 | 0.60 |
| 1:A:1223:ASP:HA | 1:A:1243:VAL:CG1 | 2.32 | 0.60 |
| 1:A:418:SER:O | 1:A:419:LYS:C | 2.40 | 0.60 |
| 1:A:1042:PHE:HE2 | 1:A:1046:LEU:HD11 | 1.67 | 0.60 |
| 1:A:68:GLN:HE22 | 1:A:80:HIS:CB | 2.15 | 0.60 |
| 1:A:1115:SER:O | 1:A:1329:THR:HG23 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:121:ASN:ND2 | 2:B:121:ASN:N | 2.50 | 0.60 |
| 2:B:995:ARG:NH1 | 2:B:995:ARG:HB2 | 2.16 | 0.60 |
| 1:A:97:ALA:HA | 1:A:100:LYS:HE3 | 1.84 | 0.60 |
| 2:B:1171:VAL:CG1 | 2:B:1191:ILE:HD13 | 2.32 | 0.60 |
| 1:A:567:LYS:O | 1:A:569:LYS:N | 2.35 | 0.59 |
| 1:A:886:ILE:CD1 | 1:A:943:LEU:HB3 | 2.31 | 0.59 |
| 1:A:337:ARG:CZ | 1:A:839:ARG:NH1 | 2.64 | 0.59 |
| 2:B:211:VAL:CG2 | 2:B:483:LEU:HD13 | 2.32 | 0.59 |
| 1:A:1158:PRO:HB3 | 1:A:1241:ARG:NH1 | 2.17 | 0.59 |
| 8:H:139:ASN:O | 8:H:140:ALA:HB2 | 2.02 | 0.59 |
| 1:A:1402:PHE:CE2 | 1:A:1403:GLU:HG3 | 2.37 | 0.59 |
| 2:B:666:TYR:C | 2:B:668:ASP:H | 2.06 | 0.59 |
| 2:B:1117:GLN:HG3 | 2:B:1156:ASP:OD1 | 2.02 | 0.59 |
| 2:B:1159:ARG:CD | 2:B:1193:GLN:HE21 | 2.15 | 0.59 |
| 9:I:8:ARG:HG3 | 9:I:9:ASP:N | 2.15 | 0.59 |
| 1:A:1149:ALA:HB2 | 9:I:47:GLU:HA | 1.84 | 0.59 |
| 2:B:803:LEU:H | 2:B:822:ASN:HD21 | 1.48 | 0.59 |
| 1:A:231:PRO:HA | 1:A:234:MET:HE2 | 1.85 | 0.59 |
| 1:A:444:PHE:HB3 | 1:A:458:HIS:HD2 | 1.67 | 0.59 |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:N | 2.17 | 0.59 |
| 2:B:1174:LYS:HB2 | 2:B:1179:GLN:O | 2.02 | 0.59 |
| 1:A:756:ILE:HG22 | 1:A:757:ASN:N | 2.17 | 0.59 |
| 1:A:151:ASP:HA | 1:A:162:VAL:O | 2.02 | 0.59 |
| 1:A:239:LEU:HD12 | 1:A:240:PRO:HD2 | 1.84 | 0.59 |
| 1:A:824:LEU:O | 1:A:827:THR:HB | 2.00 | 0.59 |
| 2:B:405:ARG:NH1 | 2:B:632:ARG:HG2 | 2.17 | 0.59 |
| 1:A:107:CYS:HB2 | 1:A:114:LEU:CD2 | 2.33 | 0.59 |
| 1:A:1399:ARG:CB | 1:A:1408:ILE:HD13 | 2.28 | 0.59 |
| 9:I:15:TYR:O | 9:I:27:PHE:HA | 2.02 | 0.59 |
| 9:I:85:PHE:CD1 | 9:I:99:LEU:HD22 | 2.37 | 0.59 |
| 1:A:93:VAL:HG11 | 1:A:308:ILE:CD1 | 2.33 | 0.59 |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:N | 2.18 | 0.59 |
| 1:A:76:GLU:O | 1:A:76:GLU:HG3 | 2.02 | 0.59 |
| 3:C:166:GLU:CG | 11:K:10:PHE:HZ | 2.14 | 0.59 |
| 11:K:49:GLU:HG3 | 11:K:94:ILE:CG1 | 2.33 | 0.59 |
| 9:I:111:THR:CG2 | 9:I:113:ASP:HB2 | 2.33 | 0.59 |
| 1:A:840:ARG:HB3 | 1:A:1384:VAL:HG12 | 1.85 | 0.59 |
| 1:A:896:ARG:NH2 | 1:A:1030:ARG:HH21 | 2.00 | 0.59 |
| 1:A:511:ILE:HG12 | 1:A:521:MET:HE3 | 1.85 | 0.59 |
| 8:H:24:CYS:HB2 | 8:H:44:VAL:HG21 | 1.85 | 0.59 |
| 8:H:84:ALA:HA | 8:H:87:ARG:CG | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:217:ARG:NH1 | 2:B:407:ASP:OD1 | 2.35 | 0.59 |
| 2:B:90:ILE:HD12 | 2:B:432:MET:SD | 2.42 | 0.59 |
| 1:A:1004:ASN:ND2 | 5:E:167:ARG:HD2 | 2.18 | 0.59 |
| 2:B:519:TRP:C | 2:B:519:TRP:CD1 | 2.76 | 0.59 |
| 1:A:469:ARG:NH2 | 2:B:976:ILE:HD13 | 2.18 | 0.59 |
| 2:B:130:VAL:HG12 | 2:B:131:ASP:H | 1.67 | 0.59 |
| 8:H:89:LEU:C | 8:H:91:ASP:N | 2.55 | 0.59 |
| 1:A:1385:THR:HG22 | 1:A:1386:ARG:H | 1.68 | 0.59 |
| 6:F:81:THR:HG22 | 6:F:82:THR:N | 2.18 | 0.59 |
| 1:A:57:ARG:O | 1:A:68:GLN:HG3 | 2.03 | 0.59 |
| 1:A:68:GLN:HE22 | 1:A:80:HIS:HB3 | 1.67 | 0.59 |
| 1:A:1336:MET:CE | 1:A:1381:LEU:HG | 2.33 | 0.59 |
| 6:F:127:GLU:O | 6:F:129:LYS:HG3 | 2.03 | 0.59 |
| 2:B:642:ASP:O | 2:B:644:GLU:N | 2.36 | 0.58 |
| 1:A:1018:PHE:O | 1:A:1021:LEU:HB3 | 2.03 | 0.58 |
| 1:A:225:ASN:ND2 | 1:A:227:VAL:HB | 2.18 | 0.58 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:CG1 | 2.33 | 0.58 |
| 8:H:109:LYS:NZ | 8:H:109:LYS:HB2 | 2.18 | 0.58 |
| 10:J:48:ARG:HE | 10:J:49:MET:CE | 2.16 | 0.58 |
| 2:B:912:ILE:HD11 | 2:B:966:VAL:HG23 | 1.84 | 0.58 |
| 11:K:47:ARG:HD3 | 11:K:59:ALA:O | 2.04 | 0.58 |
| 2:B:1102:LYS:O | 2:B:1104:HIS:N | 2.32 | 0.58 |
| 2:B:860:MET:HG2 | 2:B:861:ASP:N | 2.18 | 0.58 |
| 2:B:779:GLY:HA2 | 2:B:796:LEU:HB2 | 1.85 | 0.58 |
| 2:B:1201:LYS:HE2 | 2:B:1205:GLN:NE2 | 2.18 | 0.58 |
| 1:A:596:THR:O | 1:A:598:LEU:N | 2.36 | 0.58 |
| 1:A:1342:GLU:HG3 | 5:E:198:ILE:HG21 | 1.86 | 0.58 |
| 1:A:1325:THR:O | 5:E:148:GLU:HB2 | 2.04 | 0.58 |
| 1:A:567:LYS:NZ | 8:H:95:TYR:CE1 | 2.71 | 0.58 |
| 2:B:23:ALA:O | 2:B:654:ARG:HB3 | 2.04 | 0.58 |
| 2:B:46:GLN:O | 2:B:408:LEU:HD23 | 2.03 | 0.58 |
| 1:A:90:VAL:HG11 | 1:A:297:GLN:HA | 1.84 | 0.58 |
| 1:A:1364:ASN:ND2 | 1:A:1364:ASN:C | 2.56 | 0.58 |
| 2:B:983:ARG:HD2 | 2:B:1091:TYR:HB3 | 1.85 | 0.58 |
| 1:A:44:THR:HG22 | 1:A:44:THR:O | 2.02 | 0.58 |
| 1:A:1295:THR:HG23 | 1:A:1297:GLU:OE1 | 2.03 | 0.58 |
| 11:K:46:ILE:HG22 | 11:K:50:LEU:HD12 | 1.86 | 0.58 |
| 2:B:913:GLY:HA2 | 2:B:938:SER:CB | 2.32 | 0.58 |
| 3:C:37:MET:HG2 | 3:C:243:VAL:CG1 | 2.34 | 0.58 |
| 5:E:61:GLN:HB2 | 5:E:79:TRP:CE3 | 2.38 | 0.58 |
| 11:K:55:LYS:HB3 | 11:K:81:TYR:CD1 | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:219:PHE:O | 1:A:222:LEU:N | 2.33 | 0.58 |
| 9:I:16:PRO:HB3 | 9:I:27:PHE:CE2 | 2.38 | 0.58 |
| 5:E:157:SER:C | 5:E:159:ASP:H | 2.07 | 0.58 |
| 3:C:244:VAL:O | 3:C:248:ILE:HG13 | 2.03 | 0.58 |
| 1:A:1308:THR:HG21 | 1:A:1310:GLY:O | 2.04 | 0.58 |
| 2:B:287:ARG:NH1 | 2:B:324:ILE:O | 2.37 | 0.58 |
| 2:B:1077:THR:CG2 | 2:B:1079:LYS:HB2 | 2.34 | 0.58 |
| 1:A:353:ILE:HG22 | 1:A:468:PHE:HB2 | 1.85 | 0.58 |
| 8:H:81:PRO:CB | 8:H:82:PRO:CD | 2.81 | 0.58 |
| 1:A:260:ASP:OD1 | 1:A:261:ASP:N | 2.37 | 0.58 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:N | 2.02 | 0.58 |
| 1:A:93:VAL:HG22 | 1:A:301:ALA:HA | 1.85 | 0.58 |
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:HB3 | 1.67 | 0.58 |
| 1:A:31:SER:OG | 1:A:83:HIS:HB2 | 2.02 | 0.58 |
| 1:A:1332:PHE:N | 1:A:1332:PHE:CD2 | 2.72 | 0.58 |
| 1:A:86:LEU:HA | 1:A:273:ASN:OD1 | 2.02 | 0.58 |
| 2:B:205:ILE:N | 2:B:205:ILE:HD12 | 2.19 | 0.58 |
| 1:A:76:GLU:O | 1:A:76:GLU:CG | 2.52 | 0.58 |
| 6:F:87:LYS:HE2 | 6:F:88:TYR:CZ | 2.39 | 0.58 |
| 1:A:1400:CYS:SG | 1:A:1409:LEU:HG | 2.44 | 0.58 |
| 1:A:225:ASN:HD22 | 1:A:227:VAL:HB | 1.68 | 0.58 |
| 1:A:101:LYS:O | 1:A:105:CYS:HB2 | 2.04 | 0.58 |
| 11:K:33:ILE:HD13 | 11:K:87:LEU:HD22 | 1.85 | 0.58 |
| 2:B:23:ALA:HB1 | 2:B:24:PRO:HD2 | 1.85 | 0.57 |
| 2:B:980:PHE:CE1 | 2:B:990:ILE:HD11 | 2.39 | 0.57 |
| 1:A:385:ILE:HG22 | 1:A:386:ASP:N | 2.18 | 0.57 |
| 2:B:25:ILE:HG22 | 2:B:29:ASP:CB | 2.34 | 0.57 |
| 1:A:1155:ASP:OD2 | 1:A:1161:THR:HG23 | 2.04 | 0.57 |
| 1:A:41:MET:HB3 | 1:A:48:ALA:O | 2.04 | 0.57 |
| 5:E:61:GLN:HB2 | 5:E:79:TRP:HE3 | 1.69 | 0.57 |
| 6:F:111:LEU:N | 6:F:111:LEU:CD1 | 2.67 | 0.57 |
| 11:K:65:HIS:CD2 | 11:K:67:PHE:HB2 | 2.39 | 0.57 |
| 2:B:806:THR:HB | 2:B:809:MET:HG3 | 1.85 | 0.57 |
| 2:B:756:ILE:O | 2:B:759:PRO:HD3 | 2.04 | 0.57 |
| 1:A:537:ARG:HB2 | 8:H:20:TYR:CE2 | 2.39 | 0.57 |
| 1:A:452:LYS:HB3 | 2:B:1141:HIS:CE1 | 2.40 | 0.57 |
| 2:B:101:MET:HB2 | 2:B:169:ARG:HH12 | 1.69 | 0.57 |
| 2:B:653:VAL:HG22 | 2:B:689:LEU:HB3 | 1.85 | 0.57 |
| 1:A:901:LEU:N | 1:A:926:GLN:NE2 | 2.50 | 0.57 |
| 9:I:47:GLU:OE1 | 9:I:50:THR:HG23 | 2.04 | 0.57 |
| 1:A:1281:ARG:HB2 | 1:A:1309:ASP:HB2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:5:ASN:ND2 | 5:E:52:ARG:HG2 | 2.12 | 0.57 |
| 2:B:803:LEU:N | 2:B:822:ASN:HD21 | 2.02 | 0.57 |
| 1:A:399:HIS:O | 1:A:435:HIS:HD2 | 1.87 | 0.57 |
| 5:E:46:TYR:HA | 5:E:57:MET:SD | 2.43 | 0.57 |
| 1:A:1143:LEU:HD23 | 1:A:1267:MET:HB3 | 1.86 | 0.57 |
| 8:H:24:CYS:SG | 8:H:44:VAL:HG21 | 2.44 | 0.57 |
| 5:E:213:ILE:O | 5:E:213:ILE:HG23 | 2.04 | 0.57 |
| 1:A:882:SER:HA | 1:A:952:ALA:O | 2.05 | 0.57 |
| 1:A:1315:GLU:O | 1:A:1318:THR:HG23 | 2.04 | 0.57 |
| 8:H:12:VAL:HA | 8:H:28:ALA:HB2 | 1.86 | 0.57 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:HD2 | 1.85 | 0.57 |
| 8:H:5:LEU:CD1 | 8:H:135:LEU:HG | 2.34 | 0.57 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:H | 1.69 | 0.57 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:CG1 | 2.33 | 0.57 |
| 1:A:482:PHE:CD1 | 2:B:836:GLU:HB2 | 2.38 | 0.57 |
| 1:A:166:GLY:O | 1:A:167:CYS:HB3 | 2.03 | 0.57 |
| 1:A:337:ARG:CD | 1:A:839:ARG:HH22 | 2.17 | 0.57 |
| 11:K:10:PHE:HD1 | 11:K:11:LEU:HD13 | 1.67 | 0.57 |
| 1:A:1436:ILE:HG22 | 2:B:1142:GLY:HA2 | 1.87 | 0.57 |
| 1:A:1074:GLU:O | 1:A:1076:ALA:N | 2.37 | 0.57 |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:N | 2.13 | 0.57 |
| 1:A:879:GLU:OE2 | 1:A:962:ARG:NH2 | 2.37 | 0.57 |
| 1:A:401:GLY:O | 1:A:435:HIS:CD2 | 2.58 | 0.57 |
| 2:B:1147:LEU:HD22 | 2:B:1151:LEU:CD2 | 2.35 | 0.57 |
| 12:L:49:LYS:O | 12:L:50:ASP:HB2 | 2.03 | 0.57 |
| 1:A:567:LYS:NZ | 8:H:46:LEU:CB | 2.67 | 0.57 |
| 2:B:855:PHE:HZ | 2:B:857:ARG:HH11 | 1.52 | 0.57 |
| 6:F:111:LEU:C | 6:F:113:GLY:H | 2.07 | 0.57 |
| 2:B:429:PHE:HA | 2:B:432:MET:CE | 2.35 | 0.57 |
| 3:C:55:THR:HB | 3:C:152:GLU:H | 1.70 | 0.57 |
| 2:B:848:ARG:NH1 | 10:J:8:PHE:O | 2.35 | 0.57 |
| 3:C:148:ARG:HG3 | 10:J:61:LEU:O | 2.03 | 0.57 |
| 1:A:28:ARG:HG2 | 1:A:83:HIS:CE1 | 2.39 | 0.57 |
| 2:B:311:LEU:HB3 | 9:I:4:PHE:CE2 | 2.40 | 0.57 |
| 8:H:106:GLU:C | 8:H:108:SER:N | 2.57 | 0.57 |
| 3:C:251:LEU:O | 3:C:255:VAL:HG23 | 2.04 | 0.57 |
| 1:A:901:LEU:H | 1:A:926:GLN:HE21 | 1.50 | 0.57 |
| 1:A:40:THR:HG21 | 1:A:259:GLU:OE2 | 2.04 | 0.57 |
| 1:A:414:ASP:O | 1:A:417:TYR:O | 2.22 | 0.57 |
| 2:B:1022:THR:HG23 | 2:B:1022:THR:O | 2.05 | 0.57 |
| 2:B:973:ILE:HG23 | 2:B:974:PRO:HD2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:710:LEU:N | 1:A:710:LEU:HD12 | 2.20 | 0.57 |
| 2:B:955:THR:OG1 | 12:L:55:ILE:HA | 2.04 | 0.57 |
| 1:A:1300:LYS:NZ | 1:A:1300:LYS:HB3 | 2.20 | 0.57 |
| 5:E:46:TYR:CE2 | 5:E:58:MET:HA | 2.40 | 0.57 |
| 8:H:89:LEU:HD22 | 8:H:91:ASP:CG | 2.25 | 0.57 |
| 2:B:1116:ARG:HD2 | 2:B:1198:TYR:CG | 2.40 | 0.57 |
| 3:C:242:GLN:NE2 | 3:C:246:ARG:HE | 2.02 | 0.56 |
| 1:A:1017:LEU:HD23 | 5:E:204:THR:O | 2.05 | 0.56 |
| 2:B:806:THR:OG1 | 2:B:809:MET:HE3 | 2.04 | 0.56 |
| 2:B:979:LYS:HG2 | 2:B:1095:LEU:HD12 | 1.87 | 0.56 |
| 2:B:701:ILE:HD11 | 2:B:703:ILE:HD11 | 1.86 | 0.56 |
| 2:B:980:PHE:HE1 | 2:B:990:ILE:HD11 | 1.70 | 0.56 |
| 1:A:742:ASN:CA | 1:A:745:GLN:HB2 | 2.33 | 0.56 |
| 11:K:51:LEU:HD13 | 11:K:59:ALA:HB3 | 1.86 | 0.56 |
| 8:H:89:LEU:HD22 | 8:H:91:ASP:OD2 | 2.05 | 0.56 |
| 2:B:1180:PHE:O | 2:B:1181:GLU:HB2 | 2.05 | 0.56 |
| 2:B:844:SER:OG | 2:B:996:ARG:N | 2.33 | 0.56 |
| 3:C:229:TYR:N | 3:C:229:TYR:CD1 | 2.74 | 0.56 |
| 8:H:82:PRO:O | 8:H:83:GLN:HB2 | 2.04 | 0.56 |
| 1:A:401:GLY:C | 1:A:435:HIS:CD2 | 2.79 | 0.56 |
| 1:A:511:ILE:HA | 1:A:521:MET:HE3 | 1.87 | 0.56 |
| 2:B:864:LYS:HD3 | 2:B:871:THR:OG1 | 2.05 | 0.56 |
| 3:C:248:ILE:CD1 | 11:K:101:LEU:HD22 | 2.35 | 0.56 |
| 1:A:619:LYS:O | 1:A:623:GLY:N | 2.38 | 0.56 |
| 1:A:556:TRP:CE3 | 1:A:558:GLY:HA2 | 2.41 | 0.56 |
| 2:B:704:ALA:HB1 | 2:B:710:LEU:HD12 | 1.87 | 0.56 |
| 9:I:7:CYS:C | 9:I:8:ARG:O | 2.43 | 0.56 |
| 3:C:258:ILE:O | 3:C:261:ALA:HB3 | 2.04 | 0.56 |
| 6:F:97:ARG:NE | 6:F:124:GLU:OE1 | 2.31 | 0.56 |
| 1:A:69:THR:HB | 2:B:1174:LYS:HE2 | 1.87 | 0.56 |
| 3:C:175:ALA:HB3 | 10:J:43:ARG:NH2 | 2.20 | 0.56 |
| 2:B:522:VAL:HG11 | 2:B:537:LYS:HB3 | 1.86 | 0.56 |
| 3:C:131:HIS:O | 3:C:132:PRO:C | 2.43 | 0.56 |
| 2:B:243:ALA:HA | 2:B:250:PHE:O | 2.05 | 0.56 |
| 6:F:99:LEU:HD12 | 6:F:99:LEU:O | 2.05 | 0.56 |
| 9:I:111:THR:HG22 | 9:I:112:SER:N | 2.19 | 0.56 |
| 2:B:1079:LYS:HA | 3:C:27:LEU:HD21 | 1.87 | 0.56 |
| 1:A:577:ILE:O | 1:A:580:VAL:HG23 | 2.04 | 0.56 |
| 1:A:98:LYS:O | 1:A:102:VAL:HG23 | 2.05 | 0.56 |
| 1:A:185:TRP:CZ3 | 1:A:200:ARG:HG2 | 2.40 | 0.56 |
| 1:A:738:LYS:HZ1 | 3:C:194:GLU:C | 2.09 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:97:MET:HE2 | 8:H:142:LEU:HD23 | 1.86 | 0.56 |
| 1:A:548:ASN:HA | 11:K:60:ALA:HB1 | 1.87 | 0.56 |
| 5:E:195:VAL:HG22 | 5:E:213:ILE:HB | 1.88 | 0.56 |
| 11:K:50:LEU:CD1 | 11:K:73:LEU:HD21 | 2.35 | 0.56 |
| 10:J:1:MET:HG3 | 10:J:60:PHE:HE2 | 1.69 | 0.56 |
| 8:H:97:MET:CE | 8:H:142:LEU:HD23 | 2.35 | 0.56 |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:N | 2.53 | 0.56 |
| 2:B:839:MET:CE | 2:B:980:PHE:HB2 | 2.35 | 0.56 |
| 12:L:26:THR:HG22 | 12:L:27:LEU:N | 2.21 | 0.56 |
| 1:A:974:ASP:HB2 | 8:H:136:LYS:NZ | 2.21 | 0.56 |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:CD1 | 2.41 | 0.56 |
| 2:B:120:ARG:NH1 | 12:L:54:ARG:NH1 | 2.54 | 0.56 |
| 3:C:162:GLY:HA3 | 3:C:170:TRP:CE2 | 2.41 | 0.56 |
| 1:A:849:MET:CE | 1:A:1061:GLY:HA2 | 2.36 | 0.56 |
| 1:A:1365:TYR:O | 1:A:1366:ARG:C | 2.43 | 0.56 |
| 1:A:896:ARG:HD3 | 1:A:897:TYR:HE1 | 1.67 | 0.56 |
| 3:C:99:LEU:HD23 | 3:C:99:LEU:N | 2.20 | 0.56 |
| 1:A:1420:ASP:O | 1:A:1421:CYS:HB2 | 2.04 | 0.56 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N | 2.03 | 0.55 |
| 1:A:1328:TYR:CG | 1:A:1329:THR:N | 2.74 | 0.55 |
| 8:H:6:PHE:HE1 | 8:H:130:ARG:HE | 1.53 | 0.55 |
| 1:A:1342:GLU:HG2 | 5:E:212:ARG:NH1 | 2.20 | 0.55 |
| 2:B:118:ARG:NH2 | 2:B:194:GLU:CD | 2.60 | 0.55 |
| 2:B:864:LYS:N | 2:B:872:GLU:OE1 | 2.39 | 0.55 |
| 1:A:825:ILE:HD12 | 2:B:513:GLN:NE2 | 2.21 | 0.55 |
| 2:B:1171:VAL:HG11 | 2:B:1191:ILE:HD13 | 1.88 | 0.55 |
| 1:A:1096:SER:O | 1:A:1099:PRO:HG2 | 2.05 | 0.55 |
| 1:A:35:ILE:HG12 | 1:A:52:GLY:O | 2.06 | 0.55 |
| 3:C:145:CYS:SG | 3:C:146:LYS:N | 2.79 | 0.55 |
| 2:B:479:VAL:HG12 | 2:B:480:SER:H | 1.72 | 0.55 |
| 2:B:794:ASN:C | 2:B:795:ILE:HD12 | 2.26 | 0.55 |
| 2:B:984:HIS:HB3 | 2:B:1022:THR:OG1 | 2.05 | 0.55 |
| 1:A:92:HIS:HD2 | 1:A:94:GLY:H | 1.53 | 0.55 |
| 2:B:898:LEU:HD22 | 2:B:964:VAL:HG11 | 1.89 | 0.55 |
| 1:A:1261:LYS:HA | 1:A:1264:GLU:HB3 | 1.88 | 0.55 |
| 11:K:61:TYR:HA | 11:K:72:LYS:O | 2.07 | 0.55 |
| 2:B:1159:ARG:CD | 2:B:1193:GLN:HG3 | 2.31 | 0.55 |
| 2:B:780:VAL:HG21 | 10:J:56:LEU:HD13 | 1.88 | 0.55 |
| 3:C:56:THR:CG2 | 3:C:57:VAL:H | 2.09 | 0.55 |
| 1:A:1389:PHE:O | 1:A:1392:SER:HB3 | 2.06 | 0.55 |
| 2:B:34:ILE:O | 2:B:37:PHE:HB3 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:57:TYR:HD1 | 2:B:57:TYR:N | 2.03 | 0.55 |
| 1:A:672:ASP:HB3 | 1:A:675:THR:OG1 | 2.05 | 0.55 |
| 3:C:70:ILE:HD11 | 3:C:144:ILE:HG12 | 1.88 | 0.55 |
| 1:A:838:GLN:O | 1:A:842:VAL:HG23 | 2.06 | 0.55 |
| 1:A:867:ILE:HG22 | 1:A:872:GLY:N | 2.22 | 0.55 |
| 10:J:21:TYR:HA | 10:J:39:LEU:HD11 | 1.89 | 0.55 |
| 2:B:25:ILE:HD11 | 2:B:653:VAL:HB | 1.89 | 0.55 |
| 2:B:93:GLY:N | 2:B:131:ASP:O | 2.37 | 0.55 |
| 1:A:665:GLY:HA3 | 2:B:1086:PHE:CD1 | 2.41 | 0.55 |
| 2:B:361:LEU:N | 2:B:362:PRO:CD | 2.69 | 0.55 |
| 1:A:1111:MET:CE | 1:A:1114:PRO:HA | 2.35 | 0.55 |
| 2:B:801:LYS:O | 10:J:52:THR:CG2 | 2.52 | 0.55 |
| 1:A:1222:ASN:O | 1:A:1223:ASP:HB3 | 2.06 | 0.55 |
| 1:A:885:THR:O | 1:A:885:THR:HG22 | 2.05 | 0.55 |
| 1:A:885:THR:O | 1:A:940:ARG:HG3 | 2.07 | 0.55 |
