# WORLDWIDE wwPDB PROTEIN DATA BANK

# Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 09:25 AM JST

|  |  |  |
|---|---|---|
| PDB ID | : | 6IRH |
| EMDB ID | : | EMD-9717 |
| Title | : | Structure of the human GluN1/GluN2A NMDA receptor in the glutamate/glycine-bound state at pH 6.3, Class III |
| Authors | : | Zhang, J.; Chang, S.; Zhang, X.; Zhu, S. |
| Deposited on | : | 2018-11-12 |
| Resolution | : | 7.80 Å(reported) |
| Based on initial models | : | 5TQ0, 4PE5, 5H8F |

# 1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.80 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 | Percentile Ranks | Value |
|--------|-----------------|-------|
| Clashscore | | 36 |
| Ramachandran outliers | | 0.7% |
| Sidechain outliers | | 0.1% |

*Worse*      *Better*

▮ Percentile relative to all structures
◨ Percentile relative to all EM structures
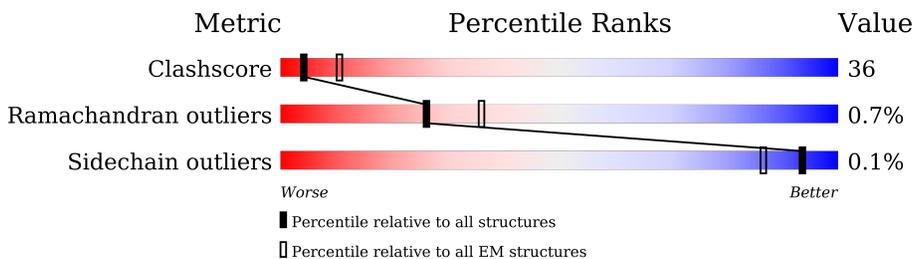
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|--------|:------------------------:|:------------------------:|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|:---:|:-----:|:------:|------------------|
| 1 | A | 847 | 15% / 51% 41% • 7% |
| 1 | C | 847 | 15% / 50% 41% • 7% |
| 2 | B | 841 | 16% / 51% 38% • 10% |
| 2 | D | 841 | 20% / 50% 39% • 10% |

# 2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 23937 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamate receptor ionotropic, NMDA 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | C | 786 | Total | C | N | O | S | 0 | 0 |
| | | | 6156 | 3922 | 1069 | 1130 | 35 | | |
| 1 | A | 785 | Total | C | N | O | S | 0 | 0 |
| | | | 6149 | 3917 | 1068 | 1129 | 35 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 612 | ARG | GLY | engineered mutation | UNP Q05586 |
| A | 612 | ARG | GLY | engineered mutation | UNP Q05586 |

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | D | 756 | Total | C | N | O | S | 1 | 0 |
| | | | 5816 | 3759 | 954 | 1067 | 36 | | |
| 2 | B | 756 | Total | C | N | O | S | 1 | 0 |
| | | | 5816 | 3759 | 954 | 1067 | 36 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 656 | ARG | GLU | engineered mutation | UNP Q12879 |
| D | 657 | ARG | GLU | engineered mutation | UNP Q12879 |
| B | 656 | ARG | GLU | engineered mutation | UNP Q12879 |
| B | 657 | ARG | GLU | engineered mutation | UNP Q12879 |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Glutamate receptor ionotropic, NMDA 1

• Molecule 1: Glutamate receptor ionotropic, NMDA 1

• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain D:

L794 W795 L796 I799 C800 H801 N802 E803 K804 N805 E806 V807 M808 S809 SER GLN LEU ASP I814 G819 V820 F821 Y822 M823 L824 A825 A826 A827 M828 A829 L830 S831 L832 F841

• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B:

16%

51% 38% 10%

MET GLY ARG VAL GLY TYR TRP THR LEU LEU VAL LEU PRO ALA LEU LEU VAL TRP ARG GLY PRO ALA PRO SER ALA ALA ALA GLU LYS GLY PRO PRO ALA L34 N35 I36 A37 V38 M39 L40 G41 H42 S43 H44 D45 R52 P57 A60 A61 G62 L63 D66 V67 N68 V69 V70

A71 L72 L73 M74 N75 R76 T77 D78 P79 K80 S81 L89 I95 H96 G97 L98 V99 F100 G101 D102 D105 Q106 M112 L113 D114 F115 I116 S117 S118 H119 P123 I124 L125 H128 G129 M135 A136 D137 K138 D139 T143 F144 F145 G148 A149 S150 Q153 V157

K160 I161 M162 Q163 D164 Y165 D166 W167 H168 V169 F170 S171 L172 V173 T174 T175 I176 Y180 R181 E182 F183 I184 T189 D192 N193 S194 F195 V196 G197 W198 D199 M200 Q201 I204 T205 L206 D207 T208 S209 F210 E211 D212 A213 K214 T215 Q216 V217 Q218 L219 K220 K221 I222 H223 S224 S225 V226

I227 L228 L229 Y230 K233 D234 S241 E242 A243 R244 S245 L246 G247 Y251 F254 W255 I256 V257 P258 S259 L260 V261 T265 K270 P273 S274 G275 L276 I277 S278 V279 S280 Y281 W284 D285 Y286 R291 V292 R293 D294 G295 I296 G297 I298 F310 S311 Y312 I313 P314 E315

A318 S319 C320 Y321 G322 Q323 M324 E325 R326 P327 E328 V329 P330 M331 L334 H335 M338 V341 T342 W343 D344 G345 K346 D347 L348 E352 Q356 V357 H358 P359 R360 L361 V362 V363 I364 V365 L366 N367 D368 D369 R370 E373 K374 V375 W378 E379 T382 L383 S384 L385 R386

H387 A388 V389 W390 P391 D398 CYS E400 P401 D402 D403 S407 I408 V409 E412 E413 F416 V417 I418 V419 E420 P424 L425 T426 E427 T428 C429 V430 R431 N432 T433 V434 P435 C436 R437 K438 F439 N443 N444 S445 T446 N447 E448 G449 M450 N451 V452 K453 K454 C455 C456 K457 G458 F459

C460 I461 K466 L467 S468 R469 Y475 D476 L477 Y478 L479 G483 K484 H485 G486 K487 N494 I497 G498 E499 V500 Q503 V506 M507 A508 V509 G510 S511 L512 T513 I514 N515 E516 E517 R518 S519 E520 V521 V522 D523 V526 P527 F528 V529 E530 I533 S534 V535 M536 V537 S538

ARG SER ASN GLY THR VAL SER PRO SER ALA PHE LEU GLU PRO PHE SER A556 S557 V558 M561 M562 F563 V564 M565 L566 L567 I568 V569 I572 F575 Y579 P582 VAL GLY TYR ASN ARG ASN LEU ALA LYS GLY LYS ALA PRO HIS GLY PRO S598 A604 I605 W606 G610

F613 ASN ASN SER VAL PRO VAL GLN ASN PRO LYS GLY T625 T626 I629 M630 V631 S632 V633 W634 A635 F636 F637 F641 L642 A643 S644 Y645 N648 L649 F652 M653 I654 Q655 ARG R657 F658 V659 D660 Q661 V662 T663 G664 L665 S666 D667 K668 Q671 R672 P673 F680 R681 F682

G683 T684 T690 E691 R692 N693 I694 R695 N696 N697 Y698 M701 H702 Q703 Y704 M705 Q710 K711 G712 V713 E714 D715 A716 L717 V718 S719 L720 K721 T722 G723 K724 L725 D726 A727 F728 I729 Y730 D731 A732 A733 V734 L735 N736 Y737 K738 A739 G740 R741 D742 E743 G744 C745 K746 L747 V748 T749 I750

G751 S752 G753 F756 A757 T758 T759 GLY TYR GLY I763 A764 L765 Q766 K767 G768 S769 P770 W771 K772 R773 D776 L777 A778 L779 L780 Q781 G784 D785 M788 E789 E790 L791 E792 T793 L794 W795 L796 I799 C800 H801 N802 E803 K804 N805 E806 V807 M808 S809 SER GLN LEU ASP I814

G819 V820 F821 Y822 M823 L824 A825 A826 A827 M828 A829 L830 S831 L832 F841

# 4   Experimental information ⓘ

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 86215 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 56 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 7.243 | Depositor |
| Minimum map value | -1.433 | Depositor |
| Average map value | 0.048 | Depositor |
| Map value standard deviation | 0.746 | Depositor |
| Recommended contour level | 3.0 | Depositor |
| Map size (Å) | 242.4, 242.4, 242.4 | wwPDB |
| Map dimensions | 240, 240, 240 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.01, 1.01, 1.01 | Depositor |

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

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 | 0.53 | 0/6273 | 0.74 | 10/8483 (0.1%) |
| 1 | C | 0.53 | 0/6282 | 0.74 | 10/8498 (0.1%) |
| 2 | B | 0.50 | 2/5946 (0.0%) | 0.71 | 9/8072 (0.1%) |
| 2 | D | 0.49 | 1/5946 (0.0%) | 0.71 | 11/8072 (0.1%) |
| All | All | 0.52 | 3/24447 (0.0%) | 0.73 | 40/33125 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 5 |
| 1 | C | 0 | 6 |
| 2 | B | 0 | 6 |
| 2 | D | 0 | 6 |
| All | All | 0 | 23 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 2 | B | 536 | MET | C-N | 6.29 | 1.48 | 1.34 |
| 2 | D | 343 | TRP | CB-CG | -6.15 | 1.39 | 1.50 |
| 2 | B | 343 | TRP | CB-CG | -6.15 | 1.39 | 1.50 |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|----------|------|----------------|-------------|
| 1 | C | 95 | PRO | N-CA-CB | 8.76 | 113.81 | 103.30 |
| 1 | A | 95 | PRO | N-CA-CB | 8.75 | 113.80 | 103.30 |
| 2 | D | 327 | PRO | N-CA-CB | 6.52 | 111.12 | 103.30 |
| 2 | B | 327 | PRO | N-CA-CB | 6.52 | 111.12 | 103.30 |
| 1 | C | 184 | LEU | CA-CB-CG | 6.45 | 130.13 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | A | 184 | LEU | CA-CB-CG | 6.44 | 130.11 | 115.30 |
| 2 | D | 424 | PRO | N-CA-CB | 6.37 | 110.95 | 103.30 |
| 2 | B | 424 | PRO | N-CA-CB | 6.37 | 110.95 | 103.30 |
| 2 | D | 529 | VAL | C-N-CA | -6.29 | 105.97 | 121.70 |
| 2 | D | 391 | PRO | N-CA-CB | 6.29 | 110.85 | 103.30 |
| 2 | B | 391 | PRO | N-CA-CB | 6.28 | 110.84 | 103.30 |
| 2 | B | 529 | VAL | C-N-CA | -6.28 | 106.01 | 121.70 |
| 1 | C | 777 | LEU | O-C-N | 6.16 | 132.55 | 122.70 |
| 1 | A | 777 | LEU | O-C-N | 6.13 | 132.51 | 122.70 |
| 1 | C | 547 | PRO | N-CA-CB | 6.08 | 110.60 | 103.30 |
| 1 | A | 547 | PRO | N-CA-CB | 6.07 | 110.58 | 103.30 |
| 2 | D | 401 | PRO | N-CA-CB | 5.90 | 110.38 | 103.30 |
| 2 | B | 401 | PRO | N-CA-CB | 5.88 | 110.36 | 103.30 |
| 2 | D | 727 | ALA | O-C-N | -5.81 | 113.41 | 122.70 |
| 1 | A | 169 | ASP | CB-CG-OD1 | -5.79 | 113.09 | 118.30 |
| 1 | C | 169 | ASP | CB-CG-OD1 | -5.76 | 113.12 | 118.30 |
| 1 | A | 96 | PRO | N-CA-CB | 5.73 | 110.18 | 103.30 |
| 1 | C | 96 | PRO | N-CA-CB | 5.72 | 110.16 | 103.30 |
| 2 | D | 330 | PRO | N-CA-CB | 5.62 | 110.04 | 103.30 |
| 2 | B | 330 | PRO | N-CA-CB | 5.61 | 110.03 | 103.30 |
| 1 | A | 98 | PRO | N-CA-CB | 5.56 | 109.97 | 103.30 |
| 1 | C | 98 | PRO | N-CA-CB | 5.53 | 109.94 | 103.30 |
| 1 | C | 777 | LEU | CA-C-N | -5.52 | 105.05 | 117.20 |
| 1 | A | 777 | LEU | CA-C-N | -5.51 | 105.07 | 117.20 |
| 2 | B | 57 | PRO | N-CA-CB | 5.48 | 109.87 | 103.30 |
| 2 | D | 57 | PRO | N-CA-CB | 5.45 | 109.84 | 103.30 |
| 2 | B | 343 | TRP | CA-CB-CG | -5.29 | 103.65 | 113.70 |
| 2 | D | 343 | TRP | CA-CB-CG | -5.29 | 103.65 | 113.70 |
| 2 | D | 729 | ILE | O-C-N | 5.22 | 131.05 | 122.70 |
| 2 | B | 176 | ILE | CG1-CB-CG2 | -5.11 | 100.16 | 111.40 |
| 2 | D | 176 | ILE | CG1-CB-CG2 | -5.11 | 100.17 | 111.40 |
| 1 | A | 254 | ILE | CG1-CB-CG2 | -5.09 | 100.19 | 111.40 |
| 1 | C | 254 | ILE | CG1-CB-CG2 | -5.08 | 100.23 | 111.40 |
| 1 | A | 238 | LEU | C-N-CA | 5.07 | 134.37 | 121.70 |
| 1 | C | 238 | LEU | C-N-CA | 5.06 | 134.35 | 121.70 |

There are no chirality outliers.