| 2:B:556:THR:HG22 | 2:B:557:PHE:N | 2.20 | 0.55 |
| 1:A:517:ASN:ND2 | 1:A:1362:TYR:HE2 | 2.05 | 0.55 |
| 2:B:1051:THR:CG2 | 2:B:1052:VAL:N | 2.70 | 0.55 |
| 1:A:23:SER:HB3 | 1:A:233:TRP:CE2 | 2.41 | 0.55 |
| 2:B:566:LEU:HD22 | 2:B:586:TRP:O | 2.06 | 0.55 |
| 6:F:109:VAL:HG13 | 6:F:127:GLU:OE1 | 2.07 | 0.55 |
| 8:H:17:PRO:HB3 | 8:H:24:CYS:SG | 2.47 | 0.55 |
| 9:I:111:THR:CG2 | 9:I:112:SER:N | 2.69 | 0.55 |
| 12:L:32:ALA:HB3 | 12:L:55:ILE:CD1 | 2.26 | 0.55 |
| 9:I:7:CYS:O | 9:I:8:ARG:O | 2.24 | 0.55 |
| 1:A:15:LYS:HD2 | 2:B:1220:ARG:HE | 1.72 | 0.55 |
| 1:A:463:ILE:HD11 | 1:A:469:ARG:HG3 | 1.89 | 0.55 |
| 2:B:130:VAL:CG2 | 2:B:167:ILE:HD12 | 2.34 | 0.55 |
| 2:B:28:GLU:CD | 2:B:807:ARG:HH22 | 2.10 | 0.55 |
| 1:A:216:VAL:O | 1:A:219:PHE:HB2 | 2.06 | 0.55 |
| 2:B:515:HIS:H | 2:B:518:HIS:CD2 | 2.24 | 0.55 |
| 2:B:63:ILE:HA | 2:B:421:PHE:CE2 | 2.42 | 0.55 |
| 1:A:704:ALA:HB2 | 1:A:710:LEU:CG | 2.23 | 0.55 |
| 2:B:958:GLN:O | 2:B:960:GLY:N | 2.33 | 0.55 |
| 1:A:399:HIS:O | 1:A:435:HIS:CD2 | 2.60 | 0.55 |
| 3:C:248:ILE:HD13 | 11:K:101:LEU:HD22 | 1.89 | 0.55 |
| 1:A:849:MET:HE1 | 1:A:1061:GLY:HA2 | 1.87 | 0.55 |
| 2:B:406:LEU:HD12 | 2:B:545:ILE:HD11 | 1.89 | 0.55 |
| 2:B:308:TRP:CH2 | 9:I:45:ARG:HG2 | 2.42 | 0.55 |
| 1:A:852:TYR:CE2 | 6:F:136:ARG:HG2 | 2.42 | 0.55 |
| 1:A:1116:LEU:O | 1:A:1308:THR:HB | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:168:TYR:HB3 | 5:E:170:LEU:CD2 | 2.36 | 0.55 |
| 1:A:843:LYS:HG3 | 1:A:1402:PHE:HD1 | 1.72 | 0.55 |
| 1:A:50:ILE:C | 1:A:52:GLY:H | 2.09 | 0.55 |
| 2:B:755:ILE:CG2 | 2:B:755:ILE:O | 2.55 | 0.55 |
| 1:A:1308:THR:CG2 | 1:A:1310:GLY:O | 2.55 | 0.54 |
| 2:B:179:CYS:SG | 2:B:181:LEU:HB2 | 2.47 | 0.54 |
| 5:E:176:PRO:HD2 | 5:E:211:TYR:O | 2.07 | 0.54 |
| 5:E:197:LYS:HG3 | 5:E:211:TYR:CE2 | 2.42 | 0.54 |
| 8:H:89:LEU:O | 8:H:91:ASP:N | 2.37 | 0.54 |
| 1:A:339:ASN:O | 1:A:343:LYS:HG2 | 2.07 | 0.54 |
| 2:B:566:LEU:HD13 | 2:B:588:GLY:CA | 2.37 | 0.54 |
| 2:B:195:CYS:CB | 2:B:782:LEU:HD22 | 2.37 | 0.54 |
| 2:B:429:PHE:HA | 2:B:432:MET:HE2 | 1.89 | 0.54 |
| 9:I:2:THR:HG22 | 9:I:2:THR:O | 2.07 | 0.54 |
| 1:A:741:ASN:ND2 | 1:A:743:VAL:H | 2.05 | 0.54 |
| 1:A:646:PHE:O | 1:A:650:GLN:HG3 | 2.07 | 0.54 |
| 1:A:122:MET:O | 1:A:126:LEU:HG | 2.07 | 0.54 |
| 8:H:59:ILE:HG22 | 8:H:60:ALA:N | 2.21 | 0.54 |
| 1:A:875:ALA:HB2 | 1:A:1366:ARG:HD2 | 1.88 | 0.54 |
| 1:A:590:ARG:O | 1:A:591:PHE:HB2 | 2.08 | 0.54 |
| 2:B:680:THR:HG22 | 2:B:681:TRP:H | 1.72 | 0.54 |
| 1:A:89:PRO:O | 1:A:204:THR:HG21 | 2.07 | 0.54 |
| 1:A:1073:GLY:O | 1:A:1076:ALA:HB3 | 2.07 | 0.54 |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:CB | 2.37 | 0.54 |
| 1:A:821:ARG:O | 1:A:822:GLU:C | 2.46 | 0.54 |
| 1:A:556:TRP:CD2 | 1:A:558:GLY:HA2 | 2.42 | 0.54 |
| 1:A:350:ARG:HB2 | 1:A:488:ASN:OD1 | 2.08 | 0.54 |
| 5:E:153:HIS:CE1 | 5:E:184:VAL:HG11 | 2.43 | 0.54 |
| 12:L:63:ARG:O | 12:L:64:LEU:O | 2.24 | 0.54 |
| 1:A:1339:LEU:HD13 | 5:E:147:HIS:CD2 | 2.42 | 0.54 |
| 2:B:783:THR:HA | 10:J:60:PHE:HE1 | 1.72 | 0.54 |
| 3:C:13:ALA:O | 11:K:114:LEU:HD13 | 2.08 | 0.54 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:CD1 | 2.37 | 0.54 |
| 1:A:451:HIS:CE1 | 1:A:1074:GLU:HG3 | 2.42 | 0.54 |
| 2:B:784:ASN:ND2 | 2:B:788:ARG:HD2 | 2.23 | 0.54 |
| 2:B:1034:VAL:HG12 | 2:B:1035:ALA:N | 2.23 | 0.54 |
| 5:E:195:VAL:HG22 | 5:E:213:ILE:CB | 2.36 | 0.54 |
| 1:A:809:THR:O | 1:A:810:PRO:C | 2.46 | 0.54 |
| 1:A:1116:LEU:H | 1:A:1308:THR:HG22 | 1.72 | 0.54 |
| 1:A:963:ILE:HD12 | 1:A:1049:ILE:HG12 | 1.88 | 0.54 |
| 5:E:46:TYR:CD2 | 5:E:58:MET:HG2 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1205:LYS:O | 1:A:1207:LEU:N | 2.41 | 0.54 |
| 6:F:107:VAL:HG12 | 6:F:109:VAL:H | 1.72 | 0.54 |
| 1:A:1225:PHE:CE2 | 1:A:1227:ILE:HD11 | 2.43 | 0.54 |
| 8:H:84:ALA:HA | 8:H:87:ARG:HG3 | 1.88 | 0.54 |
| 3:C:101:LEU:HD13 | 3:C:118:LEU:HD23 | 1.88 | 0.54 |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:C | 2.28 | 0.54 |
| 6:F:72:LYS:N | 6:F:142:SER:HA | 2.22 | 0.54 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CE2 | 2.42 | 0.54 |
| 1:A:515:GLN:HG3 | 1:A:516:SER:N | 2.22 | 0.54 |
| 2:B:292:ILE:H | 2:B:293:PRO:HD2 | 1.73 | 0.54 |
| 3:C:242:GLN:HE21 | 3:C:246:ARG:HE | 1.54 | 0.54 |
| 5:E:61:GLN:NE2 | 5:E:105:PHE:CE2 | 2.71 | 0.54 |
| 2:B:542:MET:HE2 | 2:B:747:MET:HE2 | 1.89 | 0.54 |
| 1:A:443:LEU:HD13 | 1:A:455:MET:HE1 | 1.89 | 0.54 |
| 3:C:183:TRP:CZ2 | 3:C:207:CYS:HB3 | 2.42 | 0.54 |
| 2:B:43:LEU:HD13 | 2:B:812:LEU:CD2 | 2.38 | 0.54 |
| 1:A:1366:ARG:O | 1:A:1369:ALA:HB3 | 2.08 | 0.54 |
| 2:B:640:VAL:O | 2:B:641:GLU:C | 2.46 | 0.54 |
| 3:C:238:ILE:HG23 | 3:C:242:GLN:HB2 | 1.89 | 0.54 |
| 1:A:533:LYS:O | 1:A:535:THR:N | 2.40 | 0.54 |
| 2:B:102:VAL:HG22 | 2:B:112:LEU:HD22 | 1.88 | 0.54 |
| 1:A:367:PRO:HB3 | 1:A:465:TYR:O | 2.08 | 0.54 |
| 1:A:738:LYS:HB2 | 1:A:740:LEU:HG | 1.89 | 0.54 |
| 2:B:898:LEU:CD2 | 2:B:964:VAL:HG11 | 2.38 | 0.54 |
| 2:B:758:PHE:C | 2:B:760:ASP:H | 2.10 | 0.54 |
| 1:A:710:LEU:H | 1:A:710:LEU:CD1 | 2.19 | 0.54 |
| 2:B:120:ARG:HE | 2:B:955:THR:CG2 | 2.20 | 0.54 |
| 1:A:356:ASP:OD2 | 11:K:65:HIS:HE1 | 1.91 | 0.54 |
| 2:B:288:ALA:HB1 | 2:B:331:LEU:CD1 | 2.38 | 0.54 |
| 2:B:43:LEU:HD13 | 2:B:812:LEU:HD23 | 1.90 | 0.54 |
| 1:A:337:ARG:NE | 1:A:839:ARG:NH2 | 2.55 | 0.54 |
| 2:B:864:LYS:HG3 | 2:B:865:LYS:N | 2.22 | 0.54 |
| 1:A:845:LEU:N | 1:A:845:LEU:HD23 | 2.22 | 0.54 |
| 12:L:60:ARG:CG | 12:L:61:THR:H | 1.94 | 0.53 |
| 2:B:287:ARG:CG | 2:B:292:ILE:HA | 2.26 | 0.53 |
| 1:A:154:SER:HB3 | 1:A:162:VAL:HG23 | 1.89 | 0.53 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:HA | 1.90 | 0.53 |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:O | 2.07 | 0.53 |
| 2:B:484:ASN:ND2 | 2:B:486:TYR:CD1 | 2.76 | 0.53 |
| 6:F:114:GLU:OE1 | 6:F:119:ARG:HG3 | 2.08 | 0.53 |
| 6:F:94:LEU:HD21 | 6:F:122:MET:HA | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:36:LEU:HD12 | 10:J:47:ARG:NH1 | 2.23 | 0.53 |
| 10:J:32:GLU:O | 10:J:36:LEU:HG | 2.07 | 0.53 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:N | 2.16 | 0.53 |
| 2:B:549:THR:HB | 2:B:628:THR:HG23 | 1.89 | 0.53 |
| 1:A:444:PHE:HB3 | 1:A:458:HIS:CD2 | 2.43 | 0.53 |
| 2:B:1169:MET:HE3 | 2:B:1205:GLN:HG2 | 1.90 | 0.53 |
| 2:B:837:ASP:OD1 | 2:B:1020:ARG:NH2 | 2.41 | 0.53 |
| 2:B:956:THR:CG2 | 2:B:960:GLY:HA2 | 2.38 | 0.53 |
| 1:A:1375:MET:HG2 | 1:A:1382:THR:O | 2.08 | 0.53 |
| 1:A:233:TRP:C | 1:A:235:ILE:N | 2.60 | 0.53 |
| 1:A:898:ARG:HD2 | 1:A:899:VAL:H | 1.73 | 0.53 |
| 12:L:27:LEU:HD13 | 12:L:37:LYS:HB3 | 1.90 | 0.53 |
| 1:A:92:HIS:CD2 | 1:A:94:GLY:H | 2.26 | 0.53 |
| 2:B:644:GLU:HG3 | 2:B:654:ARG:HH22 | 1.74 | 0.53 |
| 9:I:29:CYS:O | 9:I:29:CYS:SG | 2.66 | 0.53 |
| 1:A:768:GLN:HG2 | 1:A:816:HIS:CA | 2.38 | 0.53 |
| 2:B:899:ILE:HD11 | 2:B:910:VAL:O | 2.09 | 0.53 |
| 2:B:756:ILE:HG21 | 2:B:759:PRO:HB3 | 1.90 | 0.53 |
| 1:A:696:GLU:OE2 | 1:A:702:LEU:HD23 | 2.08 | 0.53 |
| 3:C:189:THR:HG22 | 3:C:190:ASP:N | 2.24 | 0.53 |
| 1:A:567:LYS:HZ2 | 8:H:46:LEU:CB | 2.21 | 0.53 |
| 1:A:1111:MET:CE | 1:A:1330:ASN:OD1 | 2.57 | 0.53 |
| 1:A:32:VAL:HG21 | 1:A:68:GLN:HE22 | 1.74 | 0.53 |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:CE1 | 2.39 | 0.53 |
| 12:L:70:ARG:HG2 | 12:L:70:ARG:NH1 | 2.22 | 0.53 |
| 2:B:405:ARG:HA | 2:B:631:GLY:O | 2.09 | 0.53 |
| 9:I:62:ILE:HG23 | 9:I:63:GLY:N | 2.22 | 0.53 |
| 2:B:235:SER:OG | 2:B:236:HIS:HD2 | 1.91 | 0.53 |
| 1:A:38:PRO:N | 1:A:270:LEU:HD23 | 2.22 | 0.53 |
| 1:A:557:ASP:OD2 | 1:A:559:VAL:HB | 2.08 | 0.53 |
| 1:A:1029:ARG:HG3 | 1:A:1029:ARG:HH11 | 1.74 | 0.53 |
| 2:B:287:ARG:HA | 2:B:291:ILE:O | 2.09 | 0.53 |
| 1:A:683:ILE:HD11 | 1:A:764:CYS:CB | 2.35 | 0.53 |
| 1:A:529:CYS:HB2 | 2:B:1015:HIS:CE1 | 2.44 | 0.53 |
| 5:E:23:VAL:HG12 | 5:E:28:TYR:HB2 | 1.89 | 0.53 |
| 1:A:1195:LEU:HD11 | 1:A:1267:MET:HE3 | 1.91 | 0.53 |
| 6:F:118:LEU:O | 6:F:122:MET:HG3 | 2.08 | 0.53 |
| 1:A:608:ILE:HD12 | 1:A:613:ILE:CD1 | 2.38 | 0.53 |
| 1:A:13:THR:HG23 | 1:A:1432:GLN:NE2 | 2.24 | 0.53 |
| 1:A:407:ARG:HD2 | 1:A:413:ILE:HD11 | 1.91 | 0.53 |
| 8:H:38:LEU:CD1 | 8:H:125:LEU:HD13 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:205:ILE:HD11 | 2:B:461:LEU:HD23 | 1.90 | 0.53 |
| 1:A:552:TRP:NE1 | 1:A:655:PHE:CD1 | 2.77 | 0.53 |
| 1:A:852:TYR:CZ | 6:F:136:ARG:HG2 | 2.44 | 0.53 |
| 9:I:46:HIS:CD2 | 9:I:48:LEU:HD21 | 2.44 | 0.53 |
| 1:A:384:ASN:OD1 | 1:A:385:ILE:N | 2.42 | 0.53 |
| 1:A:1220:PHE:O | 1:A:1222:ASN:N | 2.42 | 0.53 |
| 2:B:1069:PHE:HA | 2:B:1085:ILE:O | 2.08 | 0.53 |
| 2:B:857:ARG:HD2 | 2:B:945:GLU:OE1 | 2.08 | 0.53 |
| 2:B:542:MET:HE1 | 2:B:743:ILE:CG2 | 2.39 | 0.53 |
| 2:B:577:ALA:HB1 | 2:B:589:VAL:HG11 | 1.91 | 0.53 |
| 1:A:741:ASN:ND2 | 1:A:741:ASN:C | 2.62 | 0.53 |
| 2:B:806:THR:C | 2:B:808:ALA:H | 2.13 | 0.53 |
| 1:A:114:LEU:HD22 | 1:A:171:GLN:NE2 | 2.23 | 0.53 |
| 2:B:90:ILE:CD1 | 2:B:432:MET:SD | 2.97 | 0.53 |
| 1:A:185:TRP:HZ3 | 1:A:200:ARG:HG2 | 1.74 | 0.53 |
| 6:F:132:LEU:O | 6:F:148:VAL:HG23 | 2.09 | 0.53 |
| 1:A:1161:THR:HG22 | 1:A:1162:VAL:N | 2.24 | 0.53 |
| 1:A:902:LEU:HD21 | 1:A:923:LEU:HD23 | 1.90 | 0.53 |
| 1:A:1436:ILE:CG2 | 1:A:1437:GLY:H | 2.22 | 0.53 |
| 1:A:442:VAL:O | 1:A:457:ALA:HA | 2.09 | 0.53 |
| 2:B:59:LEU:HD11 | 2:B:417:PHE:CZ | 2.44 | 0.53 |
| 1:A:1193:LEU:HD21 | 1:A:1267:MET:HE2 | 1.91 | 0.53 |
| 2:B:120:ARG:NH2 | 12:L:54:ARG:HD2 | 2.24 | 0.53 |
| 3:C:57:VAL:HG11 | 10:J:60:PHE:HB2 | 1.88 | 0.53 |
| 8:H:6:PHE:O | 8:H:58:THR:HA | 2.08 | 0.53 |
| 5:E:28:TYR:CE1 | 5:E:78:LEU:HD12 | 2.44 | 0.53 |
| 1:A:91:PHE:HB2 | 1:A:297:GLN:OE1 | 2.09 | 0.53 |
| 3:C:46:ILE:HD13 | 3:C:157:CYS:CB | 2.39 | 0.53 |
| 9:I:73:ARG:O | 9:I:81:ARG:HA | 2.09 | 0.53 |
| 2:B:240:ILE:HG23 | 2:B:240:ILE:O | 2.09 | 0.53 |
| 2:B:547:VAL:H | 2:B:612:GLU:CD | 2.13 | 0.53 |
| 2:B:293:PRO:HA | 9:I:12:ASN:HD21 | 1.74 | 0.52 |
| 2:B:234:ILE:H | 2:B:234:ILE:CD1 | 2.16 | 0.52 |
| 2:B:234:ILE:HG21 | 2:B:257:LYS:HB3 | 1.91 | 0.52 |
| 5:E:78:LEU:HD21 | 5:E:109:ILE:HD12 | 1.90 | 0.52 |
| 12:L:38:LEU:HG | 12:L:39:SER:N | 2.24 | 0.52 |
| 3:C:241:ASP:O | 3:C:245:VAL:HG23 | 2.08 | 0.52 |
| 8:H:32:THR:HG22 | 8:H:33:GLN:HG3 | 1.90 | 0.52 |
| 2:B:484:ASN:ND2 | 2:B:486:TYR:CE1 | 2.77 | 0.52 |
| 1:A:134:ARG:HH12 | 1:A:220:THR:HG22 | 1.74 | 0.52 |
| 5:E:17:ARG:O | 5:E:21:GLU:HG3 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:928:LEU:O | 1:A:931:GLU:N | 2.43 | 0.52 |
| 5:E:12:LEU:HD22 | 5:E:55:ARG:CZ | 2.39 | 0.52 |
| 1:A:1365:TYR:O | 1:A:1367:HIS:N | 2.42 | 0.52 |
| 1:A:666:ILE:HD11 | 2:B:1030:LEU:CD1 | 2.20 | 0.52 |
| 1:A:1116:LEU:N | 1:A:1308:THR:HG22 | 2.24 | 0.52 |
| 2:B:284:ILE:HD13 | 2:B:324:ILE:HD12 | 1.91 | 0.52 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:HD12 | 1.91 | 0.52 |
| 1:A:225:ASN:O | 1:A:227:VAL:HG23 | 2.08 | 0.52 |
| 1:A:226:GLU:HG2 | 1:A:227:VAL:HG23 | 1.90 | 0.52 |
| 2:B:875:GLU:O | 2:B:877:PRO:HD3 | 2.09 | 0.52 |
| 5:E:155:ARG:HD2 | 5:E:194:GLU:OE2 | 2.09 | 0.52 |
| 6:F:77:ASP:O | 6:F:78:GLN:HB2 | 2.09 | 0.52 |
| 1:A:670:ILE:HD13 | 2:B:1067:ARG:CZ | 2.39 | 0.52 |
| 9:I:75:CYS:C | 9:I:77:LYS:N | 2.59 | 0.52 |
| 1:A:1299:VAL:CG1 | 1:A:1300:LYS:N | 2.72 | 0.52 |
| 3:C:93:ASP:OD1 | 3:C:122:SER:HB2 | 2.09 | 0.52 |
| 2:B:46:GLN:NE2 | 2:B:496:ARG:HA | 2.24 | 0.52 |
| 11:K:46:ILE:O | 11:K:50:LEU:HB2 | 2.09 | 0.52 |
| 2:B:916:THR:HG22 | 2:B:918:ILE:HG13 | 1.90 | 0.52 |
| 2:B:25:ILE:HG22 | 2:B:26:THR:N | 2.24 | 0.52 |
| 10:J:9:SER:CB | 10:J:45:CYS:HB2 | 2.40 | 0.52 |
| 1:A:1392:SER:O | 1:A:1393:ASN:CB | 2.58 | 0.52 |
| 1:A:387:ARG:O | 1:A:391:LEU:HG | 2.09 | 0.52 |
| 1:A:233:TRP:C | 1:A:235:ILE:H | 2.13 | 0.52 |
| 12:L:38:LEU:O | 12:L:39:SER:CB | 2.56 | 0.52 |
| 1:A:1147:THR:HA | 1:A:1197:LEU:HD23 | 1.90 | 0.52 |
| 2:B:271:ALA:HB3 | 2:B:285:ILE:CD1 | 2.40 | 0.52 |
| 9:I:50:THR:HG22 | 9:I:52:ILE:H | 1.75 | 0.52 |
| 10:J:52:THR:O | 10:J:52:THR:HG22 | 2.08 | 0.52 |
| 1:A:507:VAL:N | 1:A:508:PRO:CD | 2.72 | 0.52 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:HB2 | 1.74 | 0.52 |
| 1:A:1319:VAL:CG1 | 1:A:1320:PRO:HD2 | 2.39 | 0.52 |
| 7:G:141:UNK:CA | 7:G:168:UNK:CA | 2.87 | 0.52 |
| 2:B:98:THR:OG1 | 2:B:127:GLY:HA3 | 2.09 | 0.52 |
| 1:A:754:SER:O | 1:A:755:PHE:C | 2.48 | 0.52 |
| 2:B:842:ASN:HD22 | 2:B:845:SER:CB | 2.21 | 0.52 |
| 9:I:29:CYS:C | 9:I:31:THR:H | 2.13 | 0.52 |
| 1:A:261:ASP:OD2 | 1:A:323:LYS:HD2 | 2.10 | 0.52 |
| 1:A:399:HIS:C | 1:A:401:GLY:H | 2.10 | 0.52 |
| 1:A:340:LEU:HD21 | 2:B:1200:ALA:CB | 2.40 | 0.52 |
| 1:A:1336:MET:HE1 | 1:A:1381:LEU:HG | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:35:VAL:C | 5:E:37:LEU:H | 2.12 | 0.52 |
| 2:B:552:MET:N | 2:B:553:PRO:HD2 | 2.24 | 0.52 |
| 3:C:164:ALA:HA | 3:C:167:HIS:O | 2.10 | 0.52 |
| 2:B:108:VAL:CG1 | 2:B:109:THR:H | 2.18 | 0.52 |
| 1:A:219:PHE:O | 1:A:222:LEU:O | 2.28 | 0.52 |
| 6:F:109:VAL:CG1 | 6:F:110:ASP:N | 2.73 | 0.52 |
| 1:A:167:CYS:HB2 | 1:A:169:ASN:ND2 | 2.24 | 0.52 |
| 2:B:614:SER:OG | 2:B:627:PHE:HB2 | 2.09 | 0.52 |
| 2:B:1084:GLN:HG2 | 3:C:201:TRP:CZ2 | 2.45 | 0.52 |
| 1:A:817:ALA:HA | 2:B:764:SER:OG | 2.10 | 0.52 |
| 1:A:365:GLY:HA3 | 1:A:469:ARG:HB2 | 1.91 | 0.52 |
| 1:A:326:ARG:HG2 | 1:A:1406:VAL:CG2 | 2.39 | 0.52 |
| 1:A:1300:LYS:HB3 | 1:A:1300:LYS:HZ2 | 1.74 | 0.52 |
| 11:K:49:GLU:OE2 | 11:K:97:LYS:HE3 | 2.10 | 0.52 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:HG2 | 2.24 | 0.52 |
| 1:A:443:LEU:HD11 | 2:B:1138:MET:SD | 2.50 | 0.52 |
| 2:B:1197:PRO:HG2 | 2:B:1200:ALA:CB | 2.40 | 0.52 |
| 1:A:715:GLU:OE2 | 1:A:774:ARG:NH1 | 2.43 | 0.52 |
| 2:B:25:ILE:CG2 | 2:B:29:ASP:HB3 | 2.40 | 0.52 |
| 1:A:907:THR:HG22 | 1:A:908:LEU:N | 2.25 | 0.52 |
| 1:A:41:MET:HG2 | 1:A:49:LYS:HG2 | 1.92 | 0.52 |
| 1:A:384:ASN:OD1 | 1:A:388:LEU:HD12 | 2.10 | 0.52 |
| 2:B:248:SER:O | 2:B:249:ARG:HB2 | 2.09 | 0.52 |
| 1:A:737:LEU:HD11 | 1:A:758:ILE:HG21 | 1.92 | 0.52 |
| 2:B:515:HIS:H | 2:B:518:HIS:HD2 | 1.55 | 0.52 |
| 1:A:96:ILE:O | 1:A:100:LYS:HG3 | 2.10 | 0.52 |
| 2:B:755:ILE:HG22 | 2:B:755:ILE:O | 2.09 | 0.52 |
| 2:B:287:ARG:HG2 | 2:B:292:ILE:CA | 2.27 | 0.51 |
| 2:B:1163:CYS:SG | 2:B:1182:CYS:SG | 3.09 | 0.51 |
| 2:B:864:LYS:HD3 | 2:B:871:THR:HA | 1.91 | 0.51 |
| 11:K:63:VAL:HG23 | 11:K:63:VAL:O | 2.08 | 0.51 |
| 1:A:738:LYS:HZ2 | 3:C:194:GLU:HA | 1.75 | 0.51 |
| 2:B:737:THR:CG2 | 9:I:66:PRO:HB2 | 2.40 | 0.51 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:N | 1.97 | 0.51 |
| 1:A:384:ASN:O | 1:A:385:ILE:C | 2.48 | 0.51 |
| 2:B:563:MET:HG3 | 2:B:563:MET:O | 2.10 | 0.51 |
| 2:B:751:VAL:HG12 | 2:B:752:ALA:N | 2.26 | 0.51 |
| 12:L:27:LEU:HD13 | 12:L:37:LYS:CG | 2.41 | 0.51 |
| 2:B:846:ILE:HD13 | 2:B:974:PRO:HG2 | 1.91 | 0.51 |
| 1:A:50:ILE:HG22 | 1:A:51:GLY:N | 2.24 | 0.51 |
| 1:A:134:ARG:NH1 | 1:A:220:THR:O | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:L:47:ARG:HG2 | 12:L:52:GLY:CA | 2.39 | 0.51 |
| 1:A:1326:ARG:O | 1:A:1327:ILE:C | 2.49 | 0.51 |
| 5:E:5:ASN:O | 5:E:9:ILE:HG13 | 2.11 | 0.51 |
| 1:A:568:PRO:HB2 | 3:C:221:TYR:CE1 | 2.45 | 0.51 |
| 5:E:124:VAL:HG22 | 5:E:132:ILE:CG2 | 2.39 | 0.51 |
| 3:C:80:LEU:CD2 | 3:C:129:ILE:HD11 | 2.28 | 0.51 |
| 9:I:75:CYS:HG | 9:I:106:CYS:HG | 1.59 | 0.51 |
| 1:A:470:LEU:HD21 | 1:A:487:MET:HE3 | 1.92 | 0.51 |
| 1:A:836:TYR:CE2 | 1:A:840:ARG:HD2 | 2.45 | 0.51 |
| 2:B:130:VAL:CG1 | 2:B:131:ASP:N | 2.74 | 0.51 |
| 1:A:1299:VAL:CG1 | 1:A:1300:LYS:H | 2.20 | 0.51 |
| 10:J:14:VAL:HG12 | 10:J:50:ILE:HD11 | 1.92 | 0.51 |
| 1:A:675:THR:CG2 | 1:A:736:ASN:HD21 | 2.22 | 0.51 |
| 1:A:821:ARG:HG3 | 1:A:825:ILE:CD1 | 2.40 | 0.51 |
| 2:B:1035:ALA:HB1 | 2:B:1040:ASN:O | 2.10 | 0.51 |
| 8:H:84:ALA:C | 8:H:86:ASP:N | 2.64 | 0.51 |
| 1:A:1359:ASP:C | 1:A:1361:SER:H | 2.13 | 0.51 |
| 5:E:23:VAL:HG13 | 5:E:28:TYR:CD1 | 2.45 | 0.51 |
| 2:B:31:TRP:CD1 | 2:B:807:ARG:NH1 | 2.78 | 0.51 |
| 1:A:898:ARG:HD2 | 1:A:899:VAL:N | 2.26 | 0.51 |
| 1:A:929:LEU:H | 1:A:929:LEU:CD2 | 2.23 | 0.51 |
| 6:F:109:VAL:CG2 | 6:F:124:GLU:HG2 | 2.40 | 0.51 |
| 1:A:753:GLY:HA2 | 1:A:757:ASN:HD22 | 1.74 | 0.51 |
| 1:A:357:PRO:HG2 | 2:B:833:TYR:CE1 | 2.45 | 0.51 |
| 3:C:177:GLU:HG3 | 3:C:231:ASN:HB3 | 1.93 | 0.51 |
| 1:A:1362:TYR:OH | 1:A:1364:ASN:HA | 2.11 | 0.51 |
| 2:B:120:ARG:HB2 | 2:B:122:LEU:HG | 1.91 | 0.51 |
| 2:B:834:ASN:O | 2:B:1013:ASN:HB2 | 2.10 | 0.51 |
| 1:A:306:ASN:HD21 | 1:A:324:SER:N | 2.09 | 0.51 |
| 11:K:24:ASP:HB3 | 11:K:30:ALA:HB3 | 1.93 | 0.51 |
| 1:A:444:PHE:CB | 1:A:458:HIS:HD2 | 2.24 | 0.51 |
| 1:A:1150:SER:HB2 | 1:A:1195:LEU:HD23 | 1.93 | 0.51 |
| 2:B:463:THR:HG21 | 2:B:465:ASN:HD22 | 1.74 | 0.51 |
| 1:A:847:ASP:OD2 | 1:A:858:ASN:HB2 | 2.10 | 0.51 |
| 2:B:514:LEU:HD12 | 2:B:515:HIS:H | 1.74 | 0.51 |
| 1:A:27:VAL:HG13 | 1:A:240:PRO:HB3 | 1.91 | 0.51 |
| 5:E:121:MET:C | 5:E:123:LEU:H | 2.13 | 0.51 |
| 2:B:825:VAL:HG12 | 2:B:826:ALA:N | 2.24 | 0.51 |
| 12:L:62:LYS:O | 12:L:64:LEU:HG | 2.11 | 0.51 |
| 12:L:62:LYS:C | 12:L:64:LEU:H | 2.13 | 0.51 |
| 1:A:567:LYS:HD2 | 1:A:568:PRO:HD2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:HH11 | 2.09 | 0.51 |
| 10:J:7:CYS:SG | 10:J:9:SER:HB2 | 2.50 | 0.51 |
| 1:A:1152:ILE:CG2 | 1:A:1260:LEU:HD23 | 2.38 | 0.51 |
| 2:B:864:LYS:HG2 | 2:B:871:THR:HG23 | 1.93 | 0.51 |
| 6:F:101:ILE:HD13 | 6:F:120:ILE:HG22 | 1.91 | 0.51 |
| 2:B:707:PRO:CG | 2:B:708:GLU:H | 2.21 | 0.51 |
| 2:B:271:ALA:O | 2:B:279:ASP:HA | 2.11 | 0.51 |
| 1:A:817:ALA:HA | 2:B:764:SER:HG | 1.76 | 0.51 |
| 1:A:596:THR:O | 1:A:597:LEU:C | 2.48 | 0.51 |
| 1:A:332:LYS:H | 1:A:337:ARG:HD2 | 1.76 | 0.51 |
| 1:A:649:ILE:O | 1:A:653:VAL:HG23 | 2.11 | 0.51 |
| 2:B:185:THR:O | 2:B:189:LEU:HG | 2.11 | 0.51 |
| 11:K:101:LEU:HD23 | 11:K:101:LEU:O | 2.11 | 0.51 |
| 2:B:428:ILE:O | 2:B:431:TYR:HB3 | 2.10 | 0.51 |
| 1:A:1214:GLU:O | 1:A:1218:GLN:HG2 | 2.10 | 0.51 |
| 2:B:283:VAL:HG13 | 2:B:297:ILE:CD1 | 2.41 | 0.51 |
| 1:A:15:LYS:CB | 2:B:1220:ARG:HG2 | 2.33 | 0.51 |
| 8:H:83:GLN:C | 8:H:85:GLY:H | 2.14 | 0.51 |
| 5:E:54:GLN:O | 5:E:57:MET:HB3 | 2.11 | 0.51 |
| 5:E:168:TYR:HB3 | 5:E:170:LEU:CG | 2.41 | 0.51 |
| 3:C:18:VAL:HG12 | 3:C:20:PHE:HD2 | 1.76 | 0.51 |
| 1:A:115:LEU:HB2 | 1:A:122:MET:CE | 2.41 | 0.51 |
| 1:A:1351:GLU:O | 1:A:1352:VAL:C | 2.49 | 0.51 |
| 1:A:1269:GLU:OE2 | 2:B:263:GLY:HA3 | 2.10 | 0.51 |
| 1:A:722:LEU:HD11 | 1:A:794:PRO:HB3 | 1.92 | 0.51 |
| 1:A:901:LEU:HD23 | 1:A:907:THR:HG23 | 1.92 | 0.51 |
| 2:B:100:PRO:HG3 | 2:B:172:ILE:HD12 | 1.92 | 0.51 |
| 1:A:500:GLU:OE1 | 2:B:1143:ALA:HB1 | 2.11 | 0.51 |
| 1:A:107:CYS:HB2 | 1:A:114:LEU:HD23 | 1.93 | 0.51 |
| 2:B:365:THR:HG23 | 2:B:367:LEU:HG | 1.93 | 0.51 |
| 1:A:376:TYR:OH | 1:A:498:ARG:HD2 | 2.10 | 0.51 |
| 1:A:786:HIS:CE1 | 2:B:705:MET:HE1 | 2.46 | 0.50 |
| 1:A:1312:ASN:O | 1:A:1316:VAL:HG23 | 2.11 | 0.50 |
| 1:A:49:LYS:HB3 | 1:A:55:ASP:HB2 | 1.92 | 0.50 |
| 1:A:709:THR:CB | 1:A:712:GLU:HG3 | 2.41 | 0.50 |
| 2:B:1177:HIS:HB3 | 2:B:1179:GLN:HE21 | 1.74 | 0.50 |
| 2:B:101:MET:HE2 | 2:B:169:ARG:HH12 | 1.76 | 0.50 |
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:CB | 2.24 | 0.50 |
| 11:K:47:ARG:CB | 11:K:47:ARG:HH11 | 2.23 | 0.50 |
| 1:A:451:HIS:CD2 | 1:A:1074:GLU:HG3 | 2.45 | 0.50 |
| 2:B:1084:GLN:CD | 2:B:1084:GLN:H | 2.14 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:827:ILE:HG12 | 2:B:1012:ILE:HD11 | 1.93 | 0.50 |
| 8:H:95:TYR:HE2 | 8:H:97:MET:HG3 | 1.74 | 0.50 |
| 1:A:857:ARG:HG2 | 1:A:863:VAL:HA | 1.94 | 0.50 |
| 1:A:1376:THR:HG23 | 1:A:1376:THR:O | 2.12 | 0.50 |
| 1:A:1376:THR:HG23 | 5:E:212:ARG:NH2 | 2.26 | 0.50 |
| 2:B:1177:HIS:CB | 2:B:1179:GLN:HE21 | 2.24 | 0.50 |
| 8:H:84:ALA:C | 8:H:86:ASP:H | 2.13 | 0.50 |
| 5:E:157:SER:C | 5:E:159:ASP:N | 2.64 | 0.50 |
| 8:H:128:ASN:O | 8:H:131:ASN:ND2 | 2.45 | 0.50 |
| 2:B:737:THR:HG23 | 9:I:66:PRO:HB2 | 1.93 | 0.50 |
| 2:B:1119:VAL:O | 2:B:1126:GLY:HA3 | 2.11 | 0.50 |
| 2:B:485:ARG:NH2 | 2:B:782:LEU:HD11 | 2.27 | 0.50 |
| 11:K:91:CYS:O | 11:K:95:ILE:HG13 | 2.11 | 0.50 |
| 10:J:36:LEU:HD13 | 10:J:47:ARG:HG2 | 1.92 | 0.50 |
| 9:I:68:LEU:HB3 | 9:I:84:VAL:HG22 | 1.94 | 0.50 |
| 2:B:581:PHE:HB2 | 2:B:625:LYS:HG2 | 1.93 | 0.50 |
| 1:A:587:HIS:HA | 1:A:607:ILE:O | 2.11 | 0.50 |
| 2:B:271:ALA:HB3 | 2:B:285:ILE:HD11 | 1.93 | 0.50 |
| 10:J:54:VAL:O | 10:J:56:LEU:N | 2.43 | 0.50 |
| 1:A:1384:VAL:O | 1:A:1384:VAL:HG12 | 2.11 | 0.50 |
| 2:B:542:MET:CG | 2:B:747:MET:HE3 | 2.38 | 0.50 |
| 2:B:559:SER:HA | 2:B:563:MET:HB3 | 1.91 | 0.50 |
| 1:A:810:PRO:O | 1:A:813:PHE:HB3 | 2.11 | 0.50 |
| 1:A:829:VAL:C | 1:A:831:THR:H | 2.15 | 0.50 |
| 1:A:573:SER:O | 1:A:576:GLN:HB2 | 2.11 | 0.50 |
| 2:B:292:ILE:N | 2:B:293:PRO:HD2 | 2.25 | 0.50 |
| 3:C:66:ARG:NH2 | 10:J:2:ILE:CG2 | 2.74 | 0.50 |
| 9:I:75:CYS:O | 9:I:77:LYS:N | 2.44 | 0.50 |
| 2:B:800:GLN:OE1 | 2:B:822:ASN:HB2 | 2.12 | 0.50 |
| 1:A:418:SER:C | 1:A:420:ARG:N | 2.63 | 0.50 |
| 9:I:101:PHE:O | 9:I:109:ILE:HA | 2.12 | 0.50 |
| 12:L:51:CYS:C | 12:L:53:HIS:H | 2.11 | 0.50 |
| 9:I:15:TYR:CD1 | 9:I:15:TYR:N | 2.79 | 0.50 |
| 9:I:25:LEU:HD12 | 9:I:26:LEU:H | 1.76 | 0.50 |
| 2:B:1053:GLU:O | 2:B:1054:GLY:C | 2.50 | 0.50 |
| 5:E:177:ARG:O | 5:E:212:ARG:HD3 | 2.11 | 0.50 |
| 1:A:751:SER:O | 1:A:752:LYS:CG | 2.59 | 0.50 |
| 1:A:341:MET:CE | 1:A:1401:SER:HB2 | 2.40 | 0.50 |
| 1:A:100:LYS:NZ | 1:A:176:LYS:HD2 | 2.27 | 0.50 |
| 2:B:35:SER:O | 2:B:36:ALA:C | 2.50 | 0.50 |
| 2:B:519:TRP:HZ2 | 2:B:705:MET:CE | 2.24 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:642:ASP:HB3 | 2:B:649:LYS:CD | 2.41 | 0.50 |
| 2:B:653:VAL:CG2 | 2:B:689:LEU:HB3 | 2.42 | 0.50 |
| 2:B:977:GLY:CA | 2:B:1099:VAL:CG2 | 2.86 | 0.50 |
| 2:B:975:GLN:O | 2:B:990:ILE:HD12 | 2.12 | 0.50 |
| 2:B:858:SER:HA | 2:B:966:VAL:O | 2.12 | 0.50 |
| 1:A:535:THR:HG23 | 1:A:575:LYS:HE2 | 1.93 | 0.50 |
| 1:A:888:GLY:O | 1:A:940:ARG:NH2 | 2.44 | 0.50 |
| 1:A:893:PHE:CE1 | 1:A:940:ARG:HD2 | 2.46 | 0.50 |
| 5:E:80:VAL:HG22 | 5:E:109:ILE:HD12 | 1.94 | 0.50 |
| 12:L:40:LEU:HD13 | 12:L:44:ASP:OD1 | 2.11 | 0.50 |
| 3:C:142:VAL:H | 10:J:16:ASP:HB3 | 1.77 | 0.50 |
| 1:A:1153:TYR:HA | 9:I:41:PRO:O | 2.12 | 0.50 |
| 9:I:99:LEU:HB2 | 9:I:112:SER:HB3 | 1.94 | 0.50 |
| 2:B:648:HIS:NE2 | 2:B:650:GLU:OE1 | 2.43 | 0.50 |
| 6:F:82:THR:HG22 | 6:F:84:TYR:N | 2.27 | 0.50 |
| 1:A:1094:VAL:HG13 | 1:A:1113:THR:CG2 | 2.37 | 0.50 |
| 9:I:29:CYS:SG | 9:I:31:THR:HG22 | 2.52 | 0.50 |
| 1:A:1194:ARG:HH22 | 1:A:1237:ILE:HD13 | 1.73 | 0.50 |
| 1:A:612:ILE:O | 1:A:612:ILE:HG23 | 2.12 | 0.50 |
| 5:E:46:TYR:HE2 | 5:E:58:MET:HA | 1.76 | 0.50 |
| 1:A:511:ILE:HG12 | 1:A:521:MET:CE | 2.42 | 0.50 |
| 1:A:329:LEU:HD22 | 2:B:1203:LEU:CD1 | 2.41 | 0.50 |
| 3:C:254:LYS:HE2 | 11:K:42:LEU:HD13 | 1.94 | 0.50 |
| 1:A:346:ASP:CG | 2:B:1108:ARG:HA | 2.31 | 0.50 |
| 5:E:98:ILE:O | 5:E:102:GLU:HG3 | 2.12 | 0.50 |
| 1:A:332:LYS:HG3 | 1:A:333:GLU:HG2 | 1.94 | 0.49 |
| 3:C:33:LEU:HG | 3:C:37:MET:CE | 2.41 | 0.49 |
| 1:A:929:LEU:HD21 | 1:A:983:ILE:HG21 | 1.94 | 0.49 |
| 1:A:466:SER:HB3 | 11:K:2:ASN:ND2 | 2.27 | 0.49 |
| 9:I:55:THR:HG21 | 9:I:109:ILE:HD13 | 1.93 | 0.49 |
| 2:B:195:CYS:SG | 2:B:197:PHE:HB2 | 2.51 | 0.49 |
| 8:H:84:ALA:HB1 | 8:H:87:ARG:HB2 | 1.94 | 0.49 |
| 1:A:105:CYS:SG | 1:A:138:ILE:HG22 | 2.52 | 0.49 |
| 2:B:240:ILE:O | 2:B:253:THR:HG23 | 2.11 | 0.49 |
| 1:A:819:GLY:O | 1:A:820:GLY:C | 2.49 | 0.49 |
| 8:H:76:THR:HG22 | 8:H:76:THR:O | 2.11 | 0.49 |
| 2:B:708:GLU:C | 2:B:710:LEU:H | 2.16 | 0.49 |
| 3:C:75:MET:HG3 | 3:C:246:ARG:NH2 | 2.28 | 0.49 |
| 2:B:873:THR:O | 2:B:914:LYS:HA | 2.12 | 0.49 |
| 5:E:56:LYS:HG3 | 5:E:84:ASP:CB | 2.42 | 0.49 |
| 2:B:579:ARG:HB2 | 2:B:586:TRP:NE1 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:741:ASN:ND2 | 1:A:743:VAL:N | 2.60 | 0.49 |
| 1:A:1142:THR:O | 1:A:1273:LEU:HD22 | 2.12 | 0.49 |
| 2:B:1043:ASP:O | 2:B:1050:ILE:HD12 | 2.12 | 0.49 |
| 1:A:808:LEU:O | 2:B:728:ARG:NH1 | 2.43 | 0.49 |
| 2:B:570:VAL:HG11 | 2:B:573:GLN:OE1 | 2.13 | 0.49 |
| 2:B:734:HIS:O | 2:B:735:ALA:HB2 | 2.12 | 0.49 |
| 3:C:77:ILE:HG23 | 3:C:161:LYS:HE3 | 1.94 | 0.49 |
| 8:H:6:PHE:HE1 | 8:H:130:ARG:NE | 2.10 | 0.49 |
| 6:F:133:VAL:HG22 | 6:F:147:SER:HA | 1.94 | 0.49 |
| 8:H:93:TYR:HA | 8:H:145:ARG:CB | 2.41 | 0.49 |
| 1:A:394:ASN:OD1 | 1:A:398:GLU:OE1 | 2.30 | 0.49 |
| 2:B:542:MET:HG3 | 2:B:747:MET:CE | 2.38 | 0.49 |
| 1:A:135:PHE:HD1 | 1:A:222:LEU:HD22 | 1.76 | 0.49 |
| 1:A:675:THR:HG21 | 1:A:736:ASN:HD21 | 1.77 | 0.49 |
| 1:A:821:ARG:CG | 1:A:825:ILE:HD11 | 2.41 | 0.49 |
| 2:B:260:GLY:O | 2:B:267:ARG:HD3 | 2.12 | 0.49 |
| 8:H:47:PHE:HB2 | 8:H:95:TYR:HD1 | 1.76 | 0.49 |
| 2:B:1118:PRO:HD3 | 2:B:1155:SER:HA | 1.95 | 0.49 |
| 2:B:65:GLU:HG3 | 2:B:66:ASP:N | 2.27 | 0.49 |
| 8:H:31:THR:O | 8:H:32:THR:HB | 2.11 | 0.49 |
| 2:B:660:LYS:O | 2:B:663:ALA:HB3 | 2.13 | 0.49 |
| 1:A:1349:TYR:CD2 | 1:A:1349:TYR:C | 2.84 | 0.49 |
| 6:F:81:THR:HG22 | 6:F:82:THR:H | 1.78 | 0.49 |
| 12:L:52:GLY:O | 12:L:54:ARG:HG3 | 2.12 | 0.49 |
| 3:C:43:THR:CG2 | 3:C:44:LEU:N | 2.75 | 0.49 |
| 8:H:44:VAL:O | 8:H:44:VAL:HG12 | 2.12 | 0.49 |
| 11:K:97:LYS:O | 11:K:100:ALA:HB3 | 2.12 | 0.49 |
| 1:A:738:LYS:NZ | 3:C:194:GLU:HA | 2.26 | 0.49 |
| 1:A:1099:PRO:O | 1:A:1102:LYS:HB3 | 2.13 | 0.49 |
| 1:A:1134:ILE:O | 1:A:1138:ILE:HG13 | 2.12 | 0.49 |
| 2:B:896:ASP:OD2 | 12:L:58:LYS:HE3 | 2.13 | 0.49 |
| 10:J:7:CYS:O | 10:J:8:PHE:C | 2.50 | 0.49 |
| 3:C:75:MET:HG3 | 3:C:246:ARG:HH22 | 1.77 | 0.49 |
| 5:E:191:LYS:O | 5:E:192:ARG:C | 2.51 | 0.49 |
| 1:A:538:ASP:OD1 | 8:H:22:LYS:HB2 | 2.12 | 0.49 |
| 2:B:171:PRO:HD2 | 2:B:457:LEU:CD1 | 2.43 | 0.49 |
| 1:A:474:VAL:HG13 | 1:A:478:TYR:CE1 | 2.48 | 0.49 |
| 1:A:545:GLN:O | 1:A:548:ASN:N | 2.44 | 0.49 |
| 9:I:85:PHE:O | 9:I:86:PHE:HB3 | 2.12 | 0.49 |
| 2:B:726:ALA:HB1 | 2:B:1051:THR:CG2 | 2.43 | 0.49 |
| 1:A:74:MET:O | 1:A:75:ASN:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1208:MET:HA | 2:B:1212:ILE:O | 2.12 | 0.49 |
| 1:A:391:LEU:O | 1:A:394:ASN:N | 2.46 | 0.49 |
| 8:H:88:SER:O | 8:H:89:LEU:HG | 2.12 | 0.49 |
| 1:A:226:GLU:CG | 1:A:227:VAL:N | 2.75 | 0.49 |
| 1:A:974:ASP:HB2 | 8:H:136:LYS:HZ1 | 1.77 | 0.49 |
| 2:B:25:ILE:CG2 | 2:B:29:ASP:CB | 2.91 | 0.49 |
| 2:B:635:ARG:NH1 | 2:B:742:GLU:OE2 | 2.45 | 0.49 |
| 1:A:418:SER:HB3 | 1:A:421:ALA:HB2 | 1.94 | 0.49 |
| 11:K:55:LYS:CD | 11:K:78:THR:HB | 2.42 | 0.49 |
| 1:A:225:ASN:C | 1:A:227:VAL:H | 2.10 | 0.49 |
| 3:C:4:GLU:O | 3:C:5:GLY:O | 2.31 | 0.49 |
| 1:A:795:GLU:HG2 | 2:B:731:VAL:HG21 | 1.93 | 0.49 |
| 1:A:1100:ARG:NH2 | 1:A:1330:ASN:HB2 | 2.28 | 0.49 |
| 2:B:291:ILE:HD13 | 2:B:300:HIS:CD2 | 2.48 | 0.49 |
| 2:B:737:THR:CG2 | 9:I:66:PRO:CB | 2.89 | 0.49 |
| 2:B:839:MET:HE2 | 2:B:980:PHE:CD1 | 2.48 | 0.49 |
| 2:B:906:SER:O | 2:B:907:GLY:C | 2.50 | 0.49 |
| 2:B:488:TYR:CE2 | 2:B:813:LYS:HB2 | 2.48 | 0.49 |
| 2:B:756:ILE:CG2 | 2:B:759:PRO:HB3 | 2.42 | 0.49 |
| 10:J:16:ASP:OD1 | 10:J:17:LYS:HE3 | 2.12 | 0.49 |
| 2:B:225:VAL:HG11 | 2:B:388:CYS:HB3 | 1.95 | 0.49 |
| 2:B:890:TYR:O | 2:B:892:LYS:N | 2.46 | 0.49 |
| 2:B:380:TYR:CE1 | 2:B:384:ARG:HD3 | 2.48 | 0.49 |
| 1:A:5:GLN:O | 2:B:1159:ARG:NH2 | 2.46 | 0.49 |
| 1:A:378:GLU:HG2 | 1:A:388:LEU:HD11 | 1.94 | 0.49 |
| 1:A:337:ARG:CZ | 1:A:839:ARG:HH12 | 2.22 | 0.49 |
| 1:A:1392:SER:O | 1:A:1393:ASN:CG | 2.52 | 0.49 |
| 2:B:1106:ARG:HH21 | 2:B:1109:GLY:C | 2.16 | 0.49 |
| 2:B:781:PHE:O | 2:B:782:LEU:HG | 2.12 | 0.49 |
| 11:K:83:PRO:HA | 11:K:86:ALA:HB3 | 1.95 | 0.49 |
| 8:H:59:ILE:O | 8:H:60:ALA:HB3 | 2.12 | 0.49 |
| 4:D:118:UNK:CA | 4:D:119:UNK:CA | 2.91 | 0.49 |
| 2:B:1053:GLU:O | 2:B:1055:ILE:N | 2.46 | 0.48 |
| 2:B:1106:ARG:NH2 | 2:B:1109:GLY:C | 2.67 | 0.48 |
| 1:A:89:PRO:C | 1:A:204:THR:HG21 | 2.33 | 0.48 |
| 2:B:821:GLN:OE1 | 2:B:850:LEU:HD12 | 2.13 | 0.48 |
| 1:A:1001:ARG:HG2 | 1:A:1001:ARG:HH11 | 1.77 | 0.48 |
| 8:H:39:THR:O | 8:H:123:MET:HA | 2.14 | 0.48 |
| 8:H:49:VAL:CG1 | 8:H:50:ALA:N | 2.75 | 0.48 |
| 2:B:726:ALA:HB1 | 2:B:1051:THR:HG21 | 1.95 | 0.48 |
| 2:B:1065:GLN:HE22 | 2:B:1067:ARG:HG2 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:61:ILE:HA | 1:A:74:MET:SD | 2.53 | 0.48 |
| 1:A:589:GLN:OE1 | 1:A:591:PHE:HE1 | 1.96 | 0.48 |
| 1:A:332:LYS:N | 1:A:337:ARG:HD2 | 2.28 | 0.48 |
| 5:E:100:ILE:CG2 | 5:E:105:PHE:HB2 | 2.42 | 0.48 |
| 2:B:1160:VAL:HG11 | 2:B:1169:MET:SD | 2.53 | 0.48 |
| 1:A:69:THR:HG22 | 1:A:69:THR:O | 2.12 | 0.48 |
| 1:A:738:LYS:HB3 | 8:H:19:ARG:HH22 | 1.79 | 0.48 |
| 2:B:1060:ARG:O | 2:B:1063:GLY:N | 2.45 | 0.48 |
| 1:A:491:VAL:O | 1:A:493:GLN:NE2 | 2.46 | 0.48 |
| 1:A:918:GLU:O | 1:A:918:GLU:HG3 | 2.12 | 0.48 |
| 1:A:1189:SER:OG | 1:A:1190:PRO:HD2 | 2.12 | 0.48 |
| 2:B:351:TYR:O | 2:B:355:ILE:HG13 | 2.12 | 0.48 |
| 1:A:68:GLN:NE2 | 1:A:80:HIS:CB | 2.76 | 0.48 |
| 2:B:283:VAL:O | 2:B:286:PHE:HB2 | 2.11 | 0.48 |
| 2:B:227:LYS:HB2 | 2:B:395:GLN:OE1 | 2.13 | 0.48 |
| 2:B:653:VAL:HG12 | 2:B:654:ARG:N | 2.28 | 0.48 |
| 1:A:783:THR:HG21 | 1:A:815:PHE:CE2 | 2.48 | 0.48 |
| 1:A:606:LEU:HB2 | 1:A:614:PHE:CE2 | 2.47 | 0.48 |
| 1:A:1406:VAL:CG1 | 1:A:1410:PHE:HE1 | 2.26 | 0.48 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:HB2 | 1.94 | 0.48 |
| 3:C:11:ARG:NH2 | 3:C:229:TYR:CD2 | 2.68 | 0.48 |