All (23) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 162 | HIS | Peptide |
| 1 | A | 248 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 353 | ILE | Peptide |
| 1 | A | 368 | ASN | Peptide |
| 1 | A | 491 | ASN | Peptide |
| 2 | B | 170 | PHE | Peptide |
| 2 | B | 251 | TYR | Peptide |
| 2 | B | 310 | PHE | Peptide |
| 2 | B | 331 | MET | Peptide |
| 2 | B | 44 | HIS | Peptide |
| 2 | B | 796 | LEU | Peptide |
| 1 | C | 162 | HIS | Peptide |
| 1 | C | 248 | LEU | Peptide |
| 1 | C | 353 | ILE | Peptide |
| 1 | C | 368 | ASN | Peptide |
| 1 | C | 381 | TRP | Peptide |
| 1 | C | 491 | ASN | Peptide |
| 2 | D | 170 | PHE | Peptide |
| 2 | D | 251 | TYR | Peptide |
| 2 | D | 310 | PHE | Peptide |
| 2 | D | 331 | MET | Peptide |
| 2 | D | 44 | HIS | Peptide |
| 2 | D | 796 | LEU | Peptide |

## 5.2   Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 6149 | 0 | 6088 | 529 | 0 |
| 1 | C | 6156 | 0 | 6098 | 531 | 0 |
| 2 | B | 5816 | 0 | 5626 | 538 | 0 |
| 2 | D | 5816 | 0 | 5626 | 529 | 0 |
| All | All | 23937 | 0 | 23438 | 1715 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (1715) 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) |
| --- | --- | --- | --- |
| 2:B:416:PHE:CE1 | 2:B:528:PHE:CE2 | 1.91 | 1.59 |
| 2:B:416:PHE:CD1 | 2:B:528:PHE:CZ | 1.89 | 1.59 |
| 2:B:416:PHE:CD1 | 2:B:528:PHE:HZ | 1.18 | 1.59 |
| 1:A:56:TRP:CB | 1:A:59:GLN:HG3 | 1.31 | 1.58 |
| 1:C:56:TRP:CB | 1:C:59:GLN:CG | 1.81 | 1.58 |
| 2:D:534:SER:HB3 | 2:D:750:ILE:CG2 | 1.29 | 1.58 |
| 2:B:526:VAL:HG21 | 2:B:779:LEU:CD2 | 1.18 | 1.58 |
| 2:D:582:PRO:CG | 1:A:839:ARG:HH22 | 1.07 | 1.58 |
| 1:A:56:TRP:CB | 1:A:59:GLN:CG | 1.81 | 1.57 |
| 2:D:416:PHE:CD1 | 2:D:528:PHE:HZ | 1.18 | 1.57 |
| 2:D:526:VAL:HG21 | 2:D:779:LEU:CD2 | 1.18 | 1.57 |
| 1:C:839:ARG:HH22 | 2:B:582:PRO:CG | 1.04 | 1.56 |
| 2:D:416:PHE:CD1 | 2:D:528:PHE:CZ | 1.89 | 1.56 |
| 2:D:416:PHE:CE1 | 2:D:528:PHE:CE2 | 1.91 | 1.56 |
| 1:C:56:TRP:CB | 1:C:59:GLN:HG3 | 1.31 | 1.56 |
| 2:B:534:SER:HB3 | 2:B:750:ILE:CG2 | 1.29 | 1.54 |
| 2:B:537:VAL:CG1 | 2:B:727:ALA:CB | 1.80 | 1.53 |
| 1:C:817:PHE:CZ | 2:B:561:MET:HB3 | 1.44 | 1.52 |
| 2:D:416:PHE:CZ | 2:D:528:PHE:HE2 | 1.32 | 1.47 |
| 2:D:561:MET:HB3 | 1:A:817:PHE:CZ | 1.47 | 1.47 |
| 2:D:534:SER:CB | 2:D:750:ILE:HG21 | 1.44 | 1.44 |
| 1:C:521:ASN:CG | 2:B:780:LEU:HB3 | 1.35 | 1.44 |
| 2:B:537:VAL:HG12 | 2:B:727:ALA:CB | 0.99 | 1.44 |
| 2:B:416:PHE:CZ | 2:B:528:PHE:HE2 | 1.32 | 1.43 |
| 2:B:534:SER:CB | 2:B:750:ILE:HG21 | 1.44 | 1.43 |
| 1:C:521:ASN:ND2 | 2:B:780:LEU:CB | 1.78 | 1.43 |
| 2:D:526:VAL:CG2 | 2:D:779:LEU:HD22 | 1.49 | 1.42 |
| 2:B:526:VAL:CG2 | 2:B:779:LEU:HD22 | 1.49 | 1.41 |
| 2:D:780:LEU:CB | 1:A:521:ASN:ND2 | 1.83 | 1.40 |
| 2:D:780:LEU:HB3 | 1:A:521:ASN:ND2 | 1.10 | 1.38 |
| 1:C:839:ARG:NH2 | 2:B:582:PRO:HG2 | 1.08 | 1.38 |
| 2:B:537:VAL:CG1 | 2:B:727:ALA:HB2 | 1.39 | 1.38 |
| 2:D:582:PRO:HG2 | 1:A:839:ARG:NH2 | 1.08 | 1.38 |
| 2:D:629:ILE:HD11 | 1:A:608:TRP:CE2 | 1.56 | 1.37 |
| 2:B:630:MET:O | 2:B:634:TRP:CE3 | 1.77 | 1.37 |
| 2:D:780:LEU:HB3 | 1:A:521:ASN:CG | 1.39 | 1.37 |
| 1:C:531:LYS:CB | 1:C:776:ILE:HD13 | 1.54 | 1.36 |
| 1:C:521:ASN:ND2 | 2:B:780:LEU:HB3 | 1.07 | 1.36 |
| 1:C:608:TRP:CE2 | 2:B:629:ILE:HD11 | 1.58 | 1.36 |
| 2:D:533:ILE:O | 2:D:756:PHE:N | 1.57 | 1.36 |
| 2:D:634:TRP:CZ2 | 1:A:824:ILE:CG1 | 2.08 | 1.36 |
| 2:B:533:ILE:O | 2:B:756:PHE:N | 1.57 | 1.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:824:ILE:CG1 | 2:B:634:TRP:CZ2 | 2.09 | 1.35 |
| 2:D:777:LEU:HA | 1:A:521:ASN:OD1 | 1.27 | 1.35 |
| 1:A:531:LYS:CB | 1:A:776:ILE:HD13 | 1.54 | 1.35 |
| 2:D:630:MET:O | 2:D:634:TRP:CE3 | 1.77 | 1.34 |
| 2:D:526:VAL:CG2 | 2:D:779:LEU:CD2 | 2.03 | 1.34 |
| 2:B:536:MET:O | 2:B:728:PHE:N | 1.62 | 1.32 |
| 1:C:608:TRP:CE2 | 2:B:629:ILE:CD1 | 2.13 | 1.31 |
| 2:D:629:ILE:CD1 | 1:A:608:TRP:CE2 | 2.10 | 1.31 |
| 1:A:56:TRP:CB | 1:A:59:GLN:CD | 1.98 | 1.31 |
| 2:D:784:GLY:O | 1:A:696:GLN:NE2 | 1.58 | 1.31 |
| 1:C:696:GLN:NE2 | 2:B:784:GLY:O | 1.61 | 1.30 |
| 2:D:526:VAL:CG1 | 2:D:527:PRO:HD2 | 1.59 | 1.30 |
| 1:C:56:TRP:CB | 1:C:59:GLN:CD | 1.98 | 1.30 |
| 2:B:526:VAL:CG1 | 2:B:527:PRO:HD2 | 1.60 | 1.29 |
| 1:C:820:VAL:HG13 | 2:B:634:TRP:NE1 | 1.46 | 1.29 |
| 1:C:817:PHE:CZ | 2:B:561:MET:CB | 2.16 | 1.28 |
| 2:D:634:TRP:CZ2 | 1:A:824:ILE:HG12 | 1.66 | 1.28 |
| 2:B:526:VAL:HG12 | 2:B:527:PRO:CD | 1.64 | 1.28 |
| 1:C:521:ASN:OD1 | 2:B:777:LEU:HA | 1.30 | 1.28 |
| 2:D:645:TYR:OH | 1:A:810:PHE:HE2 | 1.03 | 1.27 |
| 1:C:810:PHE:HE2 | 2:B:645:TYR:OH | 0.99 | 1.26 |
| 1:A:773:SER:O | 1:A:776:ILE:HG22 | 1.09 | 1.26 |
| 2:D:526:VAL:HG12 | 2:D:527:PRO:CD | 1.64 | 1.26 |
| 1:C:521:ASN:HB2 | 2:B:780:LEU:CG | 1.56 | 1.26 |
| 2:B:526:VAL:CG2 | 2:B:779:LEU:CD2 | 2.03 | 1.26 |
| 1:C:531:LYS:HB2 | 1:C:776:ILE:CD1 | 1.66 | 1.25 |
| 1:C:233:ARG:O | 1:C:237:MET:HG2 | 1.11 | 1.25 |
| 2:D:561:MET:CB | 1:A:817:PHE:CZ | 2.18 | 1.25 |
| 1:A:233:ARG:O | 1:A:237:MET:HG2 | 1.11 | 1.24 |
| 1:A:531:LYS:HB2 | 1:A:776:ILE:CD1 | 1.66 | 1.24 |
| 2:D:536:MET:O | 2:D:728:PHE:N | 1.70 | 1.23 |
| 2:D:634:TRP:NE1 | 1:A:820:VAL:HG13 | 1.51 | 1.23 |
| 2:D:537:VAL:O | 2:D:748:VAL:N | 1.70 | 1.23 |
| 1:C:535:TYR:CE2 | 2:B:759:THR:HG22 | 1.73 | 1.23 |
| 1:C:773:SER:O | 1:C:776:ILE:HG22 | 1.10 | 1.23 |
| 2:B:537:VAL:O | 2:B:748:VAL:N | 1.70 | 1.23 |
| 1:C:521:ASN:CG | 2:B:780:LEU:CB | 2.01 | 1.22 |
| 2:D:561:MET:HB3 | 1:A:817:PHE:CE1 | 1.75 | 1.21 |
| 2:D:534:SER:O | 2:D:729:ILE:HG23 | 1.38 | 1.21 |
| 2:B:534:SER:O | 2:B:729:ILE:HG23 | 1.34 | 1.21 |
| 1:C:817:PHE:CE1 | 2:B:561:MET:HB3 | 1.76 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:629:ILE:HD11 | 1:A:608:TRP:CD2 | 1.76 | 1.21 |
| 2:D:629:ILE:HD13 | 1:A:608:TRP:NE1 | 1.55 | 1.21 |
| 2:D:780:LEU:CB | 1:A:521:ASN:CG | 2.06 | 1.21 |
| 1:C:608:TRP:NE1 | 2:B:629:ILE:HD13 | 1.56 | 1.20 |
| 1:C:521:ASN:HB2 | 2:B:780:LEU:CD2 | 1.72 | 1.20 |
| 2:D:516:GLU:HG2 | 1:A:777:LEU:CD1 | 1.72 | 1.19 |
| 1:C:777:LEU:CD1 | 2:B:516:GLU:HG2 | 1.71 | 1.19 |
| 1:C:824:ILE:HG12 | 2:B:634:TRP:CZ2 | 1.70 | 1.19 |
| 2:B:416:PHE:CE1 | 2:B:528:PHE:CZ | 2.19 | 1.19 |