| 1:A:1436:ILE:CG2 | 1:A:1437:GLY:N | 2.72 | 0.48 |
| 6:F:87:LYS:HE2 | 6:F:88:TYR:CE1 | 2.48 | 0.48 |
| 3:C:254:LYS:O | 3:C:258:ILE:HD13 | 2.13 | 0.48 |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:CD1 | 2.41 | 0.48 |
| 3:C:142:VAL:H | 10:J:16:ASP:CB | 2.26 | 0.48 |
| 5:E:102:GLU:O | 5:E:104:ASN:N | 2.46 | 0.48 |
| 6:F:82:THR:HG22 | 6:F:84:TYR:H | 1.77 | 0.48 |
| 1:A:913:LEU:HD11 | 1:A:981:LEU:O | 2.14 | 0.48 |
| 1:A:381:THR:O | 1:A:384:ASN:N | 2.41 | 0.48 |
| 1:A:874:ASP:HA | 1:A:1058:VAL:HG22 | 1.95 | 0.48 |
| 1:A:1412:ALA:HA | 1:A:1417:GLU:OE2 | 2.14 | 0.48 |
| 1:A:475:THR:CG2 | 1:A:476:SER:N | 2.76 | 0.48 |
| 1:A:154:SER:HB3 | 1:A:162:VAL:HG21 | 1.92 | 0.48 |
| 11:K:43:GLY:HA2 | 11:K:71:PHE:CZ | 2.49 | 0.48 |
| 1:A:1356:ILE:HD12 | 1:A:1368:MET:SD | 2.54 | 0.48 |
| 7:G:136:UNK:CA | 7:G:137:UNK:CA | 2.91 | 0.48 |
| 1:A:365:GLY:O | 1:A:468:PHE:HA | 2.14 | 0.48 |
| 1:A:89:PRO:HG3 | 1:A:208:LEU:CD1 | 2.44 | 0.48 |
| 1:A:31:SER:HB2 | 1:A:83:HIS:HB2 | 1.91 | 0.48 |
| 2:B:363:HIS:CD2 | 2:B:585:VAL:HG22 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:674:PRO:O | 1:A:677:ARG:HB3 | 2.13 | 0.48 |
| 2:B:298:LEU:N | 2:B:298:LEU:HD23 | 2.29 | 0.48 |
| 9:I:62:ILE:CG2 | 9:I:63:GLY:N | 2.77 | 0.48 |
| 11:K:27:ALA:HB1 | 11:K:28:PRO:HD2 | 1.96 | 0.48 |
| 3:C:212:PRO:HB3 | 3:C:213:PRO:HD2 | 1.95 | 0.48 |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:HB2 | 1.94 | 0.48 |
| 8:H:36:CYS:HA | 8:H:126:GLU:O | 2.13 | 0.48 |
| 1:A:742:ASN:O | 1:A:745:GLN:HB2 | 2.13 | 0.48 |
| 2:B:994:TYR:HD1 | 2:B:999:MET:HE3 | 1.78 | 0.48 |
| 8:H:33:GLN:OE1 | 8:H:129:TYR:CE2 | 2.67 | 0.48 |
| 2:B:284:ILE:CD1 | 2:B:324:ILE:HD12 | 2.43 | 0.48 |
| 1:A:531:ILE:CD1 | 1:A:617:VAL:HG11 | 2.44 | 0.48 |
| 2:B:821:GLN:HB2 | 2:B:851:PHE:CE2 | 2.49 | 0.48 |
| 1:A:112:LYS:HG2 | 1:A:113:LEU:H | 1.79 | 0.48 |
| 1:A:376:TYR:CD2 | 1:A:376:TYR:C | 2.87 | 0.48 |
| 1:A:178:GLY:O | 1:A:179:LEU:HD23 | 2.13 | 0.48 |
| 1:A:1410:PHE:CE2 | 2:B:1212:ILE:HD11 | 2.45 | 0.48 |
| 2:B:566:LEU:CD1 | 2:B:588:GLY:HA2 | 2.44 | 0.48 |
| 1:A:167:CYS:O | 1:A:169:ASN:N | 2.45 | 0.48 |
| 2:B:825:VAL:CG1 | 2:B:826:ALA:N | 2.76 | 0.48 |
| 1:A:1277:GLU:O | 1:A:1278:ASN:HB2 | 2.14 | 0.48 |
| 12:L:62:LYS:O | 12:L:64:LEU:N | 2.37 | 0.48 |
| 1:A:54:ASN:HA | 1:A:58:LEU:HD12 | 1.95 | 0.48 |
| 3:C:43:THR:HG22 | 3:C:44:LEU:N | 2.29 | 0.48 |
| 11:K:10:PHE:CE1 | 11:K:11:LEU:HD13 | 2.49 | 0.48 |
| 2:B:315:LYS:O | 2:B:318:VAL:N | 2.46 | 0.48 |
| 1:A:1074:GLU:C | 1:A:1076:ALA:N | 2.67 | 0.48 |
| 1:A:226:GLU:HG2 | 1:A:227:VAL:N | 2.29 | 0.48 |
| 6:F:98:ALA:O | 6:F:117:PRO:HB2 | 2.14 | 0.48 |
| 1:A:18:GLN:O | 2:B:1215:ARG:CG | 2.62 | 0.48 |
| 1:A:1066:VAL:O | 1:A:1068:ALA:N | 2.46 | 0.48 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:CA | 2.43 | 0.48 |
| 1:A:954:TRP:O | 1:A:956:LEU:HG | 2.14 | 0.48 |
| 6:F:79:ARG:HG2 | 6:F:146:TRP:CZ2 | 2.49 | 0.48 |
| 9:I:50:THR:HG22 | 9:I:51:ASN:N | 2.28 | 0.47 |
| 1:A:1192:LEU:HD11 | 1:A:1239:ARG:CB | 2.37 | 0.47 |
| 1:A:1284:MET:HG2 | 1:A:1306:LEU:CD2 | 2.43 | 0.47 |
| 2:B:55:VAL:HG12 | 2:B:56:ASP:N | 2.27 | 0.47 |
| 3:C:258:ILE:HG23 | 11:K:19:LEU:HD11 | 1.96 | 0.47 |
| 5:E:102:GLU:C | 5:E:104:ASN:N | 2.67 | 0.47 |
| 8:H:118:PHE:HB2 | 8:H:121:LEU:HB2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:291:ILE:HD13 | 2:B:300:HIS:NE2 | 2.29 | 0.47 |
| 2:B:324:ILE:HG23 | 2:B:329:THR:HB | 1.96 | 0.47 |
| 10:J:48:ARG:HE | 10:J:49:MET:HE2 | 1.79 | 0.47 |
| 2:B:778:MET:HE1 | 2:B:1094:ARG:HD3 | 1.96 | 0.47 |
| 1:A:443:LEU:CD2 | 1:A:455:MET:HB3 | 2.42 | 0.47 |
| 2:B:1156:ASP:HB3 | 2:B:1197:PRO:HA | 1.95 | 0.47 |
| 3:C:67:LEU:HD11 | 3:C:155:LEU:HD13 | 1.95 | 0.47 |
| 2:B:864:LYS:HB3 | 2:B:871:THR:HA | 1.96 | 0.47 |
| 8:H:138:GLU:O | 8:H:139:ASN:C | 2.53 | 0.47 |
| 3:C:35:ARG:O | 3:C:38:ILE:N | 2.47 | 0.47 |
| 2:B:284:ILE:HD13 | 2:B:333:PHE:CD2 | 2.49 | 0.47 |
| 3:C:62:PHE:O | 3:C:66:ARG:HG3 | 2.13 | 0.47 |
| 3:C:66:ARG:CZ | 10:J:2:ILE:HG21 | 2.44 | 0.47 |
| 2:B:269:ILE:CD1 | 2:B:386:LEU:HD21 | 2.39 | 0.47 |
| 10:J:57:ILE:HG12 | 10:J:61:LEU:HD11 | 1.94 | 0.47 |
| 11:K:59:ALA:HA | 11:K:74:ARG:O | 2.15 | 0.47 |
| 2:B:1158:PHE:HE2 | 2:B:1201:LYS:HE3 | 1.80 | 0.47 |
| 9:I:54:GLU:O | 9:I:89:GLN:HG2 | 2.14 | 0.47 |
| 2:B:871:THR:HG22 | 2:B:872:GLU:O | 2.14 | 0.47 |
| 1:A:1386:ARG:HE | 1:A:1387:HIS:CE1 | 2.32 | 0.47 |
| 8:H:40:LEU:CD2 | 8:H:42:ILE:HD11 | 2.39 | 0.47 |
| 2:B:726:ALA:CB | 2:B:1051:THR:HG21 | 2.45 | 0.47 |
| 1:A:1237:ILE:HG22 | 1:A:1238:ILE:N | 2.29 | 0.47 |
| 5:E:78:LEU:HD21 | 5:E:80:VAL:HG22 | 1.95 | 0.47 |
| 2:B:46:GLN:HE21 | 2:B:496:ARG:HG2 | 1.78 | 0.47 |
| 2:B:51:PHE:CD2 | 2:B:173:MET:HB3 | 2.49 | 0.47 |
| 2:B:1182:CYS:O | 2:B:1183:LYS:O | 2.31 | 0.47 |
| 1:A:1225:PHE:O | 1:A:1240:CYS:HA | 2.14 | 0.47 |
| 1:A:1134:ILE:HD11 | 1:A:1321:GLY:HA3 | 1.96 | 0.47 |
| 12:L:30:ILE:CD1 | 12:L:59:ALA:HA | 2.45 | 0.47 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CH2 | 2.48 | 0.47 |
| 8:H:47:PHE:CD1 | 8:H:95:TYR:HB2 | 2.50 | 0.47 |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HH11 | 1.60 | 0.47 |
| 2:B:1054:GLY:O | 2:B:1058:LEU:HG | 2.13 | 0.47 |
| 2:B:780:VAL:HG21 | 10:J:56:LEU:HD11 | 1.97 | 0.47 |
| 2:B:842:ASN:HD22 | 2:B:845:SER:HB3 | 1.80 | 0.47 |
| 9:I:75:CYS:O | 9:I:76:PRO:C | 2.52 | 0.47 |
| 1:A:994:GLN:NE2 | 1:A:1019:CYS:HB3 | 2.27 | 0.47 |
| 2:B:1169:MET:SD | 2:B:1201:LYS:HG2 | 2.54 | 0.47 |
| 10:J:44:TYR:HA | 10:J:47:ARG:HB2 | 1.95 | 0.47 |
| 1:A:20:GLY:HA2 | 1:A:1413:GLY:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1051:THR:HG21 | 2:B:1053:GLU:HB2 | 1.97 | 0.47 |
| 2:B:845:SER:HB2 | 10:J:8:PHE:HB3 | 1.96 | 0.47 |
| 1:A:14:VAL:H | 1:A:1432:GLN:HE22 | 1.61 | 0.47 |
| 2:B:230:ALA:C | 2:B:232:SER:H | 2.17 | 0.47 |
| 2:B:123:THR:O | 2:B:125:SER:N | 2.47 | 0.47 |
| 2:B:1124:ARG:O | 2:B:1125:ASP:HB3 | 2.14 | 0.47 |
| 1:A:517:ASN:ND2 | 1:A:1362:TYR:CE2 | 2.83 | 0.47 |
| 2:B:332:ASP:C | 2:B:334:ILE:N | 2.68 | 0.47 |
| 5:E:7:ARG:C | 5:E:9:ILE:H | 2.17 | 0.47 |
| 1:A:381:THR:CG2 | 1:A:383:TYR:CD1 | 2.98 | 0.47 |
| 2:B:860:MET:HB2 | 2:B:965:LYS:HG2 | 1.97 | 0.47 |
| 2:B:1013:ASN:OD1 | 2:B:1015:HIS:HB2 | 2.15 | 0.47 |
| 1:A:83:HIS:CE1 | 1:A:238:CYS:SG | 3.08 | 0.47 |
| 2:B:62:ILE:HG21 | 2:B:417:PHE:HD2 | 1.80 | 0.47 |
| 2:B:1116:ARG:NH1 | 2:B:1198:TYR:CD1 | 2.83 | 0.47 |
| 6:F:109:VAL:HG11 | 6:F:123:LYS:HG2 | 1.96 | 0.47 |
| 2:B:750:GLY:O | 2:B:751:VAL:C | 2.53 | 0.47 |
| 1:A:167:CYS:C | 1:A:169:ASN:H | 2.18 | 0.47 |
| 1:A:848:ILE:CD1 | 1:A:1374:VAL:HG21 | 2.45 | 0.47 |
| 2:B:236:HIS:CE1 | 2:B:389:ALA:HA | 2.49 | 0.47 |
| 1:A:890:ASP:H | 1:A:1296:GLY:HA3 | 1.78 | 0.47 |
| 1:A:12:ARG:HD3 | 2:B:1218:THR:HB | 1.97 | 0.47 |
| 1:A:22:PHE:HB2 | 2:B:1211:ASN:CG | 2.35 | 0.47 |
| 3:C:262:LEU:O | 3:C:265:MET:HB3 | 2.15 | 0.47 |
| 1:A:515:GLN:HA | 1:A:1367:HIS:NE2 | 2.29 | 0.47 |
| 1:A:666:ILE:O | 1:A:667:GLY:C | 2.53 | 0.47 |
| 2:B:512:ARG:NH2 | 2:B:535:LEU:HD11 | 2.02 | 0.47 |
| 8:H:125:LEU:HG | 8:H:130:ARG:CZ | 2.43 | 0.47 |
| 5:E:58:MET:O | 5:E:59:SER:C | 2.53 | 0.47 |
| 2:B:1198:TYR:HE1 | 2:B:1201:LYS:HZ2 | 1.61 | 0.47 |
| 1:A:294:SER:HA | 1:A:297:GLN:HB3 | 1.96 | 0.47 |
| 1:A:90:VAL:HG21 | 1:A:296:LEU:HG | 1.95 | 0.47 |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:N | 2.30 | 0.47 |
| 9:I:100:PHE:HZ | 9:I:118:ARG:HH12 | 1.62 | 0.47 |
| 1:A:1364:ASN:HD22 | 1:A:1365:TYR:N | 2.13 | 0.47 |
| 1:A:783:THR:CG2 | 1:A:815:PHE:CE2 | 2.97 | 0.47 |
| 9:I:74:GLU:OE1 | 9:I:79:HIS:ND1 | 2.47 | 0.47 |
| 6:F:101:ILE:HD11 | 6:F:124:GLU:OE1 | 2.15 | 0.47 |
| 11:K:83:PRO:O | 11:K:87:LEU:N | 2.46 | 0.47 |
| 1:A:829:VAL:O | 1:A:831:THR:N | 2.48 | 0.47 |
| 2:B:773:MET:SD | 2:B:987:LYS:HD2 | 2.54 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:798:TYR:CD2 | 10:J:4:PRO:HG3 | 2.49 | 0.47 |
| 1:A:567:LYS:CD | 1:A:568:PRO:HD2 | 2.45 | 0.47 |
| 8:H:49:VAL:CG1 | 8:H:50:ALA:H | 2.27 | 0.47 |
| 1:A:1237:ILE:CG2 | 1:A:1238:ILE:N | 2.78 | 0.47 |
| 1:A:1392:SER:O | 1:A:1393:ASN:ND2 | 2.48 | 0.47 |
| 1:A:530:GLY:O | 1:A:531:ILE:C | 2.54 | 0.47 |
| 5:E:96:PHE:CE1 | 5:E:100:ILE:HD11 | 2.50 | 0.47 |
| 2:B:210:LYS:HE2 | 2:B:461:LEU:O | 2.14 | 0.47 |
| 1:A:152:VAL:CG1 | 1:A:153:PRO:HD2 | 2.45 | 0.47 |
| 1:A:116:ASP:HB2 | 1:A:118:HIS:CD2 | 2.49 | 0.47 |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HG2 | 1.67 | 0.46 |
| 2:B:640:VAL:HG12 | 2:B:640:VAL:O | 2.15 | 0.46 |
| 5:E:135:PHE:HD2 | 5:E:140:LEU:HD21 | 1.79 | 0.46 |
| 1:A:540:PHE:C | 1:A:541:ILE:HD12 | 2.35 | 0.46 |
| 1:A:352:VAL:HG12 | 1:A:353:ILE:N | 2.29 | 0.46 |
| 8:H:113:ALA:HA | 8:H:125:LEU:O | 2.15 | 0.46 |
| 2:B:314:LEU:O | 2:B:315:LYS:C | 2.53 | 0.46 |
| 6:F:101:ILE:HD13 | 6:F:120:ILE:CG2 | 2.45 | 0.46 |
| 1:A:964:ILE:HD13 | 1:A:1035:TYR:CZ | 2.50 | 0.46 |
| 1:A:645:LEU:O | 1:A:649:ILE:HG13 | 2.16 | 0.46 |
| 1:A:975:HIS:ND1 | 1:A:1036:ARG:HG3 | 2.30 | 0.46 |
| 1:A:67:CYS:SG | 1:A:77:CYS:SG | 3.11 | 0.46 |
| 2:B:96:TYR:CD1 | 2:B:96:TYR:N | 2.83 | 0.46 |
| 8:H:26:ILE:HD13 | 8:H:49:VAL:HG11 | 1.97 | 0.46 |
| 2:B:519:TRP:HE1 | 2:B:635:ARG:HH22 | 1.64 | 0.46 |
| 2:B:802:PRO:HA | 2:B:822:ASN:HD21 | 1.79 | 0.46 |
| 2:B:906:SER:CB | 2:B:946:ASN:HB2 | 2.45 | 0.46 |
| 2:B:487:THR:HG22 | 2:B:489:SER:N | 2.24 | 0.46 |
| 3:C:258:ILE:N | 3:C:258:ILE:HD12 | 2.30 | 0.46 |
| 1:A:1173:HIS:CD2 | 1:A:1227:ILE:HG23 | 2.51 | 0.46 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:H | 1.79 | 0.46 |
| 1:A:573:SER:OG | 1:A:576:GLN:HG3 | 2.15 | 0.46 |
| 1:A:568:PRO:HB2 | 3:C:221:TYR:CZ | 2.50 | 0.46 |
| 10:J:1:MET:O | 10:J:2:ILE:O | 2.33 | 0.46 |
| 2:B:100:PRO:O | 2:B:180:TYR:OH | 2.31 | 0.46 |
| 1:A:804:TYR:HE1 | 2:B:1021:MET:CE | 2.28 | 0.46 |
| 2:B:864:LYS:H | 2:B:872:GLU:CG | 2.28 | 0.46 |
| 1:A:849:MET:HB2 | 1:A:1063:MET:SD | 2.55 | 0.46 |
| 2:B:377:PHE:C | 2:B:379:GLY:N | 2.68 | 0.46 |
| 1:A:923:LEU:O | 1:A:927:VAL:HG23 | 2.14 | 0.46 |
| 1:A:869:GLY:O | 5:E:204:THR:HG21 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:31:TRP:CE3 | 2:B:34:ILE:HD12 | 2.50 | 0.46 |
| 1:A:222:LEU:O | 1:A:224:PHE:N | 2.46 | 0.46 |
| 2:B:100:PRO:HD2 | 2:B:180:TYR:CE1 | 2.50 | 0.46 |
| 1:A:1209:MET:CG | 1:A:1236:LEU:HD22 | 2.45 | 0.46 |
| 2:B:851:PHE:O | 2:B:974:PRO:HD3 | 2.15 | 0.46 |
| 2:B:321:GLY:C | 2:B:323:VAL:H | 2.17 | 0.46 |
| 2:B:708:GLU:CG | 2:B:709:ASP:N | 2.69 | 0.46 |
| 1:A:549:MET:HE1 | 1:A:656:TRP:CD1 | 2.39 | 0.46 |
| 1:A:1017:LEU:O | 1:A:1018:PHE:C | 2.53 | 0.46 |
| 2:B:167:ILE:HG22 | 2:B:167:ILE:O | 2.14 | 0.46 |
| 1:A:477:PRO:HG2 | 1:A:521:MET:HG2 | 1.98 | 0.46 |
| 1:A:329:LEU:HA | 1:A:335:ARG:HB2 | 1.98 | 0.46 |
| 11:K:91:CYS:O | 11:K:94:ILE:HB | 2.16 | 0.46 |
| 2:B:653:VAL:C | 2:B:654:ARG:HG2 | 2.36 | 0.46 |
| 9:I:7:CYS:CB | 9:I:14:LEU:HD21 | 2.33 | 0.46 |
| 1:A:1410:PHE:C | 1:A:1412:ALA:N | 2.67 | 0.46 |
| 2:B:800:GLN:HB3 | 10:J:52:THR:HG22 | 1.97 | 0.46 |
| 2:B:230:ALA:N | 2:B:231:PRO:HD2 | 2.31 | 0.46 |
| 1:A:897:TYR:HD2 | 1:A:936:LEU:HD13 | 1.78 | 0.46 |
| 6:F:117:PRO:O | 6:F:120:ILE:HB | 2.16 | 0.46 |
| 1:A:889:SER:HB3 | 1:A:1297:GLU:HG3 | 1.98 | 0.46 |
| 3:C:38:ILE:HG13 | 3:C:176:ILE:HD12 | 1.97 | 0.46 |
| 1:A:1140:HIS:HB2 | 1:A:1276:VAL:O | 2.16 | 0.46 |
| 1:A:666:ILE:CD1 | 2:B:1030:LEU:HD22 | 2.41 | 0.46 |
| 1:A:852:TYR:OH | 6:F:89:GLU:OE2 | 2.28 | 0.46 |
| 2:B:294:ASP:H | 9:I:12:ASN:ND2 | 2.13 | 0.46 |
| 2:B:1100:ASP:HA | 2:B:1103:ILE:CG1 | 2.46 | 0.46 |
| 2:B:201:GLY:H | 2:B:202:TYR:HD2 | 1.63 | 0.46 |
| 1:A:1390:ASN:HD21 | 1:A:1399:ARG:HA | 1.78 | 0.46 |
| 2:B:316:PRO:HA | 2:B:319:GLU:HG2 | 1.98 | 0.46 |
| 1:A:658:LEU:HD13 | 2:B:831:SER:HA | 1.98 | 0.46 |
| 1:A:1074:GLU:C | 1:A:1076:ALA:H | 2.18 | 0.46 |
| 8:H:114:VAL:O | 8:H:124:ARG:HA | 2.16 | 0.46 |
| 9:I:2:THR:OG1 | 9:I:45:ARG:HB3 | 2.15 | 0.46 |
| 2:B:680:THR:O | 2:B:683:SER:OG | 2.34 | 0.46 |
| 2:B:282:ILE:HG13 | 2:B:283:VAL:N | 2.31 | 0.46 |
| 3:C:180:TYR:O | 3:C:181:ASP:HB3 | 2.15 | 0.46 |
| 5:E:179:GLN:OE1 | 5:E:179:GLN:HA | 2.16 | 0.46 |
| 2:B:332:ASP:C | 2:B:334:ILE:H | 2.17 | 0.46 |
| 2:B:300:HIS:ND1 | 2:B:376:PHE:CE2 | 2.83 | 0.46 |
| 1:A:55:ASP:HB3 | 1:A:56:PRO:HD3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1072:MET:O | 2:B:1081:LEU:HB2 | 2.15 | 0.46 |
| 1:A:420:ARG:O | 1:A:424:ILE:HG13 | 2.16 | 0.46 |
| 1:A:679:ILE:HG23 | 1:A:729:ALA:CB | 2.39 | 0.46 |
| 3:C:252:GLN:CG | 11:K:95:ILE:HG23 | 2.46 | 0.46 |
| 2:B:1017:ILE:HB | 2:B:1018:PRO:HD3 | 1.98 | 0.46 |
| 5:E:190:LEU:HD11 | 5:E:196:VAL:HG11 | 1.98 | 0.46 |
| 8:H:26:ILE:CD1 | 8:H:49:VAL:HG11 | 2.46 | 0.46 |
| 1:A:1327:ILE:O | 5:E:147:HIS:HE1 | 1.98 | 0.46 |
| 3:C:62:PHE:C | 3:C:62:PHE:CD2 | 2.89 | 0.46 |
| 1:A:383:TYR:HB3 | 6:F:115:THR:CG2 | 2.44 | 0.46 |
| 2:B:1085:ILE:HG22 | 2:B:1086:PHE:N | 2.31 | 0.46 |
| 1:A:112:LYS:HG2 | 1:A:113:LEU:N | 2.30 | 0.46 |
| 1:A:890:ASP:N | 1:A:1296:GLY:HA3 | 2.30 | 0.46 |
| 1:A:881:GLN:OE1 | 1:A:959:ASN:HA | 2.15 | 0.46 |
| 1:A:701:LEU:HA | 9:I:115:LYS:HE3 | 1.98 | 0.46 |
| 9:I:34:TYR:O | 9:I:35:VAL:HG23 | 2.16 | 0.46 |
| 2:B:322:PHE:CG | 2:B:322:PHE:O | 2.69 | 0.46 |
| 1:A:517:ASN:OD1 | 1:A:517:ASN:O | 2.34 | 0.46 |
| 1:A:786:HIS:CE1 | 2:B:742:GLU:OE1 | 2.64 | 0.46 |
| 2:B:280:ILE:HD13 | 2:B:334:ILE:HG12 | 1.95 | 0.46 |
| 9:I:7:CYS:HB2 | 9:I:14:LEU:CD2 | 2.34 | 0.46 |
| 2:B:1104:HIS:HB2 | 2:B:1122:ARG:CD | 2.44 | 0.46 |
| 2:B:1085:ILE:CG2 | 2:B:1086:PHE:N | 2.78 | 0.46 |
| 2:B:1106:ARG:CD | 2:B:1126:GLY:O | 2.62 | 0.46 |
| 1:A:535:THR:HG22 | 1:A:616:VAL:HA | 1.98 | 0.46 |
| 1:A:446:ARG:HG2 | 1:A:446:ARG:NH1 | 2.28 | 0.46 |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:H | 1.81 | 0.46 |
| 1:A:87:ALA:HB3 | 1:A:276:LEU:CD2 | 2.45 | 0.46 |
| 1:A:1394:THR:HG21 | 1:A:1398:MET:SD | 2.56 | 0.46 |
| 1:A:738:LYS:NZ | 3:C:194:GLU:CA | 2.79 | 0.46 |
| 1:A:50:ILE:HG22 | 1:A:51:GLY:H | 1.81 | 0.46 |
| 1:A:53:LEU:HD13 | 1:A:263:THR:HG23 | 1.97 | 0.46 |
| 10:J:32:GLU:CD | 10:J:32:GLU:H | 2.19 | 0.46 |
| 2:B:893:LEU:HD22 | 2:B:897:GLY:O | 2.16 | 0.46 |
| 1:A:958:VAL:HG22 | 1:A:1052:GLN:HB3 | 1.98 | 0.46 |
| 5:E:112:TYR:CE2 | 5:E:134:THR:HB | 2.51 | 0.46 |
| 12:L:45:ALA:O | 12:L:46:VAL:CG2 | 2.64 | 0.45 |
| 1:A:1410:PHE:C | 1:A:1412:ALA:H | 2.19 | 0.45 |
| 2:B:229:ALA:HB1 | 2:B:231:PRO:HD2 | 1.99 | 0.45 |
| 2:B:1106:ARG:HG2 | 2:B:1107:ALA:N | 2.31 | 0.45 |
| 1:A:893:PHE:CD1 | 1:A:940:ARG:HD2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:96:PHE:CE2 | 5:E:110:PHE:HB2 | 2.50 | 0.45 |
| 2:B:686:ASN:C | 2:B:688:GLY:N | 2.70 | 0.45 |