| 2:D:537:VAL:N | 2:D:748:VAL:O | 1.75 | 1.19 |
| 2:B:537:VAL:O | 2:B:748:VAL:O | 1.60 | 1.19 |
| 1:C:535:TYR:HE2 | 2:B:759:THR:CG2 | 1.56 | 1.18 |
| 2:D:537:VAL:O | 2:D:748:VAL:O | 1.60 | 1.18 |
| 2:D:416:PHE:CE1 | 2:D:528:PHE:CZ | 2.19 | 1.17 |
| 1:C:839:ARG:CZ | 2:B:582:PRO:HB2 | 1.74 | 1.17 |
| 2:B:537:VAL:CG1 | 2:B:727:ALA:HB1 | 1.58 | 1.17 |
| 2:B:537:VAL:N | 2:B:748:VAL:O | 1.75 | 1.17 |
| 1:C:608:TRP:CD2 | 2:B:629:ILE:HD11 | 1.78 | 1.17 |
| 2:D:416:PHE:CZ | 2:D:528:PHE:CE2 | 2.21 | 1.17 |
| 2:D:538:SER:HA | 2:D:747:LEU:HA | 1.21 | 1.16 |
| 2:B:416:PHE:CZ | 2:B:528:PHE:CE2 | 2.21 | 1.16 |
| 2:D:759:THR:HG22 | 1:A:535:TYR:CE2 | 1.78 | 1.16 |
| 2:D:780:LEU:CD2 | 1:A:521:ASN:HB2 | 1.75 | 1.16 |
| 1:C:521:ASN:CB | 2:B:780:LEU:CB | 2.22 | 1.16 |
| 1:C:521:ASN:CB | 2:B:780:LEU:HB3 | 1.74 | 1.16 |
| 2:D:759:THR:HG21 | 1:A:780:HIS:CE1 | 1.81 | 1.16 |
| 1:A:773:SER:O | 1:A:776:ILE:CG2 | 1.94 | 1.16 |
| 1:C:773:SER:O | 1:C:776:ILE:CG2 | 1.94 | 1.15 |
| 1:C:813:MET:CE | 2:B:558:VAL:HG13 | 1.77 | 1.15 |
| 1:C:816:VAL:HG11 | 2:B:641:PHE:CZ | 1.80 | 1.15 |
| 2:B:534:SER:O | 2:B:729:ILE:HA | 1.46 | 1.15 |
| 2:D:780:LEU:HB3 | 1:A:521:ASN:CB | 1.76 | 1.14 |
| 2:B:534:SER:O | 2:B:729:ILE:CG2 | 1.95 | 1.14 |
| 2:D:780:LEU:CB | 1:A:521:ASN:CB | 2.26 | 1.14 |
| 1:C:780:HIS:CE1 | 2:B:759:THR:HG21 | 1.81 | 1.14 |
| 2:D:641:PHE:CZ | 1:A:816:VAL:HG11 | 1.82 | 1.14 |
| 2:D:759:THR:CG2 | 1:A:535:TYR:HE2 | 1.61 | 1.14 |
| 2:D:558:VAL:HG13 | 1:A:813:MET:CE | 1.77 | 1.13 |
| 2:D:780:LEU:CG | 1:A:521:ASN:HB2 | 1.61 | 1.13 |
| 1:C:777:LEU:HB3 | 2:B:516:GLU:HB2 | 1.27 | 1.13 |
| 2:D:582:PRO:HB2 | 1:A:839:ARG:CZ | 1.78 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:534:SER:O | 2:D:729:ILE:HA | 1.47 | 1.13 |
| 2:D:558:VAL:HG13 | 1:A:813:MET:HE2 | 1.18 | 1.13 |
| 2:D:634:TRP:CZ2 | 1:A:824:ILE:HG13 | 1.78 | 1.13 |
| 1:C:773:SER:O | 1:C:777:LEU:HG | 1.49 | 1.12 |
| 1:C:777:LEU:HD12 | 2:B:516:GLU:HG2 | 1.16 | 1.12 |
| 2:D:216:GLN:O | 2:B:220:LYS:NZ | 1.82 | 1.12 |
| 2:B:534:SER:CB | 2:B:732:ALA:HB2 | 1.79 | 1.12 |
| 1:C:208:LEU:HB3 | 1:C:238:LEU:HD11 | 1.15 | 1.12 |
| 1:A:208:LEU:HB3 | 1:A:238:LEU:HD11 | 1.17 | 1.12 |
| 2:B:538:SER:HA | 2:B:747:LEU:HA | 1.21 | 1.11 |
| 2:D:534:SER:CB | 2:D:732:ALA:HB2 | 1.79 | 1.11 |
| 1:A:26:ILE:HG12 | 1:A:58:ILE:HG22 | 1.32 | 1.11 |
| 1:C:839:ARG:NH2 | 2:B:582:PRO:CB | 2.13 | 1.11 |
| 1:A:773:SER:O | 1:A:777:LEU:HG | 1.49 | 1.11 |
| 2:B:526:VAL:HG21 | 2:B:779:LEU:HD21 | 1.14 | 1.10 |
| 2:D:534:SER:HB3 | 2:D:750:ILE:HG23 | 1.31 | 1.10 |
| 1:C:520:ASN:HD22 | 1:C:523:ARG:CG | 1.64 | 1.10 |
| 2:D:220:LYS:NZ | 2:B:216:GLN:O | 1.83 | 1.09 |
| 1:C:824:ILE:HG13 | 2:B:634:TRP:CZ2 | 1.76 | 1.09 |
| 2:D:534:SER:O | 2:D:729:ILE:CG2 | 2.00 | 1.09 |
| 2:D:516:GLU:HG2 | 1:A:777:LEU:HD12 | 1.18 | 1.09 |
| 2:D:537:VAL:HG23 | 2:D:748:VAL:HB | 1.32 | 1.08 |
| 1:A:520:ASN:HD22 | 1:A:523:ARG:CG | 1.64 | 1.08 |
| 2:B:533:ILE:O | 2:B:756:PHE:CA | 2.01 | 1.08 |
| 2:B:534:SER:O | 2:B:729:ILE:CA | 2.01 | 1.08 |
| 1:C:26:ILE:HG12 | 1:C:58:ILE:O | 1.52 | 1.08 |
| 1:C:521:ASN:ND2 | 2:B:780:LEU:CA | 2.17 | 1.08 |
| 1:C:521:ASN:HB2 | 2:B:780:LEU:CB | 1.80 | 1.08 |
| 1:C:817:PHE:HZ | 2:B:561:MET:CB | 1.58 | 1.08 |
| 2:D:516:GLU:HB2 | 1:A:777:LEU:HB3 | 1.26 | 1.08 |
| 1:A:520:ASN:HD22 | 1:A:523:ARG:HG3 | 1.11 | 1.08 |
| 2:D:533:ILE:O | 2:D:756:PHE:CA | 2.01 | 1.07 |
| 2:D:526:VAL:HG21 | 2:D:779:LEU:HD21 | 1.14 | 1.07 |
| 2:B:537:VAL:HG23 | 2:B:748:VAL:HB | 1.31 | 1.07 |
| 2:B:537:VAL:HG13 | 2:B:727:ALA:HB1 | 1.28 | 1.07 |
| 1:C:839:ARG:NH2 | 2:B:582:PRO:CG | 1.79 | 1.07 |
| 1:C:520:ASN:HD22 | 1:C:523:ARG:HG3 | 1.11 | 1.07 |
| 1:C:813:MET:HE2 | 2:B:558:VAL:HG13 | 1.30 | 1.07 |
| 1:C:521:ASN:HB2 | 2:B:780:LEU:HD22 | 1.36 | 1.07 |
| 2:D:780:LEU:CB | 1:A:521:ASN:HB2 | 1.83 | 1.07 |
| 2:D:582:PRO:CB | 1:A:839:ARG:NH2 | 2.18 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:26:ILE:HG12 | 1:A:58:ILE:O | 1.55 | 1.06 |
| 1:A:520:ASN:ND2 | 1:A:523:ARG:CD | 2.19 | 1.06 |
| 1:C:520:ASN:ND2 | 1:C:523:ARG:CD | 2.19 | 1.06 |
| 1:C:820:VAL:HG13 | 2:B:634:TRP:HE1 | 0.91 | 1.06 |
| 1:C:26:ILE:HG12 | 1:C:58:ILE:HG22 | 1.32 | 1.05 |
| 1:C:648:THR:HG22 | 2:B:643:ALA:HB1 | 1.37 | 1.05 |
| 2:D:561:MET:CB | 1:A:817:PHE:HZ | 1.60 | 1.05 |
| 2:D:534:SER:O | 2:D:729:ILE:CA | 2.05 | 1.04 |
| 1:A:233:ARG:O | 1:A:237:MET:CG | 2.06 | 1.04 |
| 2:B:534:SER:HB3 | 2:B:750:ILE:HG23 | 1.31 | 1.04 |
| 1:C:242:GLY:O | 1:C:245:TYR:HD2 | 1.40 | 1.04 |
| 1:A:242:GLY:O | 1:A:245:TYR:HD2 | 1.40 | 1.04 |
| 2:B:534:SER:OG | 2:B:732:ALA:HB2 | 1.58 | 1.04 |
| 2:D:634:TRP:HE1 | 1:A:820:VAL:HG13 | 0.96 | 1.03 |
| 2:D:643:ALA:HB1 | 1:A:648:THR:HG22 | 1.36 | 1.03 |
| 1:C:820:VAL:CG1 | 2:B:634:TRP:HE1 | 1.71 | 1.02 |
| 2:D:582:PRO:CG | 1:A:839:ARG:NH2 | 1.81 | 1.02 |
| 1:A:519:ILE:HG23 | 1:A:529:PHE:CE2 | 1.94 | 1.02 |
| 1:C:519:ILE:HG23 | 1:C:529:PHE:CE2 | 1.94 | 1.02 |
| 2:D:630:MET:HB3 | 2:D:634:TRP:HZ3 | 1.24 | 1.02 |
| 2:D:780:LEU:CA | 1:A:521:ASN:ND2 | 2.22 | 1.02 |
| 1:C:233:ARG:O | 1:C:237:MET:CG | 2.06 | 1.02 |
| 2:B:630:MET:HB3 | 2:B:634:TRP:HZ3 | 1.24 | 1.02 |
| 2:D:629:ILE:CD1 | 1:A:608:TRP:NE1 | 2.19 | 1.01 |
| 2:D:534:SER:OG | 2:D:732:ALA:HB2 | 1.58 | 1.01 |
| 2:D:780:LEU:HD22 | 1:A:521:ASN:HB2 | 1.36 | 1.01 |
| 1:C:777:LEU:CD1 | 2:B:516:GLU:CG | 2.40 | 1.00 |
| 2:D:416:PHE:CG | 2:D:528:PHE:HZ | 1.80 | 1.00 |
| 2:D:534:SER:HB2 | 2:D:732:ALA:HB2 | 1.42 | 1.00 |
| 1:C:608:TRP:NE1 | 2:B:629:ILE:CD1 | 2.19 | 0.99 |
| 1:A:531:LYS:NZ | 1:A:777:LEU:HD11 | 1.77 | 0.99 |
| 1:C:531:LYS:NZ | 1:C:777:LEU:HD11 | 1.77 | 0.99 |
| 2:D:516:GLU:HA | 1:A:777:LEU:HD13 | 1.45 | 0.99 |
| 2:D:634:TRP:HE1 | 1:A:820:VAL:CG1 | 1.75 | 0.99 |
| 2:B:416:PHE:CG | 2:B:528:PHE:HZ | 1.80 | 0.99 |
| 2:D:777:LEU:CA | 1:A:521:ASN:OD1 | 2.10 | 0.99 |
| 2:D:634:TRP:HZ2 | 1:A:824:ILE:HG13 | 1.19 | 0.98 |
| 1:C:777:LEU:HD12 | 2:B:516:GLU:CG | 1.94 | 0.98 |
| 2:D:536:MET:HA | 2:D:749:THR:HA | 1.42 | 0.97 |
| 1:A:520:ASN:HD22 | 1:A:523:ARG:CD | 1.77 | 0.97 |
| 1:C:777:LEU:HD13 | 2:B:516:GLU:HA | 1.44 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:534:SER:O | 2:B:729:ILE:CB | 2.11 | 0.97 |
| 1:C:521:ASN:OD1 | 2:B:777:LEU:CA | 2.13 | 0.96 |
| 1:C:531:LYS:HD2 | 1:C:776:ILE:HG21 | 1.46 | 0.96 |
| 1:A:531:LYS:HD2 | 1:A:776:ILE:HG21 | 1.46 | 0.96 |
| 2:D:516:GLU:CG | 1:A:777:LEU:CD1 | 2.43 | 0.96 |
| 1:C:820:VAL:CG1 | 2:B:634:TRP:NE1 | 2.28 | 0.96 |
| 2:B:534:SER:HB2 | 2:B:732:ALA:HB2 | 1.42 | 0.96 |
| 1:C:520:ASN:HD22 | 1:C:523:ARG:CD | 1.77 | 0.96 |
| 1:A:466:LEU:O | 1:A:470:MET:HB2 | 1.65 | 0.96 |
| 2:D:438:LYS:O | 2:D:451:ASN:HA | 1.66 | 0.95 |
| 1:C:466:LEU:O | 1:C:470:MET:HB2 | 1.65 | 0.95 |
| 1:C:824:ILE:HG13 | 2:B:634:TRP:HZ2 | 1.18 | 0.95 |
| 2:D:630:MET:O | 2:D:634:TRP:CZ3 | 2.20 | 0.95 |
| 2:B:630:MET:O | 2:B:634:TRP:CZ3 | 2.20 | 0.95 |
| 1:C:651:LEU:HD12 | 2:B:643:ALA:HB1 | 1.48 | 0.95 |
| 1:C:773:SER:C | 1:C:776:ILE:HG22 | 1.88 | 0.94 |
| 2:D:534:SER:O | 2:D:729:ILE:CB | 2.16 | 0.94 |
| 2:B:438:LYS:O | 2:B:451:ASN:HA | 1.66 | 0.94 |
| 2:B:460:CYS:SG | 2:B:528:PHE:HE1 | 1.91 | 0.93 |
| 1:C:648:THR:HG22 | 2:B:643:ALA:CB | 1.99 | 0.93 |
| 1:A:234:ALA:O | 1:A:237:MET:HB2 | 1.67 | 0.93 |
| 1:C:820:VAL:HG13 | 2:B:634:TRP:CD1 | 2.02 | 0.93 |
| 1:C:234:ALA:O | 1:C:237:MET:HB2 | 1.67 | 0.93 |
| 2:D:538:SER:C | 2:D:748:VAL:HG23 | 1.89 | 0.92 |
| 1:A:773:SER:C | 1:A:776:ILE:HG22 | 1.88 | 0.92 |
| 2:D:634:TRP:NE1 | 1:A:820:VAL:CG1 | 2.32 | 0.92 |
| 1:A:531:LYS:O | 1:A:776:ILE:HD11 | 1.70 | 0.92 |
| 1:C:531:LYS:O | 1:C:776:ILE:HD11 | 1.70 | 0.92 |
| 1:A:242:GLY:O | 1:A:245:TYR:CD2 | 2.23 | 0.92 |
| 2:D:516:GLU:CG | 1:A:777:LEU:HD12 | 1.98 | 0.92 |
| 2:D:537:VAL:O | 2:D:747:LEU:C | 2.09 | 0.92 |
| 2:D:460:CYS:SG | 2:D:528:PHE:HE1 | 1.91 | 0.91 |
| 2:B:538:SER:C | 2:B:748:VAL:HG23 | 1.89 | 0.91 |
| 2:B:534:SER:CB | 2:B:750:ILE:CG2 | 2.19 | 0.91 |
| 1:C:242:GLY:O | 1:C:245:TYR:CD2 | 2.23 | 0.91 |
| 1:C:777:LEU:HD13 | 2:B:516:GLU:CB | 2.00 | 0.91 |
| 2:B:537:VAL:O | 2:B:747:LEU:C | 2.09 | 0.91 |
| 2:D:643:ALA:CB | 1:A:648:THR:HG22 | 2.00 | 0.91 |
| 2:B:630:MET:O | 2:B:634:TRP:HE3 | 1.30 | 0.91 |
| 1:C:26:ILE:CG1 | 1:C:58:ILE:O | 2.18 | 0.91 |
| 2:D:416:PHE:CG | 2:D:528:PHE:CZ | 2.58 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:534:SER:CB | 2:D:750:ILE:CG2 | 2.19 | 0.90 |
| 2:D:643:ALA:HB1 | 1:A:651:LEU:HD12 | 1.53 | 0.90 |
| 2:D:634:TRP:CD1 | 1:A:820:VAL:HG13 | 2.05 | 0.90 |
| 2:D:629:ILE:HD13 | 1:A:608:TRP:CD1 | 2.08 | 0.89 |
| 2:D:759:THR:HG22 | 1:A:535:TYR:HE2 | 1.16 | 0.89 |
| 1:C:817:PHE:CE2 | 2:B:561:MET:HE2 | 2.06 | 0.89 |
| 1:C:520:ASN:ND2 | 1:C:523:ARG:HD2 | 1.85 | 0.89 |
| 1:C:608:TRP:CD1 | 2:B:629:ILE:HD13 | 2.07 | 0.89 |
| 1:A:520:ASN:ND2 | 1:A:523:ARG:HD2 | 1.85 | 0.89 |
| 1:A:26:ILE:CG1 | 1:A:58:ILE:O | 2.21 | 0.88 |
| 1:A:531:LYS:NZ | 1:A:777:LEU:HD21 | 1.88 | 0.88 |
| 1:C:521:ASN:CG | 2:B:780:LEU:HB2 | 1.93 | 0.88 |
| 1:C:824:ILE:HD11 | 2:B:634:TRP:CE2 | 2.09 | 0.88 |
| 1:C:608:TRP:CH2 | 2:B:626:THR:HG22 | 2.08 | 0.88 |
| 2:B:630:MET:HB3 | 2:B:634:TRP:CZ3 | 2.09 | 0.88 |
| 2:D:533:ILE:CG2 | 2:D:729:ILE:CG2 | 2.51 | 0.88 |
| 2:D:630:MET:O | 2:D:634:TRP:HE3 | 1.30 | 0.88 |
| 2:D:634:TRP:CH2 | 1:A:824:ILE:HG12 | 2.09 | 0.88 |
| 2:B:533:ILE:HB | 2:B:757:ALA:N | 1.86 | 0.88 |
| 2:B:534:SER:OG | 2:B:732:ALA:CB | 2.22 | 0.88 |
| 1:C:531:LYS:NZ | 1:C:777:LEU:HD21 | 1.89 | 0.88 |
| 2:D:634:TRP:CE2 | 1:A:824:ILE:HD11 | 2.08 | 0.88 |
| 1:C:535:TYR:CE2 | 2:B:759:THR:CG2 | 2.43 | 0.88 |
| 2:D:641:PHE:HZ | 1:A:816:VAL:HG11 | 1.35 | 0.88 |
| 1:C:520:ASN:HB2 | 1:C:523:ARG:HB2 | 1.56 | 0.88 |
| 2:D:516:GLU:CB | 1:A:777:LEU:HD13 | 2.04 | 0.88 |
| 1:C:777:LEU:HD13 | 2:B:516:GLU:CA | 2.04 | 0.87 |
| 1:C:824:ILE:HG12 | 2:B:634:TRP:CH2 | 2.08 | 0.87 |
| 2:B:533:ILE:HG22 | 2:B:729:ILE:CG2 | 2.04 | 0.87 |
| 1:C:817:PHE:CD2 | 2:B:561:MET:HE2 | 2.10 | 0.87 |
| 2:D:630:MET:HB3 | 2:D:634:TRP:CZ3 | 2.09 | 0.87 |
| 2:B:534:SER:HB3 | 2:B:750:ILE:HG21 | 0.87 | 0.87 |
| 1:C:820:VAL:CG1 | 2:B:634:TRP:CD1 | 2.58 | 0.87 |
| 1:C:816:VAL:HG11 | 2:B:641:PHE:HZ | 1.32 | 0.87 |
| 1:C:26:ILE:CG1 | 1:C:58:ILE:HG22 | 2.04 | 0.87 |
| 1:A:520:ASN:HB2 | 1:A:523:ARG:HB2 | 1.56 | 0.87 |
| 2:B:416:PHE:CG | 2:B:528:PHE:CZ | 2.58 | 0.87 |
| 2:D:526:VAL:HG21 | 2:D:779:LEU:HD22 | 0.87 | 0.87 |
| 2:D:533:ILE:HG22 | 2:D:729:ILE:CG2 | 2.04 | 0.86 |
| 2:B:533:ILE:CG2 | 2:B:729:ILE:CG2 | 2.53 | 0.86 |
| 1:C:531:LYS:HZ3 | 1:C:777:LEU:HD21 | 1.39 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:531:LYS:HZ2 | 1:A:777:LEU:HD11 | 1.40 | 0.86 |
| 2:B:526:VAL:HG21 | 2:B:779:LEU:HD22 | 0.87 | 0.86 |
| 1:A:519:ILE:HG12 | 1:A:529:PHE:CE2 | 2.10 | 0.86 |
| 2:D:626:THR:HG22 | 1:A:608:TRP:CH2 | 2.09 | 0.86 |
| 1:C:816:VAL:CG1 | 2:B:641:PHE:HZ | 1.88 | 0.86 |
| 1:A:26:ILE:CG1 | 1:A:58:ILE:HG22 | 2.05 | 0.86 |
| 1:C:521:ASN:HD22 | 2:B:780:LEU:CB | 1.64 | 0.86 |
| 2:D:558:VAL:CG1 | 1:A:813:MET:HE2 | 2.05 | 0.86 |
| 1:A:531:LYS:HZ3 | 1:A:777:LEU:HD21 | 1.41 | 0.86 |
| 1:C:519:ILE:HG12 | 1:C:529:PHE:CE2 | 2.10 | 0.85 |
| 2:B:536:MET:HA | 2:B:749:THR:HA | 1.56 | 0.85 |
| 2:D:534:SER:OG | 2:D:732:ALA:CB | 2.22 | 0.85 |
| 1:C:531:LYS:O | 1:C:776:ILE:CD1 | 2.23 | 0.85 |
| 2:D:533:ILE:HB | 2:D:757:ALA:N | 1.86 | 0.85 |
| 2:D:759:THR:CG2 | 1:A:780:HIS:CE1 | 2.59 | 0.85 |
| 1:A:531:LYS:O | 1:A:776:ILE:CD1 | 2.23 | 0.85 |
| 1:C:521:ASN:ND2 | 2:B:780:LEU:N | 2.25 | 0.85 |
| 2:D:561:MET:HE2 | 1:A:817:PHE:CE2 | 2.11 | 0.85 |
| 2:B:537:VAL:O | 2:B:748:VAL:C | 2.15 | 0.85 |
| 1:A:208:LEU:CB | 1:A:238:LEU:HD11 | 2.05 | 0.85 |
| 1:C:780:HIS:CE1 | 2:B:759:THR:CG2 | 2.58 | 0.85 |
| 1:C:520:ASN:ND2 | 1:C:523:ARG:HG3 | 1.92 | 0.84 |
| 2:D:561:MET:HE2 | 1:A:817:PHE:CD2 | 2.12 | 0.84 |
| 2:D:516:GLU:CA | 1:A:777:LEU:HD13 | 2.07 | 0.84 |
| 1:C:208:LEU:CB | 1:C:238:LEU:HD11 | 2.05 | 0.84 |
| 2:D:538:SER:C | 2:D:748:VAL:H | 1.81 | 0.84 |
| 1:C:56:TRP:CB | 1:C:59:GLN:CB | 2.56 | 0.84 |
| 2:D:537:VAL:O | 2:D:748:VAL:C | 2.15 | 0.84 |
| 1:A:540:ILE:O | 1:A:748:THR:HA | 1.78 | 0.84 |
| 2:D:433:THR:HA | 2:D:456:CYS:O | 1.77 | 0.84 |
| 2:D:534:SER:HB3 | 2:D:750:ILE:HG21 | 0.87 | 0.84 |
| 2:D:536:MET:HA | 2:D:749:THR:CA | 2.06 | 0.84 |
| 2:D:536:MET:O | 2:D:727:ALA:C | 2.16 | 0.84 |
| 2:D:641:PHE:HZ | 1:A:816:VAL:CG1 | 1.90 | 0.84 |
| 1:A:56:TRP:CB | 1:A:59:GLN:CB | 2.56 | 0.84 |