| 1:A:556:TRP:CZ3 | 1:A:558:GLY:HA2 | 2.51 | 0.45 |
| 2:B:50:SER:O | 2:B:53:GLN:HB3 | 2.16 | 0.45 |
| 2:B:1120:GLU:HG2 | 2:B:1121:GLY:N | 2.31 | 0.45 |
| 9:I:91:ARG:HD3 | 9:I:91:ARG:HA | 1.75 | 0.45 |
| 1:A:1041:ALA:O | 1:A:1044:TRP:HB3 | 2.15 | 0.45 |
| 2:B:25:ILE:HD11 | 2:B:653:VAL:CB | 2.46 | 0.45 |
| 2:B:704:ALA:HB2 | 2:B:738:PHE:CE1 | 2.51 | 0.45 |
| 2:B:345:LYS:O | 2:B:347:LYS:N | 2.49 | 0.45 |
| 2:B:956:THR:HG21 | 2:B:960:GLY:HA2 | 1.96 | 0.45 |
| 2:B:1098:MET:O | 2:B:1099:VAL:C | 2.53 | 0.45 |
| 1:A:592:ASP:N | 1:A:595:THR:OG1 | 2.48 | 0.45 |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:HD12 | 1.98 | 0.45 |
| 2:B:914:LYS:H | 2:B:938:SER:HB3 | 1.81 | 0.45 |
| 2:B:830:TYR:CE2 | 2:B:1000:PRO:HD3 | 2.50 | 0.45 |
| 3:C:18:VAL:O | 3:C:18:VAL:HG12 | 2.15 | 0.45 |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:H | 1.81 | 0.45 |
| 2:B:515:HIS:CD2 | 2:B:517:THR:OG1 | 2.66 | 0.45 |
| 2:B:758:PHE:C | 2:B:760:ASP:N | 2.68 | 0.45 |
| 2:B:890:TYR:C | 2:B:892:LYS:H | 2.19 | 0.45 |
| 3:C:263:THR:C | 3:C:265:MET:H | 2.18 | 0.45 |
| 2:B:664:THR:HG1 | 2:B:678:GLU:N | 2.14 | 0.45 |
| 1:A:542:GLU:C | 1:A:546:VAL:HG23 | 2.36 | 0.45 |
| 1:A:567:LYS:CB | 1:A:568:PRO:CD | 2.67 | 0.45 |
| 2:B:168:GLY:H | 2:B:450:ALA:HB1 | 1.82 | 0.45 |
| 2:B:963:PHE:HE2 | 2:B:965:LYS:HE3 | 1.81 | 0.45 |
| 1:A:223:GLY:HA3 | 1:A:1415:SER:HB3 | 1.98 | 0.45 |
| 2:B:1200:ALA:O | 2:B:1201:LYS:C | 2.54 | 0.45 |
| 2:B:574:SER:HB3 | 2:B:577:ALA:HB2 | 1.98 | 0.45 |
| 1:A:1037:LEU:HD13 | 1:A:1042:PHE:HA | 1.98 | 0.45 |
| 2:B:1177:HIS:C | 2:B:1179:GLN:N | 2.68 | 0.45 |
| 1:A:848:ILE:HD13 | 1:A:864:ILE:HD13 | 1.98 | 0.45 |
| 2:B:238:ALA:HB3 | 2:B:256:VAL:HB | 1.98 | 0.45 |
| 5:E:10:SER:O | 5:E:14:ARG:HG3 | 2.16 | 0.45 |
| 8:H:40:LEU:HD13 | 8:H:123:MET:HB2 | 1.99 | 0.45 |
| 1:A:1155:ASP:CG | 1:A:1162:VAL:HG23 | 2.37 | 0.45 |
| 2:B:549:THR:H | 2:B:628:THR:HG22 | 1.81 | 0.45 |
| 2:B:515:HIS:O | 2:B:516:ASN:C | 2.54 | 0.45 |
| 1:A:1336:MET:SD | 1:A:1381:LEU:HG | 2.56 | 0.45 |
| 2:B:295:GLY:O | 2:B:299:GLU:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1171:VAL:HG13 | 2:B:1191:ILE:HD13 | 1.99 | 0.45 |
| 11:K:61:TYR:CD1 | 11:K:61:TYR:C | 2.89 | 0.45 |
| 5:E:94:LYS:O | 5:E:98:ILE:HG13 | 2.16 | 0.45 |
| 2:B:371:GLU:N | 2:B:371:GLU:OE1 | 2.49 | 0.45 |
| 2:B:955:THR:HG1 | 12:L:55:ILE:HA | 1.81 | 0.45 |
| 5:E:205:SER:O | 5:E:206:GLY:C | 2.54 | 0.45 |
| 9:I:92:ARG:CG | 9:I:93:LYS:H | 2.30 | 0.45 |
| 8:H:111:LEU:HA | 8:H:127:GLY:O | 2.17 | 0.45 |
| 1:A:1209:MET:CE | 1:A:1236:LEU:HB3 | 2.47 | 0.45 |
| 2:B:1182:CYS:O | 2:B:1183:LYS:HD2 | 2.15 | 0.45 |
| 2:B:205:ILE:HG12 | 2:B:461:LEU:HB3 | 1.99 | 0.45 |
| 3:C:249:ASP:O | 3:C:252:GLN:HB3 | 2.16 | 0.45 |
| 1:A:456:MET:HB2 | 1:A:478:TYR:OH | 2.17 | 0.45 |
| 2:B:1060:ARG:C | 2:B:1062:HIS:N | 2.69 | 0.45 |
| 5:E:185:ALA:CB | 5:E:190:LEU:HD12 | 2.47 | 0.45 |
| 1:A:1155:ASP:OD1 | 1:A:1162:VAL:HG23 | 2.17 | 0.45 |
| 2:B:276:ILE:HD13 | 2:B:334:ILE:CG2 | 2.46 | 0.45 |
| 2:B:977:GLY:C | 2:B:1099:VAL:HG23 | 2.37 | 0.45 |
| 2:B:824:ILE:CG2 | 2:B:1087:PHE:CE2 | 3.00 | 0.45 |
| 9:I:29:CYS:O | 9:I:31:THR:N | 2.49 | 0.45 |
| 3:C:242:GLN:OE1 | 3:C:242:GLN:HA | 2.16 | 0.45 |
| 1:A:1410:PHE:HD2 | 2:B:1212:ILE:HD11 | 1.70 | 0.45 |
| 2:B:121:ASN:HA | 2:B:207:GLY:CA | 2.46 | 0.45 |
| 2:B:100:PRO:HA | 2:B:125:SER:O | 2.16 | 0.45 |
| 3:C:5:GLY:O | 3:C:6:PRO:C | 2.54 | 0.45 |
| 2:B:995:ARG:HH11 | 2:B:995:ARG:HB2 | 1.81 | 0.45 |
| 8:H:84:ALA:HA | 8:H:87:ARG:HB2 | 1.98 | 0.45 |
| 2:B:215:GLN:HB2 | 2:B:407:ASP:HB2 | 1.98 | 0.45 |
| 1:A:35:ILE:HD12 | 1:A:241:VAL:HG21 | 1.98 | 0.45 |
| 2:B:260:GLY:HA3 | 2:B:267:ARG:HG2 | 1.98 | 0.45 |
| 3:C:62:PHE:C | 3:C:62:PHE:HD2 | 2.20 | 0.45 |
| 1:A:1405:THR:O | 1:A:1406:VAL:C | 2.54 | 0.45 |
| 1:A:418:SER:O | 1:A:421:ALA:N | 2.49 | 0.45 |
| 8:H:38:LEU:HD13 | 8:H:125:LEU:CD1 | 2.46 | 0.45 |
| 1:A:535:THR:HG21 | 1:A:616:VAL:CA | 2.43 | 0.45 |
| 2:B:763:GLN:CG | 2:B:765:PRO:HD2 | 2.40 | 0.45 |
| 2:B:408:LEU:HA | 2:B:408:LEU:HD12 | 1.71 | 0.45 |
| 1:A:994:GLN:HE21 | 1:A:1019:CYS:CB | 2.26 | 0.45 |
| 1:A:335:ARG:HA | 1:A:335:ARG:HD3 | 1.87 | 0.45 |
| 2:B:1117:GLN:NE2 | 2:B:1156:ASP:OD2 | 2.48 | 0.45 |
| 2:B:1185:CYS:O | 2:B:1186:ASP:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:101:ALA:HB2 | 8:H:116:TYR:CD2 | 2.51 | 0.45 |
| 10:J:5:VAL:O | 10:J:6:ARG:HB2 | 2.15 | 0.45 |
| 1:A:845:LEU:O | 1:A:848:ILE:HG13 | 2.17 | 0.45 |
| 1:A:573:SER:H | 1:A:576:GLN:HG3 | 1.81 | 0.45 |
| 3:C:52:GLU:HB3 | 3:C:154:LYS:HB3 | 1.99 | 0.45 |
| 1:A:1317:MET:CA | 1:A:1322:ILE:HD11 | 2.46 | 0.45 |
| 1:A:960:ILE:HD12 | 1:A:1021:LEU:HD21 | 1.99 | 0.45 |
| 2:B:361:LEU:O | 2:B:363:HIS:O | 2.35 | 0.45 |
| 1:A:340:LEU:HD21 | 2:B:1200:ALA:CA | 2.47 | 0.45 |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:N | 2.31 | 0.45 |
| 1:A:152:VAL:HG13 | 1:A:153:PRO:HD2 | 1.99 | 0.45 |
| 9:I:34:TYR:O | 9:I:35:VAL:CG2 | 2.65 | 0.45 |
| 3:C:69:LEU:HA | 3:C:69:LEU:HD12 | 1.76 | 0.45 |
| 1:A:1114:PRO:O | 1:A:1330:ASN:OD1 | 2.35 | 0.45 |
| 9:I:8:ARG:HG3 | 9:I:9:ASP:CG | 2.37 | 0.45 |
| 1:A:351:THR:CG2 | 2:B:1103:ILE:HA | 2.36 | 0.45 |
| 2:B:1013:ASN:OD1 | 2:B:1015:HIS:N | 2.44 | 0.45 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:CB | 2.59 | 0.45 |
| 12:L:38:LEU:HG | 12:L:39:SER:H | 1.82 | 0.45 |
| 2:B:1158:PHE:CD2 | 2:B:1198:TYR:HD1 | 2.35 | 0.45 |
| 3:C:8:VAL:CG1 | 3:C:9:LYS:N | 2.80 | 0.45 |
| 1:A:778:GLY:HA3 | 2:B:516:ASN:CB | 2.46 | 0.45 |
| 8:H:116:TYR:HE2 | 8:H:140:ALA:CB | 2.30 | 0.45 |
| 2:B:995:ARG:NH1 | 2:B:997:GLU:OE1 | 2.49 | 0.45 |
| 2:B:973:ILE:CG2 | 2:B:974:PRO:HD2 | 2.47 | 0.45 |
| 1:A:829:VAL:C | 1:A:831:THR:N | 2.70 | 0.45 |
| 3:C:17:ASN:OD1 | 3:C:233:GLU:HG2 | 2.16 | 0.45 |
| 2:B:640:VAL:HG23 | 2:B:740:HIS:HA | 1.97 | 0.45 |
| 1:A:78:PRO:O | 1:A:79:GLY:C | 2.56 | 0.45 |
| 2:B:1159:ARG:NE | 2:B:1193:GLN:NE2 | 2.33 | 0.45 |
| 1:A:80:HIS:O | 1:A:243:PRO:HB3 | 2.17 | 0.45 |
| 1:A:47:ARG:O | 1:A:48:ALA:HB2 | 2.16 | 0.45 |
| 10:J:48:ARG:HH21 | 10:J:49:MET:CE | 2.24 | 0.45 |
| 2:B:605:ARG:CZ | 2:B:639:ILE:HD13 | 2.46 | 0.45 |
| 1:A:815:PHE:O | 1:A:818:MET:N | 2.50 | 0.45 |
| 9:I:75:CYS:C | 9:I:77:LYS:H | 2.20 | 0.45 |
| 2:B:426:LYS:O | 2:B:430:ARG:HG3 | 2.17 | 0.45 |
| 2:B:361:LEU:N | 2:B:362:PRO:HD2 | 2.31 | 0.45 |
| 2:B:805:THR:HA | 2:B:809:MET:HE1 | 1.98 | 0.45 |
| 11:K:73:LEU:CD2 | 11:K:75:ILE:HD11 | 2.46 | 0.45 |
| 2:B:365:THR:CG2 | 2:B:367:LEU:H | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:98:TYR:O | 8:H:118:PHE:HD2 | 1.99 | 0.45 |
| 2:B:370:PHE:N | 2:B:371:GLU:OE1 | 2.50 | 0.45 |
| 3:C:76:ASP:OD2 | 3:C:128:ASN:N | 2.47 | 0.45 |
| 1:A:210:ILE:O | 1:A:214:ILE:HG13 | 2.17 | 0.45 |
| 2:B:707:PRO:O | 2:B:708:GLU:O | 2.35 | 0.44 |
| 5:E:147:HIS:CD2 | 5:E:149:LEU:H | 2.35 | 0.44 |
| 3:C:73:GLN:NE2 | 3:C:75:MET:H | 1.97 | 0.44 |
| 1:A:388:LEU:O | 1:A:392:VAL:HG23 | 2.17 | 0.44 |
| 8:H:57:VAL:HG12 | 8:H:58:THR:N | 2.32 | 0.44 |
| 2:B:1154:ALA:O | 2:B:1155:SER:CB | 2.64 | 0.44 |
| 1:A:1428:VAL:HG13 | 2:B:1151:LEU:HD23 | 2.00 | 0.44 |
| 1:A:1208:THR:N | 1:A:1211:GLN:OE1 | 2.49 | 0.44 |
| 3:C:31:ASN:O | 3:C:35:ARG:HG3 | 2.17 | 0.44 |
| 2:B:332:ASP:O | 2:B:334:ILE:N | 2.50 | 0.44 |
| 1:A:243:PRO:HB2 | 1:A:245:PRO:HD2 | 1.99 | 0.44 |
| 1:A:709:THR:C | 1:A:711:ARG:N | 2.67 | 0.44 |
| 1:A:1436:ILE:O | 1:A:1437:GLY:C | 2.56 | 0.44 |
| 11:K:24:ASP:HB3 | 11:K:30:ALA:CB | 2.47 | 0.44 |
| 11:K:78:THR:O | 11:K:79:GLU:C | 2.56 | 0.44 |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:HD3 | 1.97 | 0.44 |
| 1:A:1152:ILE:HG23 | 1:A:1260:LEU:CD2 | 2.43 | 0.44 |
| 2:B:758:PHE:CZ | 2:B:1044:ALA:HA | 2.52 | 0.44 |
| 5:E:102:GLU:C | 5:E:104:ASN:H | 2.20 | 0.44 |
| 2:B:847:ASP:O | 3:C:65:HIS:HE1 | 2.01 | 0.44 |
| 5:E:138:ALA:C | 5:E:140:LEU:H | 2.21 | 0.44 |
| 3:C:236:GLY:C | 3:C:238:ILE:N | 2.69 | 0.44 |
| 9:I:106:CYS:O | 9:I:107:SER:HB2 | 2.18 | 0.44 |
| 1:A:885:THR:HG23 | 1:A:893:PHE:CE1 | 2.36 | 0.44 |
| 3:C:148:ARG:HD3 | 3:C:149:LYS:H | 1.83 | 0.44 |
| 1:A:265:LYS:HZ1 | 1:A:323:LYS:H | 1.62 | 0.44 |
| 1:A:219:PHE:CE2 | 1:A:231:PRO:HD2 | 2.52 | 0.44 |
| 6:F:111:LEU:C | 6:F:113:GLY:N | 2.71 | 0.44 |
| 1:A:1207:LEU:HA | 1:A:1211:GLN:OE1 | 2.17 | 0.44 |
| 2:B:986:GLN:OE1 | 2:B:986:GLN:CA | 2.64 | 0.44 |
| 1:A:84:ILE:HG23 | 1:A:84:ILE:O | 2.17 | 0.44 |
| 1:A:50:ILE:C | 1:A:52:GLY:N | 2.69 | 0.44 |
| 3:C:120:ILE:HD11 | 3:C:130:GLY:O | 2.17 | 0.44 |
| 8:H:40:LEU:HG | 8:H:42:ILE:HG13 | 1.98 | 0.44 |
| 1:A:571:LEU:HD22 | 8:H:46:LEU:HD11 | 1.99 | 0.44 |
| 1:A:1441:PHE:HB2 | 6:F:134:ILE:HG23 | 2.00 | 0.44 |
| 5:E:7:ARG:C | 5:E:9:ILE:N | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:77:ILE:CG2 | 3:C:161:LYS:HE3 | 2.48 | 0.44 |
| 8:H:5:LEU:O | 8:H:133:ASN:HB3 | 2.17 | 0.44 |
| 2:B:247:GLY:O | 2:B:248:SER:HB3 | 2.17 | 0.44 |
| 9:I:99:LEU:HB2 | 9:I:112:SER:CB | 2.46 | 0.44 |
| 2:B:642:ASP:O | 2:B:643:ASP:C | 2.56 | 0.44 |
| 2:B:281:PRO:HG2 | 2:B:284:ILE:CD1 | 2.45 | 0.44 |
| 1:A:1149:ALA:CB | 9:I:47:GLU:HA | 2.45 | 0.44 |
| 2:B:744:HIS:CD2 | 2:B:746:SER:OG | 2.70 | 0.44 |
| 1:A:1348:LEU:CD2 | 1:A:1372:VAL:HG13 | 2.39 | 0.44 |
| 1:A:233:TRP:O | 1:A:235:ILE:N | 2.50 | 0.44 |
| 2:B:915:THR:HG21 | 2:B:934:LYS:HG2 | 2.00 | 0.44 |
| 9:I:84:VAL:CG1 | 9:I:84:VAL:O | 2.65 | 0.44 |
| 2:B:904:ARG:CZ | 2:B:948:ILE:HD11 | 2.48 | 0.44 |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:HB | 2.00 | 0.44 |
| 2:B:200:GLY:HA2 | 2:B:202:TYR:CD2 | 2.50 | 0.44 |
| 1:A:1384:VAL:O | 1:A:1389:PHE:HE2 | 2.01 | 0.44 |
| 2:B:745:PRO:C | 2:B:747:MET:N | 2.70 | 0.44 |
| 1:A:42:ASP:OD1 | 1:A:45:GLN:O | 2.36 | 0.44 |
| 2:B:288:ALA:HA | 2:B:331:LEU:HD13 | 1.99 | 0.44 |
| 1:A:974:ASP:CB | 8:H:136:LYS:NZ | 2.80 | 0.44 |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 2.00 | 0.44 |
| 8:H:47:PHE:CB | 8:H:95:TYR:HD1 | 2.31 | 0.44 |
| 2:B:1002:THR:CG2 | 2:B:1004:GLU:HB2 | 2.47 | 0.44 |
| 1:A:326:ARG:HE | 1:A:1406:VAL:HG11 | 1.82 | 0.44 |
| 2:B:800:GLN:CB | 10:J:52:THR:HG22 | 2.47 | 0.44 |
| 11:K:24:ASP:OD1 | 11:K:26:LYS:N | 2.51 | 0.44 |
| 5:E:28:TYR:CE2 | 5:E:64:PRO:HG3 | 2.53 | 0.44 |
| 1:A:367:PRO:CB | 1:A:466:SER:HA | 2.47 | 0.44 |
| 1:A:1046:LEU:O | 1:A:1047:SER:C | 2.55 | 0.44 |
| 1:A:968:GLN:NE2 | 1:A:1035:TYR:HB2 | 2.32 | 0.44 |
| 2:B:113:TYR:CD2 | 2:B:192:LEU:HD22 | 2.53 | 0.44 |
| 10:J:16:ASP:OD1 | 10:J:17:LYS:HG3 | 2.17 | 0.44 |
| 1:A:1121:GLU:O | 1:A:1122:PRO:C | 2.56 | 0.44 |
| 2:B:650:GLU:HG2 | 2:B:654:ARG:NH1 | 2.33 | 0.44 |
| 1:A:1441:PHE:HB2 | 6:F:134:ILE:CG2 | 2.47 | 0.44 |
| 5:E:133:GLU:HB3 | 5:E:135:PHE:HE1 | 1.83 | 0.44 |
| 2:B:702:LEU:HD21 | 2:B:735:ALA:HB1 | 1.98 | 0.44 |
| 1:A:591:PHE:HD2 | 1:A:595:THR:HB | 1.83 | 0.44 |
| 1:A:13:THR:HG23 | 1:A:1432:GLN:CD | 2.38 | 0.44 |
| 3:C:22:LEU:CD2 | 3:C:25:VAL:HG21 | 2.37 | 0.44 |
| 2:B:315:LYS:N | 2:B:316:PRO:HD2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:999:MET:HE2 | 2:B:1011:ILE:HD11 | 1.99 | 0.44 |
| 1:A:21:LEU:HD21 | 1:A:95:PHE:CZ | 2.53 | 0.44 |
| 2:B:56:ASP:HB3 | 2:B:57:TYR:CD1 | 2.52 | 0.44 |
| 2:B:864:LYS:HD3 | 2:B:871:THR:CB | 2.47 | 0.44 |
| 2:B:185:THR:H | 2:B:188:ASP:HB2 | 1.81 | 0.44 |
| 3:C:186:LEU:HD12 | 3:C:186:LEU:HA | 1.86 | 0.44 |
| 2:B:640:VAL:HG23 | 2:B:740:HIS:CA | 2.48 | 0.44 |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:N | 2.32 | 0.44 |
| 2:B:274:PRO:O | 2:B:276:ILE:N | 2.51 | 0.44 |
| 3:C:39:ALA:HA | 3:C:164:ALA:CB | 2.46 | 0.44 |
| 1:A:1415:SER:O | 1:A:1416:ALA:C | 2.56 | 0.44 |
| 1:A:825:ILE:C | 1:A:827:THR:N | 2.70 | 0.44 |
| 2:B:216:GLU:OE1 | 2:B:537:LYS:CE | 2.66 | 0.44 |
| 2:B:957:ASN:O | 2:B:958:GLN:C | 2.55 | 0.43 |
| 3:C:143:LEU:HD21 | 3:C:146:LYS:HE3 | 1.99 | 0.43 |
| 1:A:54:ASN:O | 1:A:55:ASP:HB2 | 2.18 | 0.43 |
| 1:A:595:THR:HG22 | 1:A:596:THR:N | 2.33 | 0.43 |
| 1:A:1166:ASP:CG | 1:A:1194:ARG:HH21 | 2.19 | 0.43 |
| 2:B:130:VAL:CG1 | 2:B:131:ASP:H | 2.29 | 0.43 |
| 1:A:533:LYS:C | 1:A:535:THR:N | 2.72 | 0.43 |
| 1:A:742:ASN:C | 1:A:745:GLN:HB2 | 2.38 | 0.43 |
| 2:B:855:PHE:HZ | 2:B:857:ARG:HH12 | 1.64 | 0.43 |
| 1:A:401:GLY:H | 1:A:435:HIS:HD2 | 1.66 | 0.43 |
| 2:B:102:VAL:HG21 | 2:B:112:LEU:HD13 | 1.99 | 0.43 |
| 11:K:55:LYS:HD3 | 11:K:78:THR:OG1 | 2.18 | 0.43 |
| 1:A:466:SER:HB3 | 11:K:2:ASN:HD22 | 1.82 | 0.43 |
| 1:A:741:ASN:HD22 | 1:A:743:VAL:N | 2.16 | 0.43 |
| 1:A:148:CYS:HB3 | 1:A:167:CYS:O | 2.18 | 0.43 |
| 1:A:69:THR:O | 2:B:1174:LYS:HG2 | 2.17 | 0.43 |
| 2:B:101:MET:HE2 | 2:B:169:ARG:NH1 | 2.33 | 0.43 |
| 1:A:115:LEU:HB2 | 1:A:122:MET:HE1 | 1.99 | 0.43 |
| 3:C:135:GLN:C | 3:C:136:ASP:O | 2.56 | 0.43 |
| 2:B:203:PHE:HE1 | 2:B:212:LEU:CD1 | 2.31 | 0.43 |
| 2:B:212:LEU:HD13 | 2:B:409:ALA:HA | 2.00 | 0.43 |
| 9:I:98:VAL:CG1 | 9:I:99:LEU:N | 2.81 | 0.43 |
| 1:A:1364:ASN:HD22 | 1:A:1366:ARG:N | 2.16 | 0.43 |
| 1:A:7:SER:OG | 2:B:1193:GLN:NE2 | 2.51 | 0.43 |
| 5:E:138:ALA:O | 5:E:140:LEU:N | 2.50 | 0.43 |
| 9:I:46:HIS:O | 9:I:47:GLU:HB2 | 2.18 | 0.43 |
| 1:A:1342:GLU:HG2 | 5:E:212:ARG:HH11 | 1.83 | 0.43 |
| 8:H:81:PRO:HD2 | 8:H:82:PRO:HD2 | 1.98 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:306:ASN:OD1 | 1:A:313:GLN:NE2 | 2.51 | 0.43 |
| 2:B:1116:ARG:CZ | 2:B:1198:TYR:CE1 | 3.01 | 0.43 |
| 1:A:673:GLY:N | 1:A:674:PRO:HD2 | 2.33 | 0.43 |
| 1:A:858:ASN:ND2 | 1:A:858:ASN:C | 2.68 | 0.43 |
| 2:B:577:ALA:HB1 | 2:B:589:VAL:HG12 | 2.00 | 0.43 |
| 2:B:864:LYS:HD3 | 2:B:871:THR:CA | 2.47 | 0.43 |
| 9:I:55:THR:HG21 | 9:I:109:ILE:CD1 | 2.48 | 0.43 |
| 2:B:806:THR:C | 2:B:808:ALA:N | 2.71 | 0.43 |
| 12:L:27:LEU:HD13 | 12:L:37:LYS:CB | 2.48 | 0.43 |
| 1:A:1097:GLY:C | 1:A:1099:PRO:HD2 | 2.39 | 0.43 |
| 3:C:59:ALA:O | 3:C:63:ILE:HG13 | 2.18 | 0.43 |
| 5:E:145:THR:HG21 | 5:E:187:TYR:CE2 | 2.53 | 0.43 |
| 1:A:1148:ILE:HD12 | 1:A:1196:GLU:HG2 | 2.01 | 0.43 |
| 1:A:131:SER:OG | 1:A:132:LYS:N | 2.51 | 0.43 |
| 2:B:705:MET:H | 2:B:710:LEU:CD1 | 2.32 | 0.43 |
| 1:A:852:TYR:CE2 | 6:F:136:ARG:NE | 2.86 | 0.43 |
| 1:A:901:LEU:HD13 | 1:A:919:ILE:CG2 | 2.48 | 0.43 |
| 2:B:1175:LEU:O | 2:B:1176:ASN:CG | 2.56 | 0.43 |
| 2:B:56:ASP:HB3 | 2:B:57:TYR:CE1 | 2.53 | 0.43 |
| 3:C:8:VAL:HA | 3:C:21:ILE:O | 2.19 | 0.43 |
| 1:A:518:LYS:HB2 | 1:A:519:PRO:HD2 | 2.00 | 0.43 |
| 11:K:92:ASN:O | 11:K:93:SER:C | 2.56 | 0.43 |
| 2:B:295:GLY:H | 2:B:298:LEU:HG | 1.84 | 0.43 |
| 2:B:1038:SER:HB3 | 2:B:1062:HIS:NE2 | 2.32 | 0.43 |
| 1:A:362:ASP:OD1 | 1:A:459:ARG:HD3 | 2.18 | 0.43 |
| 2:B:358:LYS:O | 2:B:359:GLU:OE1 | 2.36 | 0.43 |
| 1:A:103:CYS:O | 1:A:106:VAL:O | 2.35 | 0.43 |