| 2:B:433:THR:HA | 2:B:456:CYS:O | 1.77 | 0.84 |
| 1:C:540:ILE:O | 1:C:748:THR:HA | 1.78 | 0.83 |
| 2:D:516:GLU:HB2 | 1:A:777:LEU:CB | 2.08 | 0.83 |
| 1:A:520:ASN:ND2 | 1:A:523:ARG:HG3 | 1.92 | 0.83 |
| 2:D:777:LEU:O | 1:A:521:ASN:ND2 | 2.11 | 0.83 |
| 1:C:531:LYS:CB | 1:C:776:ILE:CD1 | 2.39 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:531:LYS:HZ2 | 1:C:777:LEU:HD11 | 1.40 | 0.83 |
| 2:D:634:TRP:CD1 | 1:A:820:VAL:CG1 | 2.61 | 0.83 |
| 2:B:538:SER:C | 2:B:748:VAL:H | 1.81 | 0.83 |
| 1:C:519:ILE:HG12 | 1:C:529:PHE:CZ | 2.13 | 0.83 |
| 1:C:816:VAL:CG1 | 2:B:641:PHE:CZ | 2.62 | 0.83 |
| 2:B:537:VAL:C | 2:B:748:VAL:O | 2.17 | 0.83 |
| 1:C:813:MET:HE1 | 2:B:558:VAL:HG13 | 1.60 | 0.83 |
| 2:D:558:VAL:CG1 | 1:A:813:MET:CE | 2.57 | 0.83 |
| 2:B:534:SER:CB | 2:B:732:ALA:CB | 2.56 | 0.83 |
| 2:D:759:THR:CG2 | 1:A:535:TYR:CE2 | 2.47 | 0.83 |
| 1:A:208:LEU:HB3 | 1:A:238:LEU:CD1 | 2.05 | 0.83 |
| 2:D:534:SER:CB | 2:D:732:ALA:CB | 2.56 | 0.82 |
| 2:B:538:SER:HA | 2:B:747:LEU:CA | 2.07 | 0.82 |
| 2:B:780:LEU:O | 2:B:784:GLY:N | 2.12 | 0.82 |
| 2:B:536:MET:HB2 | 2:B:735:LEU:HD22 | 1.59 | 0.82 |
| 1:C:777:LEU:CB | 2:B:516:GLU:HB2 | 2.08 | 0.82 |
| 1:C:813:MET:CE | 2:B:558:VAL:CG1 | 2.57 | 0.82 |
| 1:A:519:ILE:HG12 | 1:A:529:PHE:CZ | 2.13 | 0.82 |
| 2:D:538:SER:HA | 2:D:747:LEU:CA | 2.07 | 0.82 |
| 2:D:780:LEU:HB3 | 1:A:521:ASN:HB2 | 1.53 | 0.82 |
| 1:A:520:ASN:ND2 | 1:A:523:ARG:CG | 2.43 | 0.82 |
| 1:C:164:ILE:HB | 1:C:218:VAL:O | 1.79 | 0.82 |
| 1:C:536:GLN:O | 1:C:755:ARG:HA | 1.80 | 0.82 |
| 2:D:780:LEU:N | 1:A:521:ASN:ND2 | 2.28 | 0.82 |
| 2:D:780:LEU:O | 2:D:784:GLY:N | 2.12 | 0.82 |
| 2:D:537:VAL:C | 2:D:748:VAL:O | 2.17 | 0.81 |
| 2:D:641:PHE:CZ | 1:A:816:VAL:CG1 | 2.63 | 0.81 |
| 1:A:536:GLN:O | 1:A:755:ARG:HA | 1.80 | 0.81 |
| 1:C:839:ARG:CZ | 2:B:582:PRO:CB | 2.51 | 0.81 |
| 2:D:115:PHE:O | 2:D:119:HIS:HB2 | 1.80 | 0.81 |
| 2:B:115:PHE:O | 2:B:119:HIS:HB2 | 1.80 | 0.81 |
| 1:A:164:ILE:HB | 1:A:218:VAL:O | 1.79 | 0.81 |
| 2:B:537:VAL:O | 2:B:748:VAL:CA | 2.28 | 0.81 |
| 2:D:780:LEU:HB2 | 1:A:521:ASN:CG | 1.98 | 0.81 |
| 1:C:521:ASN:CB | 2:B:780:LEU:HD22 | 2.10 | 0.81 |
| 2:D:759:THR:HG21 | 1:A:780:HIS:HE1 | 1.46 | 0.81 |
| 1:A:76:LEU:O | 1:A:80:GLU:HB2 | 1.81 | 0.81 |
| 1:C:76:LEU:O | 1:C:80:GLU:HB2 | 1.81 | 0.81 |
| 1:C:777:LEU:HD13 | 2:B:516:GLU:HG2 | 1.63 | 0.81 |
| 2:B:460:CYS:SG | 2:B:528:PHE:CE1 | 2.74 | 0.81 |
| 2:D:537:VAL:O | 2:D:748:VAL:CA | 2.28 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:582:PRO:CB | 1:A:839:ARG:CZ | 2.54 | 0.80 |
| 1:A:144:TYR:O | 1:A:147:GLN:HB2 | 1.80 | 0.80 |
| 1:A:531:LYS:CB | 1:A:776:ILE:CD1 | 2.39 | 0.80 |
| 1:C:813:MET:HE1 | 2:B:558:VAL:CG1 | 2.12 | 0.80 |
| 1:C:839:ARG:NH1 | 2:B:582:PRO:HB2 | 1.96 | 0.80 |
| 1:C:817:PHE:HZ | 2:B:561:MET:HB2 | 1.46 | 0.80 |
| 1:C:144:TYR:O | 1:C:147:GLN:HB2 | 1.80 | 0.79 |
| 2:D:534:SER:HB2 | 2:D:732:ALA:CB | 2.11 | 0.79 |
| 2:D:780:LEU:HD22 | 1:A:521:ASN:CB | 2.12 | 0.79 |
| 2:D:460:CYS:SG | 2:D:528:PHE:CE1 | 2.74 | 0.79 |
| 2:B:534:SER:HB2 | 2:B:732:ALA:CB | 2.11 | 0.79 |
| 2:B:435:PRO:HA | 2:B:454:LYS:O | 1.83 | 0.79 |
| 2:B:751:GLY:O | 2:B:753:GLY:N | 2.16 | 0.79 |
| 1:C:780:HIS:CG | 2:B:759:THR:HG1 | 2.00 | 0.79 |
| 2:D:516:GLU:HG2 | 1:A:777:LEU:HD13 | 1.62 | 0.79 |
| 2:D:780:LEU:HB3 | 1:A:521:ASN:HD22 | 0.97 | 0.79 |
| 1:C:521:ASN:HD22 | 2:B:780:LEU:HB3 | 0.97 | 0.79 |
| 2:D:634:TRP:CE2 | 1:A:824:ILE:CG1 | 2.66 | 0.78 |
| 2:D:751:GLY:O | 2:D:753:GLY:N | 2.16 | 0.78 |
| 1:C:521:ASN:ND2 | 2:B:777:LEU:O | 2.16 | 0.78 |
| 2:D:435:PRO:HA | 2:D:454:LYS:O | 1.83 | 0.78 |
| 2:B:535:VAL:HA | 2:B:729:ILE:CA | 2.14 | 0.78 |
| 1:C:777:LEU:HB2 | 2:B:516:GLU:HG3 | 1.66 | 0.78 |
| 2:D:516:GLU:HG3 | 1:A:777:LEU:HB2 | 1.65 | 0.78 |
| 1:C:208:LEU:HB3 | 1:C:238:LEU:CD1 | 2.05 | 0.77 |
| 1:C:817:PHE:CZ | 2:B:561:MET:HE2 | 2.19 | 0.77 |
| 2:D:536:MET:HB2 | 2:D:735:LEU:HD22 | 1.65 | 0.77 |
| 2:B:537:VAL:CA | 2:B:748:VAL:O | 2.32 | 0.77 |
| 2:D:561:MET:CG | 1:A:817:PHE:CZ | 2.67 | 0.77 |
| 2:D:636:PHE:HB2 | 1:A:615:LEU:HD22 | 1.66 | 0.77 |
| 2:D:536:MET:O | 2:D:727:ALA:CA | 2.31 | 0.77 |
| 1:C:233:ARG:C | 1:C:237:MET:HG2 | 2.02 | 0.77 |
| 2:D:537:VAL:CA | 2:D:748:VAL:O | 2.32 | 0.77 |
| 1:C:521:ASN:HD21 | 2:B:780:LEU:N | 1.83 | 0.77 |
| 2:D:561:MET:HE3 | 1:A:817:PHE:CD1 | 2.20 | 0.77 |
| 1:C:817:PHE:CZ | 2:B:561:MET:CG | 2.67 | 0.76 |
| 2:D:533:ILE:HG22 | 2:D:729:ILE:HG21 | 1.67 | 0.76 |
| 1:C:839:ARG:NH2 | 2:B:582:PRO:HB2 | 1.86 | 0.76 |
| 2:B:534:SER:C | 2:B:729:ILE:HG23 | 2.04 | 0.76 |
| 2:B:533:ILE:HG22 | 2:B:729:ILE:HG21 | 1.66 | 0.76 |
| 1:A:233:ARG:C | 1:A:237:MET:HG2 | 2.02 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:582:PRO:HB2 | 1:A:839:ARG:NH1 | 2.00 | 0.76 |
| 1:C:615:LEU:HD22 | 2:B:636:PHE:HB2 | 1.67 | 0.76 |
| 1:C:824:ILE:CG1 | 2:B:634:TRP:CE2 | 2.68 | 0.76 |
| 1:A:520:ASN:ND2 | 1:A:523:ARG:NE | 2.34 | 0.76 |
| 1:C:695:ARG:HH22 | 2:B:780:LEU:CD1 | 1.99 | 0.76 |
| 1:C:77:SER:O | 1:C:81:ASP:HB2 | 1.87 | 0.75 |
| 1:C:520:ASN:ND2 | 1:C:523:ARG:NE | 2.34 | 0.75 |
| 1:C:520:ASN:HB2 | 1:C:523:ARG:CB | 2.16 | 0.75 |
| 2:D:561:MET:HE3 | 1:A:817:PHE:CE1 | 2.21 | 0.75 |
| 1:C:695:ARG:HH22 | 2:B:780:LEU:HD11 | 1.51 | 0.75 |
| 2:B:535:VAL:HA | 2:B:729:ILE:HA | 1.67 | 0.75 |
| 1:C:780:HIS:HE1 | 2:B:759:THR:HG21 | 1.47 | 0.75 |
| 2:D:516:GLU:CG | 1:A:777:LEU:HD13 | 2.14 | 0.75 |
| 1:A:77:SER:O | 1:A:81:ASP:HB2 | 1.87 | 0.75 |
| 1:C:519:ILE:HG12 | 1:C:529:PHE:CD2 | 2.21 | 0.75 |
| 2:D:416:PHE:CD1 | 2:D:528:PHE:CE2 | 2.42 | 0.75 |
| 1:A:520:ASN:HB2 | 1:A:523:ARG:CB | 2.16 | 0.74 |
| 2:D:561:MET:HB2 | 1:A:817:PHE:HZ | 1.47 | 0.74 |
| 1:C:521:ASN:ND2 | 2:B:781:GLN:H | 1.86 | 0.74 |
| 2:B:265:THR:HG1 | 2:B:284:TRP:HE1 | 1.35 | 0.74 |
| 1:C:777:LEU:HD13 | 2:B:516:GLU:CG | 2.12 | 0.74 |
| 1:C:651:LEU:CD1 | 2:B:643:ALA:HB1 | 2.17 | 0.74 |
| 2:D:117:SER:HB2 | 2:D:143:THR:H | 1.52 | 0.74 |
| 1:A:519:ILE:HG12 | 1:A:529:PHE:CD2 | 2.21 | 0.74 |
| 1:C:26:ILE:HD11 | 1:C:58:ILE:HG21 | 1.70 | 0.74 |
| 2:D:780:LEU:CB | 1:A:521:ASN:HD22 | 1.67 | 0.74 |
| 2:D:561:MET:CE | 1:A:817:PHE:CE1 | 2.71 | 0.73 |
| 1:C:521:ASN:HD22 | 2:B:781:GLN:N | 1.85 | 0.73 |