| 12:L:43:THR:HG22 | 12:L:43:THR:O | 2.18 | 0.43 |
| 2:B:1106:ARG:NH1 | 2:B:1118:PRO:CB | 2.72 | 0.43 |
| 1:A:751:SER:OG | 2:B:1015:HIS:CE1 | 2.71 | 0.43 |
| 5:E:69:ILE:O | 5:E:73:PRO:HG3 | 2.19 | 0.43 |
| 1:A:343:LYS:NZ | 2:B:1156:ASP:OD2 | 2.49 | 0.43 |
| 2:B:526:GLU:CD | 2:B:752:ALA:HB3 | 2.38 | 0.43 |
| 1:A:84:ILE:CG2 | 1:A:239:LEU:HB3 | 2.48 | 0.43 |
| 1:A:850:VAL:O | 1:A:1060:PRO:HA | 2.18 | 0.43 |
| 1:A:494:SER:HB2 | 1:A:497:THR:OG1 | 2.18 | 0.43 |
| 8:H:12:VAL:HG13 | 8:H:26:ILE:HG23 | 2.01 | 0.43 |
| 2:B:709:ASP:C | 2:B:710:LEU:HD23 | 2.38 | 0.43 |
| 2:B:276:ILE:HD13 | 2:B:334:ILE:HG23 | 1.99 | 0.43 |
| 1:A:344:ARG:O | 2:B:1118:PRO:HG2 | 2.19 | 0.43 |
| 2:B:194:GLU:HA | 2:B:194:GLU:OE1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:9:LYS:HB2 | 3:C:21:ILE:HB | 1.98 | 0.43 |
| 1:A:86:LEU:HB3 | 1:A:296:LEU:HD21 | 1.99 | 0.43 |
| 2:B:781:PHE:CE2 | 2:B:795:ILE:HD11 | 2.53 | 0.43 |
| 3:C:249:ASP:OD1 | 3:C:253:LYS:HE3 | 2.19 | 0.43 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:HA | 2.00 | 0.43 |
| 3:C:135:GLN:O | 3:C:136:ASP:O | 2.37 | 0.43 |
| 1:A:68:GLN:O | 1:A:70:CYS:N | 2.52 | 0.43 |
| 2:B:690:VAL:HG12 | 2:B:691:GLU:N | 2.33 | 0.43 |
| 1:A:1118:VAL:O | 1:A:1305:VAL:HG13 | 2.18 | 0.43 |
| 1:A:1347:ALA:O | 1:A:1348:LEU:C | 2.55 | 0.43 |
| 1:A:102:VAL:HG21 | 1:A:234:MET:HE1 | 1.99 | 0.43 |
| 2:B:562:GLY:O | 2:B:563:MET:C | 2.56 | 0.43 |
| 1:A:774:ARG:O | 1:A:775:ILE:C | 2.57 | 0.43 |
| 3:C:123:ASN:ND2 | 3:C:125:MET:HG2 | 2.31 | 0.43 |
| 2:B:969:ARG:HG2 | 2:B:970:THR:N | 2.33 | 0.43 |
| 1:A:565:ILE:HD13 | 1:A:567:LYS:HE2 | 2.01 | 0.43 |
| 6:F:89:GLU:HB3 | 6:F:134:ILE:HD13 | 2.00 | 0.43 |
| 1:A:1116:LEU:HD12 | 1:A:1329:THR:HG1 | 1.77 | 0.43 |
| 10:J:48:ARG:NH2 | 10:J:49:MET:HE1 | 2.25 | 0.43 |
| 9:I:50:THR:HG22 | 9:I:52:ILE:N | 2.33 | 0.43 |
| 5:E:9:ILE:C | 5:E:11:ARG:N | 2.71 | 0.43 |
| 1:A:404:TYR:HA | 1:A:413:ILE:O | 2.18 | 0.43 |
| 5:E:59:SER:HA | 5:E:80:VAL:O | 2.19 | 0.43 |
| 2:B:1152:MET:SD | 2:B:1197:PRO:HD3 | 2.59 | 0.43 |
| 1:A:760:GLN:HB2 | 2:B:1021:MET:HE1 | 2.00 | 0.43 |
| 3:C:5:GLY:O | 3:C:6:PRO:O | 2.37 | 0.43 |
| 1:A:1158:PRO:HB3 | 1:A:1241:ARG:HH12 | 1.83 | 0.43 |
| 2:B:781:PHE:HE2 | 2:B:795:ILE:HD11 | 1.83 | 0.43 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:CB | 2.64 | 0.43 |
| 1:A:907:THR:HG22 | 1:A:908:LEU:H | 1.82 | 0.43 |
| 2:B:329:THR:O | 2:B:332:ASP:HB3 | 2.19 | 0.43 |
| 10:J:9:SER:HB2 | 10:J:45:CYS:HB2 | 2.01 | 0.43 |
| 1:A:709:THR:HG23 | 9:I:94:ASP:HA | 2.00 | 0.43 |
| 2:B:834:ASN:HB2 | 2:B:838:SER:O | 2.19 | 0.43 |
| 2:B:214:ALA:HB2 | 2:B:408:LEU:CD1 | 2.48 | 0.43 |
| 2:B:126:SER:OG | 2:B:172:ILE:HD11 | 2.18 | 0.43 |
| 2:B:579:ARG:HB2 | 2:B:586:TRP:HE1 | 1.84 | 0.43 |
| 1:A:644:LYS:O | 1:A:645:LEU:C | 2.55 | 0.43 |
| 2:B:446:LEU:HD23 | 2:B:446:LEU:N | 2.33 | 0.43 |
| 3:C:46:ILE:HG23 | 3:C:157:CYS:HB3 | 2.00 | 0.43 |
| 11:K:95:ILE:O | 11:K:98:LEU:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:21:TYR:CA | 10:J:39:LEU:HD11 | 2.49 | 0.43 |
| 2:B:1108:ARG:O | 2:B:1108:ARG:CG | 2.67 | 0.43 |
| 1:A:1068:ALA:O | 1:A:1069:ALA:C | 2.55 | 0.43 |
| 5:E:114:ASN:O | 5:E:115:ASN:HB3 | 2.18 | 0.43 |
| 6:F:140:ASP:OD1 | 6:F:141:GLY:N | 2.52 | 0.43 |
| 5:E:82:PHE:N | 5:E:82:PHE:CD1 | 2.85 | 0.43 |
| 2:B:1103:ILE:O | 2:B:1104:HIS:C | 2.56 | 0.43 |
| 2:B:702:LEU:HD22 | 2:B:737:THR:CG2 | 2.49 | 0.43 |
| 1:A:396:PRO:HG3 | 1:A:416:ARG:HB3 | 2.00 | 0.43 |
| 1:A:709:THR:O | 1:A:712:GLU:N | 2.52 | 0.43 |
| 1:A:711:ARG:HA | 9:I:97:MET:HE1 | 2.01 | 0.43 |
| 1:A:457:ALA:O | 1:A:507:VAL:HG23 | 2.19 | 0.43 |
| 1:A:458:HIS:ND1 | 1:A:507:VAL:HG21 | 2.33 | 0.43 |
| 1:A:114:LEU:HD12 | 1:A:142:CYS:O | 2.18 | 0.43 |
| 1:A:113:LEU:HG | 1:A:218:ASP:OD1 | 2.19 | 0.43 |
| 9:I:84:VAL:O | 9:I:84:VAL:HG13 | 2.19 | 0.43 |
| 1:A:266:LEU:HD23 | 1:A:266:LEU:HA | 1.81 | 0.43 |
| 8:H:123:MET:HE1 | 8:H:142:LEU:CD1 | 2.49 | 0.43 |
| 2:B:519:TRP:CZ2 | 2:B:705:MET:CE | 2.99 | 0.43 |
| 9:I:50:THR:HG22 | 9:I:52:ILE:HG23 | 1.98 | 0.43 |
| 2:B:202:TYR:N | 2:B:202:TYR:CD2 | 2.87 | 0.43 |
| 8:H:5:LEU:O | 8:H:6:PHE:HB2 | 2.19 | 0.43 |
| 1:A:89:PRO:HG3 | 1:A:208:LEU:HD12 | 2.00 | 0.43 |
| 1:A:679:ILE:O | 1:A:682:THR:HB | 2.18 | 0.43 |
| 2:B:55:VAL:O | 2:B:59:LEU:HB3 | 2.19 | 0.43 |
| 1:A:1409:LEU:HD23 | 1:A:1409:LEU:HA | 1.83 | 0.43 |
| 1:A:1150:SER:HB2 | 1:A:1195:LEU:CD2 | 2.49 | 0.43 |
| 1:A:672:ASP:O | 1:A:675:THR:HB | 2.19 | 0.43 |
| 1:A:1336:MET:HE1 | 1:A:1381:LEU:N | 2.34 | 0.43 |
| 1:A:633:VAL:HG11 | 1:A:645:LEU:HD22 | 2.00 | 0.43 |
| 8:H:84:ALA:CA | 8:H:87:ARG:HB2 | 2.48 | 0.43 |
| 2:B:850:LEU:CD2 | 2:B:1009:ASP:HB3 | 2.48 | 0.43 |
| 2:B:484:ASN:CG | 2:B:486:TYR:HE1 | 2.23 | 0.43 |
| 6:F:94:LEU:HD23 | 6:F:94:LEU:HA | 1.83 | 0.43 |
| 12:L:61:THR:HG22 | 12:L:62:LYS:N | 2.33 | 0.42 |
| 1:A:815:PHE:C | 1:A:817:ALA:N | 2.72 | 0.42 |
| 1:A:541:ILE:HG12 | 1:A:549:MET:HE3 | 2.01 | 0.42 |
| 1:A:337:ARG:CZ | 1:A:839:ARG:CZ | 2.97 | 0.42 |
| 8:H:83:GLN:C | 8:H:85:GLY:N | 2.73 | 0.42 |
| 1:A:30:ILE:O | 1:A:31:SER:O | 2.37 | 0.42 |
| 2:B:115:GLN:HG2 | 2:B:193:LYS:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:111:LEU:HD23 | 8:H:127:GLY:O | 2.18 | 0.42 |
| 5:E:168:TYR:O | 5:E:170:LEU:HD23 | 2.19 | 0.42 |
| 2:B:877:PRO:O | 2:B:878:GLN:HG2 | 2.19 | 0.42 |
| 2:B:366:GLN:O | 2:B:367:LEU:O | 2.36 | 0.42 |
| 3:C:228:PHE:HB2 | 3:C:230:MET:HE2 | 2.01 | 0.42 |
| 1:A:545:GLN:O | 1:A:546:VAL:C | 2.55 | 0.42 |
| 2:B:705:MET:N | 2:B:710:LEU:HD12 | 2.34 | 0.42 |
| 1:A:1390:ASN:HD22 | 1:A:1399:ARG:CA | 2.30 | 0.42 |
| 1:A:614:PHE:C | 1:A:614:PHE:CD1 | 2.92 | 0.42 |
| 1:A:534:LEU:HD13 | 1:A:656:TRP:CD1 | 2.54 | 0.42 |
| 8:H:93:TYR:CA | 8:H:145:ARG:HB3 | 2.45 | 0.42 |
| 2:B:310:MET:O | 2:B:313:MET:HB2 | 2.18 | 0.42 |
| 3:C:148:ARG:H | 3:C:151:GLN:HG3 | 1.84 | 0.42 |
| 5:E:117:THR:C | 5:E:119:SER:N | 2.73 | 0.42 |
| 1:A:645:LEU:HD11 | 1:A:649:ILE:HD11 | 2.01 | 0.42 |
| 1:A:782:ARG:NH2 | 9:I:67:THR:HG22 | 2.34 | 0.42 |
| 1:A:412:ARG:CZ | 2:B:1108:ARG:NH2 | 2.81 | 0.42 |
| 8:H:143:LEU:HD12 | 8:H:143:LEU:N | 2.34 | 0.42 |
| 1:A:373:THR:HG21 | 2:B:1105:ALA:O | 2.18 | 0.42 |
| 1:A:1155:ASP:O | 1:A:1190:PRO:O | 2.37 | 0.42 |
| 1:A:49:LYS:NZ | 1:A:60:SER:HA | 2.34 | 0.42 |
| 1:A:1049:ILE:O | 1:A:1050:GLU:C | 2.56 | 0.42 |
| 5:E:79:TRP:HD1 | 5:E:96:PHE:HE1 | 1.67 | 0.42 |
| 2:B:880:THR:O | 2:B:881:ASN:HB2 | 2.20 | 0.42 |
| 2:B:1073:TYR:N | 2:B:1073:TYR:CD1 | 2.87 | 0.42 |
| 2:B:784:ASN:HB3 | 10:J:63:TYR:OH | 2.18 | 0.42 |
| 1:A:845:LEU:O | 1:A:846:GLU:C | 2.57 | 0.42 |
| 6:F:85:MET:HE1 | 6:F:148:VAL:HG13 | 2.00 | 0.42 |
| 1:A:134:ARG:O | 1:A:137:ALA:N | 2.52 | 0.42 |
| 1:A:1161:THR:OG1 | 1:A:1170:ILE:HD11 | 2.20 | 0.42 |
| 1:A:80:HIS:N | 1:A:243:PRO:HB3 | 2.34 | 0.42 |
| 2:B:1033:LYS:NZ | 2:B:1070:GLU:OE1 | 2.46 | 0.42 |
| 1:A:541:ILE:N | 1:A:541:ILE:HD12 | 2.34 | 0.42 |
| 2:B:980:PHE:HE1 | 2:B:990:ILE:CD1 | 2.30 | 0.42 |
| 1:A:1242:VAL:CG1 | 1:A:1243:VAL:H | 2.22 | 0.42 |
| 2:B:831:SER:CB | 2:B:994:TYR:OH | 2.67 | 0.42 |
| 1:A:151:ASP:OD1 | 1:A:163:SER:HA | 2.19 | 0.42 |
| 5:E:168:TYR:CB | 5:E:170:LEU:HG | 2.49 | 0.42 |
| 2:B:1197:PRO:O | 2:B:1200:ALA:HB3 | 2.19 | 0.42 |
| 2:B:806:THR:O | 2:B:808:ALA:N | 2.53 | 0.42 |
| 2:B:794:ASN:O | 2:B:795:ILE:HD12 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:251:LEU:HG | 11:K:98:LEU:HD11 | 2.01 | 0.42 |
| 1:A:753:GLY:HA2 | 1:A:757:ASN:ND2 | 2.34 | 0.42 |
| 2:B:546:SER:OG | 2:B:631:GLY:N | 2.52 | 0.42 |
| 1:A:1004:ASN:O | 1:A:1008:GLN:HB2 | 2.19 | 0.42 |
| 1:A:1066:VAL:O | 1:A:1067:LEU:C | 2.55 | 0.42 |
| 2:B:203:PHE:HE1 | 2:B:212:LEU:HD12 | 1.85 | 0.42 |
| 2:B:1204:PHE:O | 2:B:1207:LEU:HB2 | 2.19 | 0.42 |
| 10:J:53:HIS:CD2 | 10:J:54:VAL:N | 2.88 | 0.42 |
| 1:A:337:ARG:HH11 | 1:A:839:ARG:HH12 | 1.62 | 0.42 |
| 2:B:269:ILE:HB | 2:B:317:CYS:SG | 2.60 | 0.42 |
| 2:B:34:ILE:HG12 | 2:B:542:MET:CE | 2.49 | 0.42 |
| 2:B:34:ILE:HG12 | 2:B:542:MET:HE1 | 2.00 | 0.42 |
| 9:I:101:PHE:HD1 | 9:I:110:PHE:O | 2.02 | 0.42 |
| 1:A:88:LYS:HD2 | 1:A:293:GLU:OE1 | 2.20 | 0.42 |
| 1:A:1385:THR:HG22 | 1:A:1386:ARG:N | 2.34 | 0.42 |
| 2:B:758:PHE:CE2 | 2:B:1044:ALA:HA | 2.53 | 0.42 |
| 1:A:568:PRO:CB | 3:C:221:TYR:CZ | 3.03 | 0.42 |
| 2:B:955:THR:HA | 12:L:54:ARG:O | 2.19 | 0.42 |
| 2:B:300:HIS:ND1 | 2:B:376:PHE:CD2 | 2.81 | 0.42 |
| 5:E:113:GLN:HG2 | 5:E:137:GLU:OE1 | 2.19 | 0.42 |
| 1:A:1242:VAL:CG1 | 1:A:1243:VAL:N | 2.83 | 0.42 |
| 1:A:1027:ALA:O | 1:A:1030:ARG:HB2 | 2.20 | 0.42 |
| 1:A:99:ILE:O | 1:A:102:VAL:HB | 2.18 | 0.42 |
| 1:A:451:HIS:HB2 | 1:A:454:SER:OG | 2.19 | 0.42 |
| 1:A:84:ILE:HG21 | 1:A:239:LEU:HD23 | 2.01 | 0.42 |
| 2:B:666:TYR:C | 2:B:668:ASP:N | 2.72 | 0.42 |
| 2:B:1177:HIS:O | 2:B:1179:GLN:N | 2.52 | 0.42 |
| 8:H:84:ALA:CB | 8:H:87:ARG:HB2 | 2.49 | 0.42 |
| 1:A:35:ILE:HD13 | 1:A:53:LEU:HD23 | 2.01 | 0.42 |
| 3:C:31:ASN:O | 3:C:32:SER:C | 2.56 | 0.42 |
| 2:B:749:LEU:HD22 | 2:B:753:ALA:CB | 2.49 | 0.42 |
| 5:E:16:PHE:CZ | 5:E:20:LYS:HE2 | 2.54 | 0.42 |
| 1:A:567:LYS:CD | 8:H:95:TYR:CD1 | 3.00 | 0.42 |
| 10:J:53:HIS:CE1 | 10:J:55:ASP:HA | 2.54 | 0.42 |
| 1:A:383:TYR:O | 6:F:115:THR:HG22 | 2.20 | 0.42 |
| 1:A:873:MET:C | 1:A:1058:VAL:HG23 | 2.40 | 0.42 |
| 10:J:52:THR:CG2 | 10:J:52:THR:O | 2.68 | 0.42 |
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:CA | 2.33 | 0.42 |
| 2:B:315:LYS:O | 2:B:317:CYS:N | 2.53 | 0.42 |
| 1:A:751:SER:O | 1:A:752:LYS:CB | 2.67 | 0.42 |
| 11:K:24:ASP:OD2 | 11:K:74:ARG:NH1 | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:28:TYR:CE1 | 5:E:78:LEU:CD1 | 3.03 | 0.42 |
| 1:A:760:GLN:CB | 2:B:1021:MET:HE1 | 2.49 | 0.42 |
| 1:A:756:ILE:CG2 | 1:A:757:ASN:N | 2.80 | 0.42 |
| 12:L:60:ARG:CG | 12:L:61:THR:N | 2.62 | 0.42 |
| 1:A:514:PRO:HB2 | 1:A:875:ALA:HB3 | 2.01 | 0.42 |
| 1:A:1329:THR:HG22 | 1:A:1330:ASN:N | 2.35 | 0.42 |
| 1:A:908:LEU:O | 1:A:909:ASP:C | 2.58 | 0.42 |
| 5:E:137:GLU:O | 5:E:138:ALA:C | 2.57 | 0.42 |
| 1:A:530:GLY:O | 1:A:532:ARG:N | 2.53 | 0.42 |
| 1:A:533:LYS:C | 1:A:535:THR:H | 2.23 | 0.42 |
| 2:B:487:THR:O | 2:B:488:TYR:C | 2.56 | 0.42 |
| 1:A:458:HIS:CE1 | 1:A:507:VAL:CG2 | 3.00 | 0.42 |
| 1:A:1015:VAL:O | 1:A:1015:VAL:HG12 | 2.18 | 0.42 |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:N | 2.34 | 0.42 |
| 8:H:24:CYS:CB | 8:H:44:VAL:HG21 | 2.47 | 0.42 |
| 1:A:108:MET:O | 1:A:109:HIS:CB | 2.66 | 0.42 |
| 1:A:166:GLY:O | 1:A:167:CYS:CB | 2.67 | 0.42 |
| 2:B:634:TYR:CD1 | 2:B:692:TYR:HB3 | 2.55 | 0.42 |
| 1:A:14:VAL:O | 1:A:15:LYS:HD3 | 2.20 | 0.42 |
| 1:A:683:ILE:O | 1:A:686:ALA:N | 2.53 | 0.42 |
| 1:A:1173:HIS:NE2 | 1:A:1227:ILE:HG23 | 2.35 | 0.42 |
| 2:B:39:ARG:HG2 | 2:B:39:ARG:HH11 | 1.85 | 0.42 |
| 6:F:138:LEU:HD23 | 6:F:138:LEU:HA | 1.83 | 0.42 |
| 2:B:995:ARG:HH11 | 2:B:995:ARG:CB | 2.33 | 0.42 |
| 1:A:1349:TYR:O | 1:A:1350:LYS:C | 2.56 | 0.42 |
| 1:A:474:VAL:HG13 | 1:A:474:VAL:O | 2.20 | 0.42 |
| 3:C:214:ASN:CB | 3:C:217:ASP:OD2 | 2.68 | 0.42 |
| 2:B:1115:THR:CG2 | 2:B:1199:ALA:HB2 | 2.50 | 0.42 |
| 2:B:435:THR:O | 2:B:435:THR:HG22 | 2.20 | 0.42 |
| 1:A:1366:ARG:HG2 | 1:A:1366:ARG:HH11 | 1.84 | 0.42 |
| 2:B:640:VAL:HG22 | 2:B:651:LEU:CD2 | 2.50 | 0.42 |
| 2:B:280:ILE:CG2 | 2:B:285:ILE:HG13 | 2.47 | 0.42 |
| 1:A:76:GLU:O | 1:A:78:PRO:CD | 2.68 | 0.42 |
| 3:C:146:LYS:O | 3:C:147:LEU:HD23 | 2.20 | 0.42 |
| 2:B:737:THR:HG23 | 9:I:66:PRO:HB3 | 2.01 | 0.42 |
| 3:C:242:GLN:O | 3:C:246:ARG:N | 2.52 | 0.42 |
| 1:A:14:VAL:HB | 1:A:1430:LEU:HD13 | 2.02 | 0.42 |
| 3:C:166:GLU:CG | 11:K:10:PHE:CZ | 2.96 | 0.42 |
| 2:B:911:ILE:HG21 | 2:B:966:VAL:HG11 | 2.01 | 0.42 |
| 5:E:100:ILE:O | 5:E:101:GLN:C | 2.58 | 0.42 |
| 2:B:1148:LYS:O | 2:B:1152:MET:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:138:GLU:HG2 | 8:H:139:ASN:N | 2.35 | 0.42 |
| 2:B:1177:HIS:C | 2:B:1179:GLN:H | 2.22 | 0.42 |
| 8:H:109:LYS:HZ2 | 8:H:109:LYS:HB2 | 1.84 | 0.42 |
| 9:I:63:GLY:O | 9:I:70:ARG:NH2 | 2.53 | 0.42 |
| 2:B:368:GLU:O | 2:B:371:GLU:OE1 | 2.37 | 0.42 |
| 2:B:499:ASN:OD1 | 2:B:500:THR:N | 2.53 | 0.42 |
| 2:B:1149:GLU:HG3 | 2:B:1153:GLU:OE1 | 2.20 | 0.42 |
| 1:A:1126:ALA:O | 1:A:1128:GLN:N | 2.53 | 0.42 |
| 2:B:640:VAL:HG22 | 2:B:651:LEU:HD23 | 2.01 | 0.41 |
| 2:B:707:PRO:HG2 | 2:B:708:GLU:N | 2.27 | 0.41 |
| 3:C:14:SER:HA | 11:K:114:LEU:HD22 | 2.02 | 0.41 |
| 3:C:27:LEU:HD12 | 3:C:27:LEU:O | 2.20 | 0.41 |
| 1:A:598:LEU:HD22 | 8:H:25:ARG:CZ | 2.50 | 0.41 |
| 2:B:230:ALA:O | 2:B:232:SER:N | 2.47 | 0.41 |
| 2:B:167:ILE:O | 2:B:168:GLY:O | 2.38 | 0.41 |
| 1:A:760:GLN:OE1 | 2:B:1021:MET:HE2 | 2.20 | 0.41 |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:O | 2.19 | 0.41 |
| 2:B:1177:HIS:O | 2:B:1179:GLN:HG3 | 2.19 | 0.41 |
| 9:I:25:LEU:HD12 | 9:I:26:LEU:N | 2.35 | 0.41 |
| 1:A:101:LYS:HG2 | 1:A:139:TRP:CZ2 | 2.55 | 0.41 |
| 1:A:1254:ALA:O | 1:A:1255:GLU:HB2 | 2.19 | 0.41 |
| 1:A:1168:GLU:O | 1:A:1172:LEU:HG | 2.19 | 0.41 |
| 11:K:82:ASP:O | 11:K:85:ASP:HB2 | 2.20 | 0.41 |
| 1:A:481:ASP:C | 1:A:481:ASP:OD1 | 2.58 | 0.41 |
| 2:B:92:PHE:HD2 | 2:B:130:VAL:HG11 | 1.85 | 0.41 |
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:HA | 1.85 | 0.41 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:CB | 2.33 | 0.41 |
| 2:B:1182:CYS:SG | 2:B:1185:CYS:HB2 | 2.60 | 0.41 |
| 6:F:109:VAL:HG12 | 6:F:110:ASP:H | 1.82 | 0.41 |
| 1:A:982:THR:HB | 1:A:985:ASP:CG | 2.40 | 0.41 |
| 2:B:405:ARG:CZ | 2:B:632:ARG:HG2 | 2.49 | 0.41 |
| 9:I:16:PRO:HA | 9:I:26:LEU:O | 2.20 | 0.41 |
| 2:B:757:PRO:HG2 | 2:B:984:HIS:CE1 | 2.54 | 0.41 |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:HD1 | 1.84 | 0.41 |
| 1:A:474:VAL:HG13 | 1:A:478:TYR:HE1 | 1.85 | 0.41 |
| 1:A:1343:ALA:O | 1:A:1346:ALA:HB3 | 2.20 | 0.41 |
| 1:A:639:PRO:HG2 | 1:A:640:GLN:H | 1.84 | 0.41 |
| 2:B:901:PRO:O | 2:B:949:VAL:O | 2.38 | 0.41 |
| 2:B:350:GLN:O | 2:B:351:TYR:C | 2.59 | 0.41 |
| 1:A:399:HIS:C | 1:A:401:GLY:N | 2.71 | 0.41 |
| 1:A:629:LEU:CD1 | 1:A:645:LEU:HD21 | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1177:HIS:HB2 | 2:B:1179:GLN:HG3 | 2.03 | 0.41 |
| 8:H:84:ALA:HA | 8:H:87:ARG:CB | 2.50 | 0.41 |
| 1:A:808:LEU:HD12 | 1:A:808:LEU:N | 2.35 | 0.41 |
| 1:A:59:GLY:HA2 | 1:A:67:CYS:SG | 2.60 | 0.41 |
| 12:L:28:LYS:O | 12:L:29:TYR:CG | 2.74 | 0.41 |
| 5:E:19:VAL:O | 5:E:19:VAL:HG12 | 2.20 | 0.41 |
| 1:A:913:LEU:CD1 | 1:A:981:LEU:O | 2.69 | 0.41 |
| 2:B:1033:LYS:NZ | 2:B:1087:PHE:O | 2.51 | 0.41 |
| 1:A:388:LEU:HA | 1:A:388:LEU:HD23 | 1.88 | 0.41 |
| 1:A:871:ASP:CB | 5:E:204:THR:CG2 | 2.99 | 0.41 |