| 2:D:780:LEU:CD1 | 1:A:695:ARG:HH22 | 2.01 | 0.73 |
| 1:C:521:ASN:ND2 | 2:B:781:GLN:N | 2.36 | 0.73 |
| 2:B:117:SER:HB2 | 2:B:143:THR:H | 1.52 | 0.73 |
| 1:C:438:GLY:HA3 | 1:C:478:LEU:HB2 | 1.71 | 0.73 |
| 1:A:26:ILE:HD11 | 1:A:58:ILE:HG21 | 1.70 | 0.73 |
| 1:A:540:ILE:HA | 1:A:729:PHE:O | 1.88 | 0.73 |
| 2:D:629:ILE:CD1 | 1:A:608:TRP:CZ2 | 2.71 | 0.73 |
| 1:C:510:ALA:O | 1:C:763:ARG:NH2 | 2.22 | 0.73 |
| 2:D:759:THR:HG1 | 1:A:780:HIS:CG | 2.06 | 0.73 |
| 2:D:781:GLN:N | 1:A:521:ASN:HD22 | 1.87 | 0.73 |
| 2:D:781:GLN:H | 1:A:521:ASN:ND2 | 1.87 | 0.72 |
| 2:D:561:MET:CE | 1:A:817:PHE:CD1 | 2.71 | 0.72 |
| 2:D:533:ILE:HG23 | 2:D:729:ILE:HG22 | 1.70 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:817:PHE:CD1 | 2:B:561:MET:CE | 2.73 | 0.72 |
| 1:C:540:ILE:HA | 1:C:729:PHE:O | 1.88 | 0.72 |
| 2:D:780:LEU:N | 1:A:521:ASN:HD21 | 1.88 | 0.72 |
| 1:A:510:ALA:O | 1:A:763:ARG:NH2 | 2.22 | 0.72 |
| 2:D:626:THR:HG22 | 1:A:608:TRP:HH2 | 1.52 | 0.72 |
| 2:D:780:LEU:HD11 | 1:A:695:ARG:HH22 | 1.55 | 0.72 |
| 2:D:534:SER:C | 2:D:729:ILE:HG23 | 2.10 | 0.72 |
| 1:C:535:TYR:HE2 | 2:B:759:THR:HG21 | 1.51 | 0.71 |
| 1:C:817:PHE:CE1 | 2:B:561:MET:CE | 2.73 | 0.71 |
| 1:C:839:ARG:HH21 | 2:B:582:PRO:HG2 | 1.47 | 0.71 |
| 1:A:438:GLY:HA3 | 1:A:478:LEU:HB2 | 1.71 | 0.71 |
| 2:B:432:ASN:HB2 | 2:B:457:LYS:HE2 | 1.72 | 0.71 |
| 1:C:608:TRP:CD1 | 2:B:629:ILE:CD1 | 2.71 | 0.71 |
| 2:D:634:TRP:NE1 | 1:A:824:ILE:HD11 | 2.05 | 0.71 |
| 2:D:643:ALA:HB1 | 1:A:651:LEU:CD1 | 2.21 | 0.71 |
| 2:B:533:ILE:HG23 | 2:B:729:ILE:HG22 | 1.71 | 0.71 |
| 2:D:781:GLN:N | 1:A:521:ASN:ND2 | 2.38 | 0.71 |
| 1:C:531:LYS:HD2 | 1:C:776:ILE:CG2 | 2.20 | 0.71 |
| 1:C:535:TYR:CD2 | 2:B:759:THR:HG22 | 2.24 | 0.71 |
| 2:D:558:VAL:HG13 | 1:A:813:MET:HE1 | 1.73 | 0.71 |
| 2:B:413:GLU:H | 2:B:417:VAL:HB | 1.55 | 0.71 |
| 2:D:413:GLU:H | 2:D:417:VAL:HB | 1.55 | 0.71 |
| 1:C:817:PHE:CD1 | 2:B:561:MET:HE3 | 2.26 | 0.70 |
| 2:D:533:ILE:O | 2:D:756:PHE:C | 2.18 | 0.70 |
| 1:C:25:LYS:HB3 | 1:C:59:GLN:HG2 | 1.72 | 0.70 |
| 2:D:634:TRP:CE2 | 1:A:824:ILE:CD1 | 2.74 | 0.70 |
| 2:D:582:PRO:HG2 | 1:A:839:ARG:HH21 | 1.48 | 0.70 |
| 2:D:759:THR:HG21 | 1:A:535:TYR:HE2 | 1.54 | 0.70 |
| 2:B:416:PHE:CD1 | 2:B:528:PHE:CE2 | 2.42 | 0.70 |
| 1:C:26:ILE:CD1 | 1:C:58:ILE:CG2 | 2.68 | 0.70 |
| 1:A:520:ASN:CB | 1:A:523:ARG:H | 2.04 | 0.70 |
| 2:D:630:MET:CB | 2:D:634:TRP:HZ3 | 2.02 | 0.70 |
| 2:D:432:ASN:HB2 | 2:D:457:LYS:HE2 | 1.72 | 0.70 |
| 2:D:561:MET:HE2 | 1:A:817:PHE:CZ | 2.26 | 0.70 |
| 2:B:536:MET:HA | 2:B:749:THR:CA | 2.20 | 0.70 |
| 1:C:520:ASN:CB | 1:C:523:ARG:H | 2.04 | 0.69 |
| 1:A:25:LYS:HB3 | 1:A:59:GLN:HG2 | 1.74 | 0.69 |
| 2:D:629:ILE:CD1 | 1:A:608:TRP:CD1 | 2.73 | 0.69 |
| 2:B:630:MET:CB | 2:B:634:TRP:HZ3 | 2.02 | 0.69 |
| 2:D:36:ILE:O | 2:D:69:VAL:HA | 1.91 | 0.69 |
| 1:A:56:TRP:CB | 1:A:59:GLN:NE2 | 2.56 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:26:ILE:CD1 | 1:A:58:ILE:CG2 | 2.70 | 0.69 |
| 1:C:26:ILE:HD11 | 1:C:58:ILE:CG2 | 2.22 | 0.69 |
| 2:D:572:ILE:HD13 | 1:A:828:ILE:HD11 | 1.75 | 0.69 |
| 2:B:416:PHE:HA | 2:B:459:PHE:HB2 | 1.75 | 0.69 |
| 1:C:519:ILE:HG12 | 1:C:529:PHE:CE1 | 2.28 | 0.69 |
| 2:B:407:SER:HA | 2:B:476:ASP:HB2 | 1.75 | 0.69 |
| 1:A:531:LYS:HD2 | 1:A:776:ILE:CG2 | 2.20 | 0.69 |
| 2:B:765:LEU:HD13 | 2:B:772:LYS:HG2 | 1.75 | 0.69 |
| 1:C:608:TRP:CZ2 | 2:B:629:ILE:CD1 | 2.75 | 0.68 |
| 2:D:416:PHE:HA | 2:D:459:PHE:HB2 | 1.75 | 0.68 |
| 1:C:824:ILE:HD11 | 2:B:634:TRP:NE1 | 2.09 | 0.68 |
| 1:C:824:ILE:CD1 | 2:B:634:TRP:CE2 | 2.76 | 0.68 |
| 1:A:520:ASN:HB2 | 1:A:523:ARG:H | 1.58 | 0.68 |
| 1:A:521:ASN:O | 1:A:525:GLN:HG3 | 1.93 | 0.68 |
| 2:B:536:MET:O | 2:B:727:ALA:CA | 2.40 | 0.68 |
| 1:C:608:TRP:HH2 | 2:B:626:THR:HG22 | 1.53 | 0.68 |
| 2:D:407:SER:HA | 2:D:476:ASP:HB2 | 1.75 | 0.68 |
| 2:B:769:SER:HB2 | 2:B:771:TRP:HD1 | 1.59 | 0.68 |
| 1:C:775:SER:C | 1:C:777:LEU:H | 1.96 | 0.68 |
| 1:C:810:PHE:HE2 | 2:B:645:TYR:CZ | 2.08 | 0.68 |
| 2:B:36:ILE:O | 2:B:69:VAL:HA | 1.91 | 0.68 |
| 2:B:536:MET:C | 2:B:728:PHE:H | 1.90 | 0.68 |
| 1:C:521:ASN:O | 1:C:525:GLN:HG3 | 1.93 | 0.68 |
| 2:D:416:PHE:CE2 | 2:D:528:PHE:HE2 | 2.06 | 0.68 |
| 1:C:520:ASN:HB2 | 1:C:523:ARG:H | 1.58 | 0.68 |
| 1:A:519:ILE:HG12 | 1:A:529:PHE:CE1 | 2.28 | 0.68 |
| 2:B:161:ILE:HA | 2:B:386:ARG:HH12 | 1.59 | 0.68 |
| 2:B:416:PHE:CE2 | 2:B:528:PHE:HE2 | 2.06 | 0.68 |
| 1:C:839:ARG:NH2 | 2:B:582:PRO:O | 2.27 | 0.67 |
| 2:D:161:ILE:HA | 2:D:386:ARG:HH12 | 1.59 | 0.67 |
| 2:D:750:ILE:O | 2:D:750:ILE:HG12 | 1.92 | 0.67 |
| 2:D:759:THR:HG22 | 1:A:535:TYR:CD2 | 2.26 | 0.67 |
| 1:A:775:SER:C | 1:A:777:LEU:H | 1.96 | 0.67 |
| 1:C:56:TRP:CB | 1:C:59:GLN:NE2 | 2.56 | 0.67 |
| 2:D:765:LEU:HD13 | 2:D:772:LYS:HG2 | 1.75 | 0.67 |
| 2:B:533:ILE:N | 2:B:757:ALA:HB3 | 2.06 | 0.67 |
| 2:B:682:PHE:HE1 | 2:B:727:ALA:HB3 | 1.58 | 0.67 |
| 2:D:769:SER:HB2 | 2:D:771:TRP:HD1 | 1.59 | 0.67 |
| 1:A:410:TYR:HB2 | 1:A:456:TYR:HB2 | 1.77 | 0.67 |
| 1:C:521:ASN:HB2 | 2:B:780:LEU:HB3 | 1.52 | 0.67 |
| 1:C:696:GLN:HE21 | 2:B:784:GLY:C | 1.89 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:410:TYR:HB2 | 1:C:456:TYR:HB2 | 1.77 | 0.67 |
| 2:D:265:THR:HG1 | 2:D:284:TRP:HE1 | 1.40 | 0.67 |
| 1:A:531:LYS:C | 1:A:776:ILE:HD11 | 2.14 | 0.67 |
| 2:D:280:SER:O | 2:D:362:VAL:HB | 1.95 | 0.67 |
| 2:B:750:ILE:O | 2:B:750:ILE:HG12 | 1.92 | 0.67 |
| 1:C:531:LYS:C | 1:C:776:ILE:HD11 | 2.14 | 0.67 |
| 2:D:270:LYS:O | 2:D:370:ARG:NH1 | 2.28 | 0.67 |
| 1:A:302:THR:HG21 | 1:A:316:LYS:HB2 | 1.77 | 0.67 |
| 2:B:526:VAL:CG2 | 2:B:779:LEU:HD21 | 1.91 | 0.67 |
| 1:A:26:ILE:HD11 | 1:A:58:ILE:CG2 | 2.23 | 0.66 |
| 2:B:270:LYS:O | 2:B:370:ARG:NH1 | 2.28 | 0.66 |
| 2:B:280:SER:O | 2:B:362:VAL:HB | 1.95 | 0.66 |
| 1:C:828:ILE:HD11 | 2:B:572:ILE:HD13 | 1.77 | 0.66 |
| 2:D:629:ILE:HD11 | 1:A:608:TRP:CZ2 | 2.27 | 0.66 |
| 2:D:343:TRP:HB2 | 2:D:348:LEU:HD12 | 1.78 | 0.66 |
| 2:D:526:VAL:CG2 | 2:D:779:LEU:HD21 | 1.91 | 0.66 |
| 2:D:582:PRO:CG | 1:A:839:ARG:CZ | 2.72 | 0.66 |
| 1:C:777:LEU:CD1 | 2:B:516:GLU:CB | 2.73 | 0.66 |
| 2:D:536:MET:O | 2:D:727:ALA:HB1 | 1.96 | 0.66 |
| 2:D:759:THR:OG1 | 1:A:780:HIS:CG | 2.49 | 0.66 |
| 2:B:416:PHE:HD1 | 2:B:528:PHE:CZ | 2.02 | 0.66 |
| 2:B:534:SER:HB2 | 2:B:750:ILE:HG21 | 1.69 | 0.65 |
| 1:C:521:ASN:ND2 | 2:B:780:LEU:H | 1.95 | 0.65 |
| 2:B:36:ILE:HB | 2:B:69:VAL:HG22 | 1.77 | 0.65 |
| 2:B:776:ASP:O | 2:B:779:LEU:HB3 | 1.96 | 0.65 |
| 1:C:28:ASN:ND2 | 1:C:85:SER:O | 2.30 | 0.65 |
| 1:C:651:LEU:CD1 | 2:B:643:ALA:CB | 2.73 | 0.65 |
| 1:C:302:THR:HG21 | 1:C:316:LYS:HB2 | 1.77 | 0.65 |
| 2:D:36:ILE:HB | 2:D:69:VAL:HG22 | 1.77 | 0.65 |
| 2:D:526:VAL:HG22 | 2:D:779:LEU:CD2 | 2.24 | 0.65 |
| 1:C:817:PHE:CE1 | 2:B:561:MET:HE3 | 2.30 | 0.65 |
| 1:C:558:PHE:HA | 2:D:814:ILE:HG13 | 1.79 | 0.65 |
| 2:D:516:GLU:CB | 1:A:777:LEU:HB3 | 2.15 | 0.65 |
| 2:B:486:GLY:O | 2:B:692:ARG:NH2 | 2.30 | 0.65 |
| 1:C:351:TYR:O | 1:C:366:ILE:HA | 1.97 | 0.65 |
| 1:A:433:LYS:HA | 1:A:455:CYS:O | 1.97 | 0.65 |
| 1:A:531:LYS:HZ2 | 1:A:777:LEU:CD1 | 2.08 | 0.65 |
| 1:C:26:ILE:CD1 | 1:C:58:ILE:HG22 | 2.27 | 0.64 |
| 2:D:537:VAL:HA | 2:D:727:ALA:HA | 1.77 | 0.64 |
| 2:B:343:TRP:HB2 | 2:B:348:LEU:HD12 | 1.78 | 0.64 |
| 1:C:780:HIS:CG | 2:B:759:THR:OG1 | 2.50 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:582:PRO:O | 1:A:839:ARG:NH2 | 2.30 | 0.64 |
| 1:C:220:ILE:HA | 1:C:248:LEU:HB2 | 1.79 | 0.64 |
| 1:C:433:LYS:HA | 1:C:455:CYS:O | 1.97 | 0.64 |
| 2:D:486:GLY:O | 2:D:692:ARG:NH2 | 2.30 | 0.64 |
| 2:D:533:ILE:N | 2:D:757:ALA:HB3 | 2.06 | 0.64 |
| 2:D:776:ASP:O | 2:D:779:LEU:HB3 | 1.96 | 0.64 |
| 2:B:533:ILE:CG2 | 2:B:729:ILE:HG21 | 2.23 | 0.64 |
| 1:C:534:LYS:O | 1:C:757:GLY:HA2 | 1.97 | 0.64 |
| 2:D:665:LEU:O | 2:D:671:GLN:NE2 | 2.31 | 0.64 |
| 1:A:351:TYR:O | 1:A:366:ILE:HA | 1.97 | 0.64 |
| 2:D:533:ILE:CG2 | 2:D:729:ILE:HG21 | 2.23 | 0.64 |
| 2:D:537:VAL:HG23 | 2:D:748:VAL:CB | 2.20 | 0.64 |
| 2:B:533:ILE:O | 2:B:756:PHE:CB | 2.45 | 0.64 |
| 1:C:685:LYS:HE3 | 1:C:710:ASN:HB2 | 1.78 | 0.64 |
| 1:C:839:ARG:CZ | 2:B:582:PRO:O | 2.46 | 0.64 |
| 1:A:220:ILE:HA | 1:A:248:LEU:HB2 | 1.79 | 0.64 |
| 1:A:242:GLY:O | 1:A:243:SER:C | 2.35 | 0.64 |
| 1:A:534:LYS:O | 1:A:757:GLY:HA2 | 1.97 | 0.64 |
| 1:C:531:LYS:HZ2 | 1:C:777:LEU:CD1 | 2.08 | 0.64 |
| 2:D:533:ILE:O | 2:D:756:PHE:CB | 2.45 | 0.64 |
| 1:C:432:LYS:HD3 | 1:C:464:ILE:HD12 | 1.80 | 0.63 |
| 2:B:483:GLY:HA3 | 2:B:494:ASN:HB3 | 1.80 | 0.63 |
| 1:C:777:LEU:HB3 | 2:B:516:GLU:CB | 2.16 | 0.63 |
| 2:D:534:SER:HB2 | 2:D:750:ILE:HG21 | 1.69 | 0.63 |
| 1:A:685:LYS:HE3 | 1:A:710:ASN:HB2 | 1.79 | 0.63 |
| 1:A:26:ILE:CD1 | 1:A:58:ILE:HG22 | 2.28 | 0.63 |
| 1:A:28:ASN:ND2 | 1:A:85:SER:O | 2.29 | 0.63 |
| 1:A:558:PHE:HA | 2:B:814:ILE:HG13 | 1.79 | 0.63 |
| 2:D:558:VAL:CG1 | 1:A:813:MET:HE1 | 2.27 | 0.63 |
| 2:D:483:GLY:HA3 | 2:D:494:ASN:HB3 | 1.80 | 0.63 |
| 1:A:432:LYS:HD3 | 1:A:464:ILE:HD12 | 1.80 | 0.63 |
| 1:A:531:LYS:HB2 | 1:A:776:ILE:HD13 | 0.71 | 0.63 |
| 1:C:521:ASN:HD22 | 2:B:780:LEU:C | 2.02 | 0.63 |
| 1:C:697:VAL:O | 2:D:431:ARG:NH1 | 2.31 | 0.63 |
| 2:D:434:VAL:O | 2:D:456:CYS:HB2 | 1.99 | 0.63 |
| 2:D:780:LEU:H | 1:A:521:ASN:ND2 | 1.97 | 0.63 |
| 1:C:519:ILE:HG23 | 1:C:529:PHE:CD2 | 2.34 | 0.62 |
| 2:B:533:ILE:CG2 | 2:B:729:ILE:HG22 | 2.28 | 0.62 |
| 2:B:665:LEU:O | 2:B:671:GLN:NE2 | 2.31 | 0.62 |
| 1:C:242:GLY:O | 1:C:243:SER:C | 2.35 | 0.62 |
| 1:C:531:LYS:HB2 | 1:C:776:ILE:HD13 | 0.71 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:535:VAL:HA | 2:D:729:ILE:HA | 1.78 | 0.62 |
| 2:D:636:PHE:CB | 1:A:615:LEU:HD22 | 2.28 | 0.62 |
| 1:A:242:GLY:O | 1:A:243:SER:O | 2.17 | 0.62 |
| 2:B:538:SER:CA | 2:B:748:VAL:H | 2.12 | 0.62 |
| 1:C:125:MET:SD | 1:C:252:ARG:NH2 | 2.73 | 0.62 |
| 2:D:220:LYS:HZ2 | 2:B:220:LYS:HG3 | 1.64 | 0.62 |
| 2:D:510:GLY:O | 2:D:528:PHE:CE1 | 2.53 | 0.62 |
| 2:D:759:THR:OG1 | 1:A:780:HIS:ND1 | 2.28 | 0.62 |
| 1:A:124:ARG:NH1 | 1:A:251:GLU:OE1 | 2.33 | 0.62 |
| 1:C:817:PHE:CG | 2:B:561:MET:HE2 | 2.34 | 0.62 |
| 1:A:152:PHE:O | 1:A:155:MET:HB2 | 1.99 | 0.62 |
| 2:B:434:VAL:O | 2:B:456:CYS:HB2 | 1.99 | 0.62 |
| 1:A:697:VAL:O | 2:B:431:ARG:NH1 | 2.31 | 0.62 |
| 2:B:510:GLY:O | 2:B:528:PHE:CE1 | 2.53 | 0.62 |
| 1:C:366:ILE:HB | 1:C:373:ILE:HB | 1.82 | 0.62 |
| 2:D:738:LYS:HA | 2:D:741:ARG:HB2 | 1.82 | 0.62 |
| 1:A:125:MET:SD | 1:A:252:ARG:NH2 | 2.73 | 0.62 |
| 2:D:538:SER:CA | 2:D:748:VAL:H | 2.13 | 0.62 |
| 1:C:242:GLY:O | 1:C:243:SER:O | 2.17 | 0.62 |
| 1:C:519:ILE:CG2 | 1:C:529:PHE:CE2 | 2.79 | 0.62 |
| 2:D:643:ALA:CB | 1:A:651:LEU:CD1 | 2.78 | 0.62 |
| 1:A:234:ALA:C | 1:A:237:MET:HB2 | 2.20 | 0.62 |
| 1:C:124:ARG:NH1 | 1:C:251:GLU:OE1 | 2.33 | 0.61 |
| 1:A:73:GLN:HG2 | 2:B:321:TYR:HD1 | 1.64 | 0.61 |
| 1:A:519:ILE:HG23 | 1:A:529:PHE:HE2 | 1.59 | 0.61 |
| 1:A:519:ILE:CG2 | 1:A:529:PHE:CE2 | 2.79 | 0.61 |
| 2:B:682:PHE:CD1 | 2:B:727:ALA:O | 2.53 | 0.61 |
| 1:C:152:PHE:O | 1:C:155:MET:HB2 | 1.99 | 0.61 |
| 2:D:216:GLN:HA | 2:D:219:LEU:HB2 | 1.82 | 0.61 |
| 1:C:55:SER:N | 1:C:293:HIS:CE1 | 2.68 | 0.61 |
| 1:C:615:LEU:HD22 | 2:B:636:PHE:CB | 2.31 | 0.61 |
| 2:D:35:ASN:HA | 2:D:68:ASN:O | 2.01 | 0.61 |
| 2:D:535:VAL:HA | 2:D:729:ILE:CA | 2.30 | 0.61 |
| 2:D:791:LEU:HD23 | 2:D:794:LEU:HD12 | 1.82 | 0.61 |
| 2:B:216:GLN:HA | 2:B:219:LEU:HB2 | 1.83 | 0.61 |
| 1:C:55:SER:O | 1:C:293:HIS:HE1 | 1.84 | 0.61 |
| 1:C:372:VAL:HG12 | 1:C:374:PRO:HD3 | 1.83 | 0.61 |
| 2:D:741:ARG:NH2 | 2:D:795:TRP:O | 2.32 | 0.61 |
| 2:D:777:LEU:O | 1:A:521:ASN:CG | 2.38 | 0.61 |
| 1:A:352:SER:HA | 1:A:365:GLY:O | 2.01 | 0.61 |
| 1:A:355:ASN:HB2 | 1:A:362:VAL:HB | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:26:ILE:CD1 | 1:C:58:ILE:HG21 | 2.30 | 0.61 |
| 1:C:537:GLY:H | 1:C:752:LEU:HD22 | 1.65 | 0.61 |
| 1:C:608:TRP:CD2 | 2:B:629:ILE:CD1 | 2.64 | 0.61 |
| 1:A:146:HIS:NE2 | 1:A:345:ASP:OD2 | 2.34 | 0.61 |
| 1:A:372:VAL:HG12 | 1:A:374:PRO:HD3 | 1.83 | 0.61 |
| 2:B:738:LYS:HA | 2:B:741:ARG:HB2 | 1.82 | 0.61 |
| 1:C:73:GLN:HG2 | 2:D:321:TYR:HD1 | 1.64 | 0.61 |
| 1:C:234:ALA:C | 1:C:237:MET:HB2 | 2.20 | 0.61 |
| 1:A:537:GLY:H | 1:A:752:LEU:HD22 | 1.65 | 0.61 |
| 2:B:536:MET:O | 2:B:727:ALA:C | 2.35 | 0.61 |
| 1:C:146:HIS:NE2 | 1:C:345:ASP:OD2 | 2.34 | 0.60 |
| 2:D:561:MET:HE2 | 1:A:817:PHE:CG | 2.36 | 0.60 |
| 2:B:791:LEU:HD23 | 2:B:794:LEU:HD12 | 1.83 | 0.60 |