| 1:A:1406:VAL:CG1 | 1:A:1410:PHE:CE1 | 3.03 | 0.41 |
| 1:A:894:GLU:C | 1:A:896:ARG:N | 2.74 | 0.41 |
| 2:B:879:ARG:O | 2:B:880:THR:HB | 2.20 | 0.41 |
| 3:C:252:GLN:HG3 | 11:K:95:ILE:HG23 | 2.03 | 0.41 |
| 3:C:252:GLN:NE2 | 11:K:99:GLY:N | 2.68 | 0.41 |
| 2:B:797:TYR:HB3 | 2:B:798:TYR:CD1 | 2.55 | 0.41 |
| 11:K:106:GLU:O | 11:K:110:ASN:ND2 | 2.54 | 0.41 |
| 1:A:567:LYS:NZ | 8:H:95:TYR:CD1 | 2.80 | 0.41 |
| 2:B:276:ILE:HD11 | 2:B:355:ILE:CD1 | 2.50 | 0.41 |
| 2:B:175:ARG:CG | 2:B:175:ARG:HH11 | 2.34 | 0.41 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:CB | 2.51 | 0.41 |
| 1:A:679:ILE:CG2 | 1:A:729:ALA:HB1 | 2.43 | 0.41 |
| 2:B:835:GLN:HE21 | 2:B:835:GLN:HB2 | 1.74 | 0.41 |
| 5:E:71:LYS:C | 5:E:73:PRO:HD3 | 2.40 | 0.41 |
| 2:B:1020:ARG:O | 2:B:1021:MET:C | 2.58 | 0.41 |
| 2:B:865:LYS:HB3 | 2:B:866:TYR:H | 1.72 | 0.41 |
| 1:A:984:LYS:O | 1:A:988:LEU:HB2 | 2.19 | 0.41 |
| 1:A:771:GLU:N | 1:A:822:GLU:OE1 | 2.53 | 0.41 |
| 1:A:113:LEU:C | 1:A:115:LEU:H | 2.23 | 0.41 |
| 2:B:1120:GLU:CG | 2:B:1121:GLY:N | 2.84 | 0.41 |
| 1:A:441:PRO:HG2 | 1:A:441:PRO:O | 2.20 | 0.41 |
| 1:A:1026:LEU:HA | 1:A:1026:LEU:HD23 | 1.90 | 0.41 |
| 9:I:98:VAL:HG12 | 9:I:99:LEU:N | 2.36 | 0.41 |
| 2:B:329:THR:O | 2:B:333:PHE:N | 2.48 | 0.41 |
| 10:J:3:VAL:CG2 | 10:J:18:TRP:CG | 3.02 | 0.41 |
| 2:B:601:ARG:O | 2:B:605:ARG:HG3 | 2.19 | 0.41 |
| 1:A:338:GLY:CA | 2:B:1129:ARG:HH22 | 2.17 | 0.41 |
| 1:A:960:ILE:HD12 | 1:A:1021:LEU:CD2 | 2.50 | 0.41 |
| 1:A:960:ILE:O | 1:A:961:ARG:C | 2.57 | 0.41 |
| 2:B:234:ILE:N | 2:B:234:ILE:HD12 | 2.29 | 0.41 |
| 1:A:407:ARG:HG2 | 1:A:430:TRP:CZ2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:4:THR:O | 8:H:5:LEU:HD23 | 2.20 | 0.41 |
| 1:A:531:ILE:CG2 | 1:A:532:ARG:N | 2.84 | 0.41 |
| 2:B:418:LYS:O | 2:B:420:LEU:N | 2.54 | 0.41 |
| 1:A:1193:LEU:HD21 | 1:A:1267:MET:CE | 2.51 | 0.41 |
| 1:A:339:ASN:HB3 | 2:B:1117:GLN:HE22 | 1.85 | 0.41 |
| 11:K:93:SER:O | 11:K:97:LYS:HG3 | 2.20 | 0.41 |
| 2:B:307:ASP:O | 2:B:308:TRP:C | 2.59 | 0.41 |
| 1:A:38:PRO:CA | 1:A:270:LEU:HD23 | 2.49 | 0.41 |
| 2:B:53:GLN:HG2 | 2:B:547:VAL:HG13 | 2.02 | 0.41 |
| 9:I:40:SER:HB2 | 9:I:41:PRO:HD2 | 2.03 | 0.41 |
| 11:K:71:PHE:CD1 | 11:K:71:PHE:C | 2.93 | 0.41 |
| 5:E:13:TRP:O | 5:E:16:PHE:HB3 | 2.21 | 0.41 |
| 1:A:1139:GLU:HG3 | 1:A:1280:GLU:O | 2.20 | 0.41 |
| 9:I:59:VAL:HG12 | 9:I:60:GLN:N | 2.34 | 0.41 |
| 1:A:542:GLU:OE1 | 1:A:569:LYS:HE2 | 2.20 | 0.41 |
| 2:B:955:THR:CG2 | 12:L:54:ARG:O | 2.65 | 0.41 |
| 2:B:702:LEU:HA | 2:B:702:LEU:HD12 | 1.76 | 0.41 |
| 2:B:185:THR:N | 2:B:188:ASP:HB2 | 2.36 | 0.41 |
| 2:B:240:ILE:C | 2:B:253:THR:HG23 | 2.41 | 0.41 |
| 5:E:72:PHE:CD2 | 5:E:155:ARG:NH2 | 2.83 | 0.41 |
| 11:K:35:PHE:O | 11:K:70:ARG:HB2 | 2.21 | 0.41 |
| 1:A:515:GLN:CG | 1:A:516:SER:N | 2.84 | 0.41 |
| 2:B:346:GLU:O | 2:B:347:LYS:C | 2.58 | 0.41 |
| 2:B:1104:HIS:HB2 | 2:B:1122:ARG:CB | 2.51 | 0.41 |
| 5:E:7:ARG:HG3 | 5:E:8:ASN:N | 2.36 | 0.41 |
| 2:B:800:GLN:CB | 10:J:52:THR:CG2 | 2.89 | 0.41 |
| 1:A:1187:GLN:HA | 1:A:1243:VAL:HG23 | 2.02 | 0.41 |
| 1:A:407:ARG:HG2 | 1:A:430:TRP:CE2 | 2.54 | 0.41 |
| 8:H:126:GLU:N | 8:H:130:ARG:HH12 | 2.19 | 0.41 |
| 9:I:92:ARG:CG | 9:I:93:LYS:N | 2.84 | 0.41 |
| 1:A:525:GLN:HB2 | 2:B:835:GLN:HG2 | 2.00 | 0.41 |
| 2:B:1152:MET:O | 2:B:1156:ASP:O | 2.39 | 0.41 |
| 1:A:225:ASN:C | 1:A:227:VAL:N | 2.71 | 0.41 |
| 12:L:41:SER:O | 12:L:44:ASP:HB2 | 2.21 | 0.41 |
| 1:A:866:PHE:C | 1:A:867:ILE:HG13 | 2.40 | 0.41 |
| 2:B:105:SER:O | 2:B:106:ASP:HB2 | 2.20 | 0.41 |
| 10:J:27:GLU:C | 10:J:29:GLU:H | 2.23 | 0.41 |
| 9:I:99:LEU:HB2 | 9:I:112:SER:OG | 2.21 | 0.41 |
| 2:B:120:ARG:HH12 | 12:L:54:ARG:NH1 | 2.18 | 0.41 |
| 1:A:1116:LEU:CD2 | 1:A:1316:VAL:HG21 | 2.51 | 0.41 |
| 1:A:909:ASP:OD1 | 1:A:910:PRO:HD2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:66:ARG:NH2 | 10:J:3:VAL:O | 2.54 | 0.41 |
| 1:A:598:LEU:O | 1:A:599:SER:C | 2.59 | 0.41 |
| 8:H:57:VAL:CG1 | 8:H:58:THR:N | 2.83 | 0.41 |
| 1:A:530:GLY:O | 1:A:533:LYS:N | 2.53 | 0.41 |
| 2:B:51:PHE:O | 2:B:54:PHE:N | 2.54 | 0.41 |
| 2:B:1197:PRO:O | 2:B:1200:ALA:N | 2.51 | 0.41 |
| 3:C:51:VAL:HG22 | 3:C:155:LEU:CD2 | 2.47 | 0.41 |
| 5:E:117:THR:O | 5:E:120:ALA:N | 2.54 | 0.41 |
| 5:E:116:ILE:CG2 | 5:E:117:THR:N | 2.84 | 0.41 |
| 3:C:5:GLY:HA3 | 3:C:6:PRO:HD2 | 1.78 | 0.41 |
| 2:B:872:GLU:HA | 2:B:915:THR:O | 2.21 | 0.41 |
| 2:B:784:ASN:HD21 | 2:B:788:ARG:HD2 | 1.84 | 0.41 |
| 2:B:616:ILE:HG12 | 2:B:696:GLU:HG3 | 2.03 | 0.41 |
| 3:C:46:ILE:CG2 | 3:C:157:CYS:HB3 | 2.51 | 0.41 |
| 11:K:98:LEU:O | 11:K:99:GLY:C | 2.58 | 0.41 |
| 1:A:134:ARG:O | 1:A:136:ALA:N | 2.53 | 0.41 |
| 1:A:18:GLN:O | 2:B:1215:ARG:HG3 | 2.21 | 0.41 |
| 9:I:34:TYR:C | 9:I:35:VAL:HG23 | 2.41 | 0.41 |
| 11:K:103:THR:O | 11:K:106:GLU:N | 2.53 | 0.41 |
| 2:B:387:LEU:HD23 | 2:B:393:LYS:HD2 | 2.03 | 0.41 |
| 2:B:199:MET:N | 2:B:199:MET:SD | 2.87 | 0.41 |
| 9:I:6:PHE:HD2 | 9:I:13:MET:HA | 1.86 | 0.41 |
| 2:B:843:GLN:HB2 | 2:B:993:THR:OG1 | 2.20 | 0.41 |
| 2:B:818:PRO:HG3 | 10:J:54:VAL:HG21 | 2.03 | 0.41 |
| 2:B:941:LEU:HD21 | 2:B:946:ASN:HA | 2.02 | 0.41 |
| 1:A:399:HIS:CB | 1:A:400:PRO:HD3 | 2.45 | 0.41 |
| 1:A:401:GLY:N | 1:A:435:HIS:HD2 | 2.18 | 0.41 |
| 1:A:354:SER:CA | 1:A:482:PHE:CD2 | 3.03 | 0.41 |
| 2:B:850:LEU:HD22 | 2:B:1009:ASP:HB3 | 2.01 | 0.41 |
| 5:E:72:PHE:CD1 | 5:E:72:PHE:N | 2.89 | 0.41 |
| 2:B:1084:GLN:NE2 | 3:C:192:TRP:HB2 | 2.37 | 0.41 |
| 1:A:725:ALA:HA | 1:A:728:LYS:HE2 | 2.02 | 0.41 |
| 10:J:34:THR:O | 10:J:35:ALA:C | 2.58 | 0.41 |
| 2:B:284:ILE:HG12 | 2:B:324:ILE:HD12 | 2.03 | 0.40 |
| 2:B:1103:ILE:HG13 | 2:B:1103:ILE:H | 1.52 | 0.40 |
| 1:A:15:LYS:HD2 | 2:B:1220:ARG:NE | 2.35 | 0.40 |
| 1:A:878:ILE:HG22 | 1:A:879:GLU:N | 2.37 | 0.40 |
| 1:A:962:ARG:O | 1:A:963:ILE:C | 2.57 | 0.40 |
| 1:A:379:VAL:HG22 | 1:A:431:LYS:HG2 | 2.03 | 0.40 |
| 1:A:751:SER:OG | 2:B:1015:HIS:HE1 | 2.03 | 0.40 |
| 2:B:992:ILE:CD1 | 2:B:994:TYR:CE2 | 3.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:399:HIS:NE2 | 1:A:462:VAL:HG21 | 2.36 | 0.40 |
| 5:E:127:ILE:CG1 | 5:E:127:ILE:O | 2.63 | 0.40 |
| 2:B:627:PHE:O | 2:B:632:ARG:NH1 | 2.54 | 0.40 |
| 1:A:738:LYS:CB | 8:H:19:ARG:HH22 | 2.34 | 0.40 |
| 2:B:758:PHE:HB2 | 2:B:1024:ALA:HB1 | 2.04 | 0.40 |
| 2:B:321:GLY:C | 2:B:323:VAL:N | 2.74 | 0.40 |
| 3:C:29:MET:O | 3:C:30:ALA:C | 2.59 | 0.40 |
| 8:H:40:LEU:HD13 | 8:H:123:MET:HE2 | 2.02 | 0.40 |
| 2:B:707:PRO:O | 2:B:708:GLU:C | 2.59 | 0.40 |
| 1:A:1322:ILE:HD12 | 1:A:1327:ILE:HD12 | 2.03 | 0.40 |
| 5:E:3:GLN:HG3 | 5:E:5:ASN:H | 1.85 | 0.40 |
| 1:A:598:LEU:HD22 | 8:H:25:ARG:HH12 | 1.83 | 0.40 |
| 1:A:384:ASN:O | 1:A:386:ASP:N | 2.54 | 0.40 |
| 2:B:801:LYS:HE2 | 10:J:51:LEU:O | 2.22 | 0.40 |
| 1:A:1345:ARG:CG | 1:A:1372:VAL:HG12 | 2.51 | 0.40 |
| 1:A:508:PRO:O | 1:A:511:ILE:HG13 | 2.22 | 0.40 |
| 1:A:804:TYR:HE1 | 2:B:1021:MET:HE3 | 1.85 | 0.40 |
| 2:B:1073:TYR:CE2 | 2:B:1080:LYS:HG2 | 2.57 | 0.40 |
| 2:B:446:LEU:HG | 2:B:446:LEU:O | 2.21 | 0.40 |
| 5:E:157:SER:OG | 5:E:159:ASP:HB2 | 2.22 | 0.40 |
| 1:A:172:PRO:HB3 | 1:A:185:TRP:CZ2 | 2.56 | 0.40 |
| 1:A:270:LEU:O | 1:A:274:ILE:HG13 | 2.21 | 0.40 |
| 1:A:19:PHE:HB3 | 1:A:1413:GLY:HA2 | 2.03 | 0.40 |
| 2:B:593:PRO:HG2 | 2:B:617:ARG:NH2 | 2.36 | 0.40 |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:NH1 | 2.19 | 0.40 |
| 2:B:348:ARG:HG2 | 2:B:348:ARG:H | 1.67 | 0.40 |
| 2:B:345:LYS:N | 2:B:348:ARG:HE | 2.15 | 0.40 |
| 1:A:1316:VAL:O | 1:A:1322:ILE:HD13 | 2.21 | 0.40 |
| 1:A:332:LYS:H | 1:A:337:ARG:CB | 2.33 | 0.40 |
| 2:B:233:PRO:HG2 | 2:B:234:ILE:HG13 | 2.03 | 0.40 |
| 1:A:1039:LYS:NZ | 1:A:1043:ASP:OD1 | 2.47 | 0.40 |
| 1:A:403:LYS:O | 1:A:404:TYR:O | 2.39 | 0.40 |
| 2:B:952:VAL:HG13 | 2:B:966:VAL:HG22 | 2.03 | 0.40 |
| 2:B:244:LEU:HB2 | 2:B:249:ARG:HA | 2.03 | 0.40 |
| 2:B:840:ILE:HB | 2:B:1011:ILE:HB | 2.03 | 0.40 |
| 2:B:549:THR:HG22 | 2:B:550:ASP:N | 2.36 | 0.40 |
| 2:B:56:ASP:CB | 2:B:57:TYR:HD1 | 2.33 | 0.40 |
| 2:B:288:ALA:HB2 | 2:B:330:ALA:HB1 | 2.04 | 0.40 |
| 2:B:864:LYS:H | 2:B:872:GLU:HB2 | 1.87 | 0.40 |
| 1:A:1224:LEU:HD11 | 1:A:1240:CYS:HB3 | 2.03 | 0.40 |
| 8:H:33:GLN:OE1 | 8:H:129:TYR:HE2 | 2.05 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:113:TYR:CE2 | 2:B:192:LEU:HD22 | 2.57 | 0.40 |
| 2:B:188:ASP:O | 2:B:192:LEU:HG | 2.21 | 0.40 |
| 1:A:556:TRP:CE2 | 1:A:558:GLY:HA2 | 2.56 | 0.40 |
| 3:C:175:ALA:HB3 | 10:J:43:ARG:CZ | 2.51 | 0.40 |
| 1:A:1029:ARG:O | 1:A:1032:LEU:N | 2.55 | 0.40 |
| 5:E:131:THR:HG21 | 5:E:191:LYS:HE2 | 2.02 | 0.40 |
| 1:A:19:PHE:HA | 2:B:1213:THR:O | 2.22 | 0.40 |
| 2:B:348:ARG:O | 2:B:349:ILE:C | 2.60 | 0.40 |
| 1:A:336:ILE:CD1 | 1:A:1405:THR:HG21 | 2.45 | 0.40 |
| 1:A:331:GLY:O | 1:A:332:LYS:O | 2.39 | 0.40 |
| 1:A:1220:PHE:O | 1:A:1221:LYS:C | 2.60 | 0.40 |
| 1:A:709:THR:CG2 | 9:I:94:ASP:HA | 2.52 | 0.40 |
| 1:A:1283:VAL:O | 1:A:1306:LEU:HA | 2.21 | 0.40 |
| 1:A:535:THR:O | 1:A:536:LEU:C | 2.59 | 0.40 |
| 2:B:994:TYR:CD1 | 2:B:999:MET:HE3 | 2.56 | 0.40 |
| 9:I:101:PHE:HB2 | 9:I:110:PHE:CE2 | 2.57 | 0.40 |
| 3:C:114:TYR:CG | 3:C:140:ASN:HB3 | 2.56 | 0.40 |
| 11:K:46:ILE:CG2 | 11:K:50:LEU:HD12 | 2.51 | 0.40 |
| 2:B:283:VAL:HG13 | 2:B:297:ILE:HD12 | 2.03 | 0.40 |
| 2:B:365:THR:HG22 | 2:B:367:LEU:H | 1.87 | 0.40 |
| 2:B:380:TYR:O | 2:B:384:ARG:HG2 | 2.21 | 0.40 |
| 8:H:117:SER:HA | 8:H:122:LEU:HD23 | 2.02 | 0.40 |
| 1:A:432:VAL:O | 1:A:434:ARG:N | 2.54 | 0.40 |
| 1:A:553:VAL:HG22 | 1:A:652:VAL:CG2 | 2.51 | 0.40 |
| 2:B:424:LEU:HD12 | 2:B:424:LEU:HA | 1.91 | 0.40 |
| 1:A:1116:LEU:H | 1:A:1308:THR:CG2 | 2.35 | 0.40 |
| 2:B:637:LEU:O | 2:B:690:VAL:HG13 | 2.22 | 0.40 |
| 1:A:783:THR:CG2 | 1:A:815:PHE:CZ | 2.98 | 0.40 |
| 1:A:768:GLN:HG2 | 1:A:816:HIS:N | 2.37 | 0.40 |
| 1:A:396:PRO:HB3 | 1:A:403:LYS:HG2 | 2.03 | 0.40 |
| 2:B:121:ASN:HD21 | 2:B:965:LYS:HE3 | 1.86 | 0.40 |
| 2:B:56:ASP:CB | 2:B:57:TYR:CD1 | 3.04 | 0.40 |
| 2:B:57:TYR:O | 2:B:58:THR:C | 2.60 | 0.40 |
| 1:A:929:LEU:N | 1:A:929:LEU:CD2 | 2.85 | 0.40 |
| 2:B:1114:LEU:O | 2:B:1198:TYR:HE2 | 2.04 | 0.40 |
| 1:A:17:VAL:HA | 2:B:1215:ARG:O | 2.22 | 0.40 |
| 3:C:214:ASN:HB2 | 3:C:217:ASP:OD2 | 2.22 | 0.40 |
| 5:E:182:ASP:O | 5:E:186:LEU:HG | 2.21 | 0.40 |
| 1:A:1378:GLN:O | 1:A:1380:GLY:N | 2.55 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:419:LYS:NZ | 3:C:90:ASP:N[4_555] | 1.74 | 0.46 |

## 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 | 1365/1733 (79%) | 1022 (75%) | 251 (18%) | 92 (7%) | 1 25 |
| 2 | B | 1077/1224 (88%) | 839 (78%) | 169 (16%) | 69 (6%) | 2 26 |
| 3 | C | 264/318 (83%) | 208 (79%) | 40 (15%) | 16 (6%) | 2 27 |
| 5 | E | 212/215 (99%) | 170 (80%) | 33 (16%) | 9 (4%) | 3 36 |
| 6 | F | 82/155 (53%) | 64 (78%) | 15 (18%) | 3 (4%) | 4 40 |
| 8 | H | 129/146 (88%) | 93 (72%) | 21 (16%) | 15 (12%) | 0 9 |
| 9 | I | 117/122 (96%) | 93 (80%) | 15 (13%) | 9 (8%) | 1 20 |
| 10 | J | 63/70 (90%) | 47 (75%) | 12 (19%) | 4 (6%) | 2 27 |
| 11 | K | 112/120 (93%) | 96 (86%) | 15 (13%) | 1 (1%) | 21 67 |
| 12 | L | 44/70 (63%) | 22 (50%) | 13 (30%) | 9 (20%) | 0 2 |
| All | All | 3465/4173 (83%) | 2654 (77%) | 584 (17%) | 227 (7%) | 1 25 |

All (227) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 31 | SER |
| 1 | A | 48 | ALA |
| 1 | A | 55 | ASP |
| 1 | A | 56 | PRO |
| 1 | A | 74 | MET |
| 1 | A | 75 | ASN |
| 1 | A | 167 | CYS |
| 1 | A | 322 | VAL |
| 1 | A | 404 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 418 | SER |
| 1 | A | 543 | LEU |
| 1 | A | 567 | LYS |
| 1 | A | 597 | LEU |
| 1 | A | 598 | LEU |
| 1 | A | 628 | GLY |
| 1 | A | 752 | LYS |
| 1 | A | 846 | GLU |
| 1 | A | 998 | LEU |
| 1 | A | 1036 | ARG |
| 1 | A | 1127 | ASP |
| 1 | A | 1206 | ASP |
| 1 | A | 1221 | LYS |
| 1 | A | 1223 | ASP |
| 1 | A | 1392 | SER |
| 1 | A | 1393 | ASN |
| 1 | A | 1403 | GLU |
| 1 | A | 1406 | VAL |
| 1 | A | 1416 | ALA |
| 2 | B | 65 | GLU |
| 2 | B | 124 | TYR |
| 2 | B | 174 | LEU |
| 2 | B | 175 | ARG |
| 2 | B | 200 | GLY |
| 2 | B | 229 | ALA |
| 2 | B | 364 | ILE |
| 2 | B | 367 | LEU |
| 2 | B | 531 | GLN |
| 2 | B | 708 | GLU |
| 2 | B | 709 | ASP |
| 2 | B | 731 | VAL |
| 2 | B | 751 | VAL |
| 2 | B | 958 | GLN |
| 2 | B | 959 | ASP |
| 2 | B | 1046 | PRO |
| 2 | B | 1103 | ILE |
| 2 | B | 1167 | GLY |
| 2 | B | 1176 | ASN |
| 2 | B | 1183 | LYS |
| 3 | C | 4 | GLU |
| 3 | C | 5 | GLY |
| 3 | C | 6 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 110 | THR |
| 3 | C | 142 | VAL |
| 3 | C | 215 | GLU |
| 6 | F | 73 | ALA |
| 8 | H | 32 | THR |
| 8 | H | 81 | PRO |
| 8 | H | 140 | ALA |
| 9 | I | 8 | ARG |
| 10 | J | 2 | ILE |
| 10 | J | 55 | ASP |
| 12 | L | 27 | LEU |
| 12 | L | 38 | LEU |
| 12 | L | 64 | LEU |
| 1 | A | 35 | ILE |
| 1 | A | 54 | ASN |
| 1 | A | 62 | ASP |
| 1 | A | 87 | ALA |
| 1 | A | 109 | HIS |
| 1 | A | 135 | PHE |
| 1 | A | 168 | GLY |
| 1 | A | 332 | LYS |
| 1 | A | 385 | ILE |
| 1 | A | 419 | LYS |
| 1 | A | 534 | LEU |
| 1 | A | 568 | PRO |
| 1 | A | 790 | ASP |
| 1 | A | 986 | ILE |
| 1 | A | 1114 | PRO |
| 1 | A | 1365 | TYR |
| 1 | A | 1366 | ARG |
| 1 | A | 1379 | GLY |
| 2 | B | 55 | VAL |
| 2 | B | 168 | GLY |
| 2 | B | 275 | TYR |
| 2 | B | 346 | GLU |
| 2 | B | 410 | GLY |
| 2 | B | 480 | SER |
| 2 | B | 641 | GLU |
| 2 | B | 643 | ASP |
| 2 | B | 792 | MET |
| 2 | B | 864 | LYS |
| 2 | B | 866 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 884 | ARG |
| 2 | B | 891 | ASP |
| 2 | B | 992 | ILE |
| 2 | B | 1066 | SER |
| 2 | B | 1155 | SER |
| 3 | C | 136 | ASP |
| 6 | F | 142 | SER |
| 8 | H | 61 | SER |
| 8 | H | 77 | ARG |
| 8 | H | 88 | SER |
| 8 | H | 128 | ASN |
| 9 | I | 30 | ARG |
| 9 | I | 79 | HIS |
| 12 | L | 39 | SER |
| 12 | L | 52 | GLY |
| 1 | A | 6 | TYR |
| 1 | A | 45 | GLN |
| 1 | A | 59 | GLY |
| 1 | A | 67 | CYS |
| 1 | A | 69 | THR |
| 1 | A | 335 | ARG |
| 1 | A | 433 | GLU |
| 1 | A | 596 | THR |
| 1 | A | 737 | LEU |
| 1 | A | 775 | ILE |
| 1 | A | 830 | LYS |
| 1 | A | 920 | LEU |
| 2 | B | 28 | GLU |
| 2 | B | 249 | ARG |
| 2 | B | 277 | LYS |
| 2 | B | 447 | ALA |
| 2 | B | 629 | ASP |
| 2 | B | 735 | ALA |
| 2 | B | 880 | THR |
| 2 | B | 1017 | ILE |
| 2 | B | 1099 | VAL |
| 2 | B | 1104 | HIS |
| 2 | B | 1178 | ASN |
| 3 | C | 48 | SER |
| 3 | C | 212 | PRO |
| 3 | C | 227 | THR |
| 5 | E | 31 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 102 | GLU |
| 5 | E | 103 | LYS |
| 5 | E | 122 | LYS |
| 5 | E | 139 | ALA |
| 5 | E | 206 | GLY |
| 6 | F | 128 | LYS |
| 8 | H | 8 | ASP |
| 8 | H | 17 | PRO |
| 8 | H | 82 | PRO |
| 8 | H | 135 | LEU |
| 8 | H | 139 | ASN |
| 9 | I | 9 | ASP |
| 9 | I | 33 | SER |
| 9 | I | 86 | PHE |
| 10 | J | 9 | SER |
| 12 | L | 63 | ARG |
| 1 | A | 101 | LYS |
| 1 | A | 134 | ARG |
| 1 | A | 139 | TRP |
| 1 | A | 424 | ILE |
| 1 | A | 599 | SER |
| 1 | A | 1067 | LEU |
| 1 | A | 1097 | GLY |
| 1 | A | 1115 | SER |
| 1 | A | 1122 | PRO |
| 1 | A | 1405 | THR |
| 2 | B | 248 | SER |
| 2 | B | 304 | ASP |
| 2 | B | 436 | VAL |
| 2 | B | 501 | PRO |
| 2 | B | 667 | GLN |
| 2 | B | 791 | THR |
| 2 | B | 807 | ARG |
| 2 | B | 1054 | GLY |
| 2 | B | 1097 | HIS |
| 3 | C | 18 | VAL |
| 3 | C | 149 | LYS |
| 3 | C | 174 | ALA |
| 5 | E | 59 | SER |
| 10 | J | 6 | ARG |
| 12 | L | 50 | ASP |
| 12 | L | 56 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 58 | LEU |
| 1 | A | 223 | GLY |
| 1 | A | 399 | HIS |
| 1 | A | 400 | PRO |
| 1 | A | 958 | VAL |
| 1 | A | 972 | HIS |
| 1 | A | 1098 | VAL |
| 1 | A | 1130 | GLN |
| 1 | A | 1282 | VAL |
| 1 | A | 1351 | GLU |
| 1 | A | 1378 | GLN |
| 2 | B | 419 | THR |
| 2 | B | 619 | ILE |
| 2 | B | 648 | HIS |
| 2 | B | 687 | GLU |
| 2 | B | 707 | PRO |
| 2 | B | 712 | PRO |
| 2 | B | 764 | SER |
| 2 | B | 907 | GLY |
| 2 | B | 982 | SER |
| 2 | B | 1108 | ARG |
| 5 | E | 36 | GLU |
| 8 | H | 62 | SER |
| 8 | H | 89 | LEU |
| 9 | I | 47 | GLU |
| 9 | I | 88 | SER |
| 1 | A | 226 | GLU |
| 1 | A | 368 | LYS |
| 1 | A | 465 | TYR |
| 1 | A | 531 | ILE |
| 1 | A | 903 | ASN |
| 1 | A | 1014 | ALA |
| 1 | A | 1314 | SER |
| 1 | A | 1352 | VAL |
| 2 | B | 27 | ALA |
| 5 | E | 167 | ARG |
| 8 | H | 138 | GLU |
| 9 | I | 98 | VAL |
| 11 | K | 107 | THR |
| 2 | B | 247 | GLY |
| 1 | A | 336 | ILE |
| 1 | A | 1104 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | L | 55 | ILE |
| 1 | A | 810 | PRO |
| 1 | A | 1075 | PRO |
| 1 | A | 1242 | VAL |
| 3 | C | 172 | PRO |
| 3 | C | 216 | GLY |
| 2 | B | 511 | PRO |
| 3 | C | 218 | PRO |

### 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 | 1206/1520 (79%) | 1128 (94%) | 78 (6%) | 21 61 |
| 2 | B | 952/1061 (90%) | 886 (93%) | 66 (7%) | 19 59 |
| 3 | C | 234/274 (85%) | 222 (95%) | 12 (5%) | 29 68 |
| 5 | E | 196/197 (100%) | 189 (96%) | 7 (4%) | 42 76 |
| 6 | F | 74/137 (54%) | 68 (92%) | 6 (8%) | 15 53 |
| 8 | H | 117/128 (91%) | 112 (96%) | 5 (4%) | 35 72 |
| 9 | I | 113/116 (97%) | 104 (92%) | 9 (8%) | 15 53 |
| 10 | J | 60/65 (92%) | 56 (93%) | 4 (7%) | 20 60 |
| 11 | K | 99/102 (97%) | 90 (91%) | 9 (9%) | 12 47 |
| 12 | L | 40/57 (70%) | 35 (88%) | 5 (12%) | 6 32 |
| All | All | 3091/3657 (84%) | 2890 (94%) | 201 (6%) | 21 61 |

All (201) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 18 | GLN |
| 1 | A | 22 | PHE |
| 1 | A | 31 | SER |
| 1 | A | 56 | PRO |
| 1 | A | 70 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 93 | VAL |
| 1 | A | 122 | MET |
| 1 | A | 247 | ARG |
| 1 | A | 269 | ILE |
| 1 | A | 302 | THR |
| 1 | A | 322 | VAL |
| 1 | A | 326 | ARG |
| 1 | A | 351 | THR |
| 1 | A | 375 | THR |
| 1 | A | 381 | THR |
| 1 | A | 385 | ILE |
| 1 | A | 397 | ASN |
| 1 | A | 412 | ARG |
| 1 | A | 434 | ARG |
| 1 | A | 443 | LEU |
| 1 | A | 445 | ASN |
| 1 | A | 450 | LEU |
| 1 | A | 451 | HIS |
| 1 | A | 461 | LYS |
| 1 | A | 474 | VAL |
| 1 | A | 475 | THR |
| 1 | A | 493 | GLN |
| 1 | A | 503 | GLN |
| 1 | A | 524 | VAL |
| 1 | A | 538 | ASP |
| 1 | A | 590 | ARG |
| 1 | A | 596 | THR |
| 1 | A | 597 | LEU |
| 1 | A | 598 | LEU |
| 1 | A | 618 | GLU |
| 1 | A | 629 | LEU |
| 1 | A | 666 | ILE |
| 1 | A | 682 | THR |
| 1 | A | 740 | LEU |
| 1 | A | 741 | ASN |
| 1 | A | 745 | GLN |
| 1 | A | 756 | ILE |
| 1 | A | 768 | GLN |
| 1 | A | 774 | ARG |
| 1 | A | 821 | ARG |
| 1 | A | 845 | LEU |
| 1 | A | 849 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 855 | THR |
| 1 | A | 858 | ASN |
| 1 | A | 920 | LEU |
| 1 | A | 929 | LEU |
| 1 | A | 948 | VAL |
| 1 | A | 949 | ASP |
| 1 | A | 979 | SER |
| 1 | A | 1029 | ARG |
| 1 | A | 1035 | TYR |
| 1 | A | 1043 | ASP |
| 1 | A | 1055 | ARG |
| 1 | A | 1057 | VAL |
| 1 | A | 1077 | THR |
| 1 | A | 1128 | GLN |
| 1 | A | 1222 | ASN |
| 1 | A | 1232 | ASN |
| 1 | A | 1258 | HIS |
| 1 | A | 1264 | GLU |
| 1 | A | 1295 | THR |
| 1 | A | 1308 | THR |
| 1 | A | 1318 | THR |
| 1 | A | 1332 | PHE |
| 1 | A | 1335 | ILE |
| 1 | A | 1351 | GLU |
| 1 | A | 1359 | ASP |
| 1 | A | 1364 | ASN |
| 1 | A | 1366 | ARG |
| 1 | A | 1375 | MET |
| 1 | A | 1376 | THR |
| 1 | A | 1425 | SER |
| 1 | A | 1442 | ASP |
| 2 | B | 20 | ASP |
| 2 | B | 43 | LEU |
| 2 | B | 57 | TYR |
| 2 | B | 61 | ASP |
| 2 | B | 63 | ILE |
| 2 | B | 98 | THR |
| 2 | B | 109 | THR |
| 2 | B | 121 | ASN |
| 2 | B | 175 | ARG |
| 2 | B | 194 | GLU |
| 2 | B | 232 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 234 | ILE |
| 2 | B | 261 | ARG |
| 2 | B | 268 | THR |
| 2 | B | 278 | GLN |
| 2 | B | 309 | GLN |
| 2 | B | 313 | MET |
| 2 | B | 317 | CYS |
| 2 | B | 320 | ASP |
| 2 | B | 331 | LEU |
| 2 | B | 376 | PHE |
| 2 | B | 387 | LEU |
| 2 | B | 396 | ASP |
| 2 | B | 408 | LEU |
| 2 | B | 466 | TRP |
| 2 | B | 485 | ARG |
| 2 | B | 513 | GLN |
| 2 | B | 514 | LEU |
| 2 | B | 538 | ASN |
| 2 | B | 547 | VAL |
| 2 | B | 570 | VAL |
| 2 | B | 576 | ASP |
| 2 | B | 624 | LEU |
| 2 | B | 629 | ASP |
| 2 | B | 644 | GLU |
| 2 | B | 680 | THR |
| 2 | B | 723 | VAL |
| 2 | B | 732 | SER |
| 2 | B | 762 | ASN |
| 2 | B | 764 | SER |
| 2 | B | 780 | VAL |
| 2 | B | 791 | THR |
| 2 | B | 835 | GLN |
| 2 | B | 901 | PRO |
| 2 | B | 909 | ASP |
| 2 | B | 915 | THR |
| 2 | B | 944 | THR |
| 2 | B | 951 | GLN |
| 2 | B | 953 | LEU |
| 2 | B | 976 | ILE |
| 2 | B | 986 | GLN |
| 2 | B | 987 | LYS |
| 2 | B | 996 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 999 | MET |
| 2 | B | 1007 | VAL |
| 2 | B | 1021 | MET |
| 2 | B | 1049 | ASP |
| 2 | B | 1103 | ILE |
| 2 | B | 1111 | MET |
| 2 | B | 1118 | PRO |
| 2 | B | 1132 | GLU |
| 2 | B | 1147 | LEU |
| 2 | B | 1150 | ARG |
| 2 | B | 1151 | LEU |
| 2 | B | 1183 | LYS |
| 2 | B | 1185 | CYS |
| 3 | C | 22 | LEU |
| 3 | C | 25 | VAL |
| 3 | C | 26 | ASP |
| 3 | C | 62 | PHE |
| 3 | C | 69 | LEU |
| 3 | C | 77 | ILE |
| 3 | C | 133 | ILE |
| 3 | C | 148 | ARG |
| 3 | C | 229 | TYR |
| 3 | C | 233 | GLU |
| 3 | C | 240 | VAL |
| 3 | C | 264 | GLN |
| 5 | E | 40 | GLU |
| 5 | E | 60 | PHE |
| 5 | E | 74 | ASP |
| 5 | E | 84 | ASP |
| 5 | E | 92 | THR |
| 5 | E | 104 | ASN |
| 5 | E | 183 | PRO |
| 6 | F | 79 | ARG |
| 6 | F | 90 | ARG |
| 6 | F | 103 | MET |
| 6 | F | 111 | LEU |
| 6 | F | 115 | THR |
| 6 | F | 133 | VAL |
| 8 | H | 21 | ASN |
| 8 | H | 27 | GLU |
| 8 | H | 109 | LYS |
| 8 | H | 110 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 134 | ASN |
| 9 | I | 7 | CYS |
| 9 | I | 12 | ASN |
| 9 | I | 29 | CYS |
| 9 | I | 31 | THR |
| 9 | I | 52 | ILE |
| 9 | I | 75 | CYS |
| 9 | I | 76 | PRO |
| 9 | I | 87 | GLN |
| 9 | I | 103 | CYS |
| 10 | J | 2 | ILE |
| 10 | J | 7 | CYS |
| 10 | J | 47 | ARG |
| 10 | J | 48 | ARG |
| 11 | K | 20 | LYS |
| 11 | K | 25 | THR |
| 11 | K | 31 | VAL |
| 11 | K | 47 | ARG |
| 11 | K | 50 | LEU |
| 11 | K | 61 | TYR |
| 11 | K | 77 | THR |
| 11 | K | 81 | TYR |
| 11 | K | 114 | LEU |
| 12 | L | 50 | ASP |
| 12 | L | 54 | ARG |
| 12 | L | 55 | ILE |
| 12 | L | 68 | GLU |
| 12 | L | 70 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 68 | GLN |
| 1 | A | 92 | HIS |
| 1 | A | 118 | HIS |
| 1 | A | 169 | ASN |
| 1 | A | 225 | ASN |
| 1 | A | 339 | ASN |
| 1 | A | 358 | ASN |
| 1 | A | 435 | HIS |
| 1 | A | 445 | ASN |
| 1 | A | 493 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 503 | GLN |
| 1 | A | 517 | ASN |
| 1 | A | 631 | HIS |
| 1 | A | 723 | ASN |
| 1 | A | 736 | ASN |
| 1 | A | 741 | ASN |
| 1 | A | 757 | ASN |
| 1 | A | 768 | GLN |
| 1 | A | 786 | HIS |
| 1 | A | 858 | ASN |
| 1 | A | 926 | GLN |
| 1 | A | 965 | GLN |
| 1 | A | 968 | GLN |
| 1 | A | 994 | GLN |
| 1 | A | 1364 | ASN |
| 1 | A | 1387 | HIS |
| 1 | A | 1390 | ASN |
| 1 | A | 1432 | GLN |
| 2 | B | 46 | GLN |
| 2 | B | 53 | GLN |
| 2 | B | 178 | ASN |
| 2 | B | 215 | GLN |
| 2 | B | 236 | HIS |
| 2 | B | 325 | GLN |
| 2 | B | 363 | HIS |
| 2 | B | 465 | ASN |
| 2 | B | 484 | ASN |
| 2 | B | 513 | GLN |
| 2 | B | 515 | HIS |
| 2 | B | 516 | ASN |
| 2 | B | 518 | HIS |
| 2 | B | 538 | ASN |
| 2 | B | 657 | HIS |
| 2 | B | 744 | HIS |
| 2 | B | 822 | ASN |
| 2 | B | 842 | ASN |
| 2 | B | 862 | GLN |
| 2 | B | 957 | ASN |
| 2 | B | 975 | GLN |
| 2 | B | 1015 | HIS |
| 2 | B | 1065 | GLN |
| 2 | B | 1117 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 1179 | GLN |
| 2 | B | 1193 | GLN |
| 3 | C | 65 | HIS |
| 3 | C | 73 | GLN |
| 3 | C | 112 | ASN |
| 3 | C | 123 | ASN |
| 3 | C | 167 | HIS |
| 3 | C | 242 | GLN |
| 3 | C | 252 | GLN |
| 5 | E | 5 | ASN |
| 5 | E | 32 | GLN |
| 5 | E | 101 | GLN |
| 5 | E | 104 | ASN |
| 5 | E | 114 | ASN |
| 5 | E | 147 | HIS |
| 8 | H | 33 | GLN |
| 9 | I | 12 | ASN |
| 10 | J | 53 | HIS |
| 11 | K | 52 | ASN |
| 11 | K | 65 | HIS |
| 11 | K | 76 | GLN |
| 11 | K | 110 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 1388/1733 (80%) | -0.05 | 42 (3%) 54 41 | 20, 181, 283, 321 | 0 |
| 2 | B | 1097/1224 (89%) | 0.01 | 31 (2%) 56 45 | 74, 189, 297, 321 | 0 |
| 3 | C | 266/318 (83%) | 0.00 | 5 (1%) 70 60 | 87, 180, 262, 321 | 0 |
| 4 | D | 0/161 | - | - | - | - |
| 5 | E | 214/215 (99%) | 0.21 | 10 (4%) 35 27 | 88, 223, 305, 321 | 0 |
| 6 | F | 84/155 (54%) | 0.08 | 3 (3%) 46 36 | 90, 163, 254, 321 | 0 |
| 7 | G | 0/170 | - | - | - | - |
| 8 | H | 133/146 (91%) | 0.41 | 6 (4%) 37 28 | 139, 242, 318, 321 | 0 |
| 9 | I | 119/122 (97%) | 0.74 | 14 (11%) 6 6 | 139, 241, 318, 321 | 0 |
| 10 | J | 65/70 (92%) | -0.12 | 3 (4%) 36 27 | 68, 173, 284, 313 | 0 |
| 11 | K | 114/120 (95%) | -0.04 | 1 (0%) 85 79 | 98, 170, 245, 304 | 0 |
| 12 | L | 46/70 (65%) | 0.24 | 5 (10%) 7 6 | 134, 233, 304, 321 | 0 |
| All | All | 3526/4504 (78%) | 0.04 | 120 (3%) 49 38 | 20, 189, 294, 321 | 0 |

All (120) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 114 | LEU | 5.5 |
| 2 | B | 715 | ALA | 5.2 |
| 1 | A | 199 | LEU | 4.8 |
| 3 | C | 4 | GLU | 4.5 |
| 2 | B | 869 | SER | 4.5 |
| 5 | E | 88 | VAL | 4.5 |
| 12 | L | 46 | VAL | 4.3 |
| 2 | B | 882 | THR | 4.2 |
| 9 | I | 119 | THR | 4.2 |
| 2 | B | 887 | HIS | 4.2 |
| 9 | I | 73 | ARG | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 1236 | LEU | 4.1 |
| 1 | A | 149 | GLU | 3.8 |
| 1 | A | 69 | THR | 3.8 |
| 2 | B | 933 | SER | 3.8 |
| 1 | A | 1159 | ARG | 3.7 |
| 9 | I | 83 | ASN | 3.7 |
| 9 | I | 72 | ASP | 3.7 |
| 2 | B | 428 | ILE | 3.6 |
| 8 | H | 35 | GLN | 3.6 |
| 8 | H | 107 | VAL | 3.6 |
| 9 | I | 74 | GLU | 3.6 |
| 8 | H | 8 | ASP | 3.5 |
| 5 | E | 113 | GLN | 3.3 |
| 1 | A | 1256 | GLU | 3.3 |
| 9 | I | 76 | PRO | 3.3 |
| 9 | I | 34 | TYR | 3.3 |
| 1 | A | 282 | ASN | 3.2 |
| 3 | C | 266 | ASP | 3.2 |
| 1 | A | 593 | GLU | 3.1 |
| 1 | A | 426 | LEU | 3.1 |
| 2 | B | 133 | LYS | 3.1 |
| 2 | B | 714 | GLU | 3.0 |
| 1 | A | 1221 | LYS | 2.9 |
| 8 | H | 2 | SER | 2.9 |
| 1 | A | 153 | PRO | 2.9 |
| 9 | I | 18 | GLU | 2.9 |
| 1 | A | 1188 | GLN | 2.9 |
| 10 | J | 26 | GLN | 2.8 |
| 5 | E | 114 | ASN | 2.8 |
| 9 | I | 71 | SER | 2.8 |
| 2 | B | 346 | GLU | 2.8 |
| 8 | H | 110 | ASP | 2.7 |
| 5 | E | 93 | MET | 2.7 |
| 1 | A | 161 | LEU | 2.7 |
| 6 | F | 110 | ASP | 2.7 |
| 1 | A | 115 | LEU | 2.7 |
| 10 | J | 28 | ASP | 2.7 |
| 2 | B | 106 | ASP | 2.6 |
| 1 | A | 124 | GLN | 2.6 |
| 1 | A | 66 | LYS | 2.6 |
| 2 | B | 92 | PHE | 2.6 |
| 1 | A | 1126 | ALA | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | C | 3 | GLU | 2.5 |
| 2 | B | 1224 | PHE | 2.5 |
| 1 | A | 1161 | THR | 2.5 |
| 2 | B | 881 | ASN | 2.5 |
| 2 | B | 437 | GLU | 2.5 |
| 11 | K | 74 | ARG | 2.5 |
| 3 | C | 127 | ARG | 2.5 |
| 1 | A | 44 | THR | 2.5 |
| 5 | E | 126 | SER | 2.5 |
| 9 | I | 8 | ARG | 2.5 |
| 2 | B | 643 | ASP | 2.5 |
| 1 | A | 1108 | ALA | 2.5 |
| 12 | L | 45 | ALA | 2.4 |
| 2 | B | 870 | ILE | 2.4 |
| 2 | B | 888 | GLY | 2.4 |
| 2 | B | 108 | VAL | 2.4 |
| 2 | B | 679 | TYR | 2.4 |
| 2 | B | 865 | LYS | 2.4 |
| 5 | E | 118 | PRO | 2.4 |
| 8 | H | 85 | GLY | 2.4 |
| 5 | E | 86 | PRO | 2.3 |
| 2 | B | 91 | SER | 2.3 |
| 1 | A | 259 | GLU | 2.3 |
| 2 | B | 164 | LYS | 2.3 |
| 1 | A | 164 | ARG | 2.3 |
| 1 | A | 168 | GLY | 2.3 |
| 1 | A | 1127 | ASP | 2.3 |
| 5 | E | 83 | CYS | 2.3 |
| 1 | A | 287 | HIS | 2.3 |
| 1 | A | 323 | LYS | 2.3 |
| 2 | B | 1188 | LYS | 2.3 |
| 9 | I | 118 | ARG | 2.2 |
| 2 | B | 424 | LEU | 2.2 |
| 12 | L | 43 | THR | 2.2 |
| 1 | A | 152 | VAL | 2.2 |
| 9 | I | 84 | VAL | 2.2 |
| 1 | A | 1158 | PRO | 2.2 |
| 1 | A | 118 | HIS | 2.2 |
| 2 | B | 425 | THR | 2.2 |
| 6 | F | 104 | ASN | 2.2 |
| 1 | A | 279 | LEU | 2.2 |
| 9 | I | 104 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 1175 | SER | 2.2 |
| 2 | B | 1223 | ASP | 2.2 |
| 1 | A | 1079 | MET | 2.2 |
| 1 | A | 1003 | LYS | 2.2 |
| 1 | A | 283 | GLY | 2.1 |
| 1 | A | 186 | LYS | 2.1 |
| 2 | B | 432 | MET | 2.1 |
| 1 | A | 1206 | ASP | 2.1 |
| 5 | E | 115 | ASN | 2.1 |
| 2 | B | 349 | ILE | 2.1 |
| 3 | C | 199 | LYS | 2.1 |
| 2 | B | 259 | TYR | 2.1 |
| 10 | J | 27 | GLU | 2.1 |
| 12 | L | 49 | LYS | 2.1 |
| 1 | A | 1095 | THR | 2.1 |
| 6 | F | 101 | ILE | 2.1 |
| 5 | E | 52 | ARG | 2.0 |
| 12 | L | 47 | ARG | 2.0 |
| 2 | B | 866 | TYR | 2.0 |
| 1 | A | 1243 | VAL | 2.0 |
| 1 | A | 170 | THR | 2.0 |
| 2 | B | 886 | LYS | 2.0 |
| 1 | A | 1255 | GLU | 2.0 |
| 9 | I | 102 | VAL | 2.0 |
| 1 | A | 920 | LEU | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 13 | ZN | I | 203 | 1/1 | 0.90 | 0.18 | -0.86 | 172,172,172,172 | 0 |
| 13 | ZN | A | 1735 | 1/1 | 0.90 | 0.12 | -1.14 | 172,172,172,172 | 0 |
| 13 | ZN | C | 319 | 1/1 | 0.94 | 0.07 | -1.15 | 172,172,172,172 | 0 |
| 13 | ZN | I | 204 | 1/1 | 0.93 | 0.23 | -1.45 | 172,172,172,172 | 0 |
| 13 | ZN | J | 101 | 1/1 | 0.94 | 0.12 | -1.90 | 172,172,172,172 | 0 |
| 13 | ZN | A | 1734 | 1/1 | 0.94 | 0.16 | -2.14 | 172,172,172,172 | 0 |
| 13 | ZN | B | 1307 | 1/1 | 0.99 | 0.06 | - | 172,172,172,172 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.