| 2:D:582:PRO:O | 1:A:839:ARG:CZ | 2.49 | 0.60 |
| 1:C:352:SER:HA | 1:C:365:GLY:O | 2.01 | 0.60 |
| 1:C:817:PHE:CE1 | 2:B:561:MET:HE2 | 2.36 | 0.60 |
| 1:A:335:THR:OG1 | 1:A:346:ARG:NH1 | 2.33 | 0.60 |
| 1:A:366:ILE:HB | 1:A:373:ILE:HB | 1.82 | 0.60 |
| 1:A:519:ILE:HG23 | 1:A:529:PHE:CD2 | 2.34 | 0.60 |
| 2:B:35:ASN:HA | 2:B:68:ASN:O | 2.01 | 0.60 |
| 2:B:515:ASN:HB2 | 2:B:518:ARG:H | 1.66 | 0.60 |
| 1:C:335:THR:OG1 | 1:C:346:ARG:NH1 | 2.33 | 0.60 |
| 1:C:531:LYS:NZ | 1:C:777:LEU:CD1 | 2.58 | 0.60 |
| 2:D:516:GLU:CB | 1:A:777:LEU:CD1 | 2.77 | 0.60 |
| 1:A:193:LYS:NZ | 1:A:210:GLU:O | 2.35 | 0.60 |
| 2:B:175:THR:HG22 | 2:B:206:LEU:HB2 | 1.84 | 0.60 |
| 2:D:220:LYS:HG3 | 2:B:220:LYS:HZ2 | 1.67 | 0.60 |
| 2:D:645:TYR:CZ | 1:A:810:PHE:HE2 | 2.11 | 0.60 |
| 1:A:531:LYS:NZ | 1:A:777:LEU:CD1 | 2.58 | 0.60 |
| 2:B:536:MET:HB3 | 2:B:728:PHE:HB2 | 1.83 | 0.60 |
| 2:B:741:ARG:NH2 | 2:B:795:TRP:O | 2.32 | 0.60 |
| 2:B:537:VAL:HG23 | 2:B:748:VAL:CB | 2.20 | 0.60 |
| 1:C:839:ARG:HH22 | 2:B:582:PRO:HG2 | 0.43 | 0.60 |
| 2:D:175:THR:HG22 | 2:D:206:LEU:HB2 | 1.84 | 0.60 |
| 1:A:519:ILE:HG12 | 1:A:529:PHE:CG | 2.36 | 0.60 |
| 1:C:488:GLU:HB2 | 1:C:499:ASN:HD21 | 1.67 | 0.60 |
| 2:D:515:ASN:HB2 | 2:D:518:ARG:H | 1.66 | 0.60 |
| 2:D:740:GLY:HA2 | 2:D:800:CYS:H | 1.66 | 0.60 |
| 1:A:26:ILE:CD1 | 1:A:58:ILE:HG21 | 2.31 | 0.60 |
| 1:A:488:GLU:HB2 | 1:A:499:ASN:HD21 | 1.67 | 0.60 |
| 1:A:775:SER:C | 1:A:777:LEU:N | 2.55 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:648:THR:CG2 | 2:B:643:ALA:CB | 2.78 | 0.60 |
| 1:C:682:ALA:HB1 | 1:C:710:ASN:HA | 1.83 | 0.60 |
| 2:D:35:ASN:O | 2:D:97:GLY:N | 2.35 | 0.60 |
| 1:A:55:SER:N | 1:A:293:HIS:CE1 | 2.70 | 0.60 |
| 2:B:720:LEU:HB3 | 2:B:747:LEU:HD22 | 1.84 | 0.60 |
| 1:C:519:ILE:HG12 | 1:C:529:PHE:CG | 2.36 | 0.59 |
| 1:A:341:ASN:HD22 | 1:A:345:ASP:HB2 | 1.67 | 0.59 |
| 1:A:682:ALA:HB1 | 1:A:710:ASN:HA | 1.83 | 0.59 |
| 2:B:291:ARG:HG2 | 2:B:360:ARG:HH12 | 1.66 | 0.59 |
| 1:C:341:ASN:HD22 | 1:C:345:ASP:HB2 | 1.67 | 0.59 |
| 1:C:751:GLU:HB3 | 1:C:755:ARG:HH21 | 1.67 | 0.59 |
| 1:A:55:SER:O | 1:A:293:HIS:HE1 | 1.84 | 0.59 |
| 2:B:35:ASN:O | 2:B:97:GLY:N | 2.35 | 0.59 |
| 2:D:582:PRO:HG2 | 1:A:839:ARG:HH22 | 0.42 | 0.59 |
| 1:A:160:TRP:HZ3 | 1:A:391:GLY:H | 1.49 | 0.59 |
| 1:C:193:LYS:NZ | 1:C:210:GLU:O | 2.34 | 0.59 |
| 1:C:521:ASN:CG | 2:B:777:LEU:O | 2.41 | 0.59 |
| 1:C:839:ARG:CZ | 2:B:582:PRO:CG | 2.71 | 0.59 |
| 2:D:291:ARG:HG2 | 2:D:360:ARG:HH12 | 1.66 | 0.59 |
| 2:D:162:MET:HE1 | 2:D:228:LEU:HD11 | 1.84 | 0.59 |
| 1:C:160:TRP:HZ3 | 1:C:391:GLY:H | 1.49 | 0.59 |
| 2:D:561:MET:HG3 | 1:A:817:PHE:CZ | 2.38 | 0.59 |
| 1:A:751:GLU:HB3 | 1:A:755:ARG:HH21 | 1.68 | 0.59 |
| 1:C:355:ASN:HB2 | 1:C:362:VAL:HB | 1.83 | 0.59 |
| 2:B:361:LEU:HB2 | 2:B:378:TRP:HB2 | 1.85 | 0.59 |
| 1:C:364:VAL:HA | 1:C:375:ASN:HB2 | 1.85 | 0.59 |
| 1:C:531:LYS:C | 1:C:776:ILE:CD1 | 2.72 | 0.59 |
| 1:C:820:VAL:HG11 | 2:B:634:TRP:CD1 | 2.38 | 0.59 |
| 1:A:317:THR:O | 1:A:321:PHE:N | 2.34 | 0.59 |
| 2:D:536:MET:HB3 | 2:D:728:PHE:HB2 | 1.84 | 0.58 |
| 2:D:720:LEU:HB3 | 2:D:747:LEU:HD22 | 1.84 | 0.58 |
| 1:A:145:SER:O | 1:A:148:SER:OG | 2.19 | 0.58 |
| 2:B:162:MET:HE1 | 2:B:228:LEU:HD11 | 1.86 | 0.58 |
| 2:B:503:GLN:HA | 2:B:766:GLN:HE22 | 1.68 | 0.58 |
| 2:B:538:SER:C | 2:B:746:LYS:O | 2.42 | 0.58 |
| 1:C:79:CYS:HB3 | 2:D:80:LYS:HE3 | 1.86 | 0.58 |
| 1:C:536:GLN:HE22 | 1:C:734:ALA:HB2 | 1.68 | 0.58 |
| 1:A:406:GLU:HG2 | 1:A:410:TYR:HA | 1.84 | 0.58 |
| 1:A:79:CYS:HB3 | 2:B:80:LYS:HE3 | 1.85 | 0.58 |
| 2:B:38:VAL:O | 2:B:71:ALA:HA | 2.02 | 0.58 |
| 1:C:55:SER:H | 1:C:293:HIS:CE1 | 2.21 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:C:494:ASN:HB3 | 2:D:193:ASN:HB3 | 1.85 | 0.58 |
| 1:C:519:ILE:HG23 | 1:C:529:PHE:HE2 | 1.59 | 0.58 |
| 1:C:521:ASN:HD21 | 2:B:780:LEU:H | 1.47 | 0.58 |
| 2:D:38:VAL:O | 2:D:71:ALA:HA | 2.02 | 0.58 |
| 2:D:503:GLN:HA | 2:D:766:GLN:HE22 | 1.68 | 0.58 |
| 2:D:780:LEU:HB2 | 1:A:521:ASN:CB | 2.30 | 0.58 |
| 1:A:155:MET:O | 1:A:159:SER:N | 2.37 | 0.58 |
| 1:A:494:ASN:HB3 | 2:B:193:ASN:HB3 | 1.85 | 0.58 |
| 2:B:740:GLY:HA2 | 2:B:800:CYS:H | 1.66 | 0.58 |
| 2:D:216:GLN:C | 2:B:220:LYS:NZ | 2.55 | 0.58 |
| 1:A:364:VAL:HA | 1:A:375:ASN:HB2 | 1.85 | 0.58 |
| 2:D:35:ASN:HB3 | 2:D:95:ILE:HG23 | 1.84 | 0.58 |
| 2:D:536:MET:O | 2:D:727:ALA:CB | 2.52 | 0.58 |
| 1:C:610:SER:O | 1:C:614:LEU:HB2 | 2.04 | 0.58 |
| 2:D:216:GLN:C | 2:B:220:LYS:HZ1 | 2.05 | 0.58 |
| 2:D:538:SER:C | 2:D:746:LYS:O | 2.42 | 0.58 |
| 1:A:531:LYS:C | 1:A:776:ILE:CD1 | 2.72 | 0.58 |
| 1:A:610:SER:O | 1:A:614:LEU:HB2 | 2.04 | 0.58 |
| 1:C:406:GLU:HG2 | 1:C:410:TYR:HA | 1.84 | 0.58 |
| 2:D:572:ILE:CD1 | 1:A:828:ILE:HD11 | 2.34 | 0.58 |
| 1:C:813:MET:HE2 | 2:B:558:VAL:CG1 | 2.20 | 0.58 |
| 2:D:437:ARG:HD3 | 2:D:451:ASN:HB3 | 1.85 | 0.58 |
| 1:C:138:LEU:HD22 | 1:C:344:GLY:HA3 | 1.86 | 0.57 |
| 1:C:531:LYS:HZ3 | 1:C:777:LEU:CD2 | 2.16 | 0.57 |
| 2:D:780:LEU:C | 1:A:521:ASN:HD22 | 2.06 | 0.57 |
| 2:B:535:VAL:N | 2:B:729:ILE:HG12 | 2.04 | 0.57 |
| 1:C:780:HIS:ND1 | 2:B:759:THR:OG1 | 2.29 | 0.57 |
| 2:D:361:LEU:HB2 | 2:D:378:TRP:HB2 | 1.85 | 0.57 |
| 2:B:437:ARG:HD3 | 2:B:451:ASN:HB3 | 1.85 | 0.57 |
| 2:D:220:LYS:NZ | 2:B:220:LYS:HG3 | 2.19 | 0.57 |
| 2:D:538:SER:C | 2:D:748:VAL:CG2 | 2.70 | 0.57 |
| 1:A:56:TRP:CB | 1:A:59:GLN:HB2 | 2.34 | 0.57 |
| 1:A:138:LEU:HD22 | 1:A:344:GLY:HA3 | 1.87 | 0.57 |
| 1:A:531:LYS:NZ | 1:A:777:LEU:CD2 | 2.66 | 0.57 |
| 1:C:775:SER:C | 1:C:777:LEU:N | 2.55 | 0.57 |
| 2:D:123:PRO:HG3 | 2:D:334:LEU:HD12 | 1.87 | 0.57 |
| 2:D:157:VAL:HG21 | 2:D:361:LEU:HD13 | 1.87 | 0.57 |
| 2:D:220:LYS:HZ1 | 2:B:216:GLN:C | 2.07 | 0.57 |
| 2:D:226:VAL:HG22 | 2:D:254:PHE:HB2 | 1.87 | 0.57 |
| 1:A:58:ILE:HG22 | 1:A:58:ILE:O | 2.04 | 0.57 |
| 2:B:526:VAL:HG22 | 2:B:779:LEU:CD2 | 2.24 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:694:ILE:O | 2:B:698:TYR:N | 2.36 | 0.57 |
| 1:C:436:CYS:O | 1:C:452:PRO:HA | 2.05 | 0.57 |
| 1:C:521:ASN:CB | 2:B:780:LEU:HB2 | 2.26 | 0.57 |
| 2:D:102:ASP:HB2 | 2:D:129:GLY:HA3 | 1.86 | 0.57 |
| 2:D:561:MET:CE | 1:A:817:PHE:CZ | 2.87 | 0.57 |
| 2:B:35:ASN:HB3 | 2:B:95:ILE:HG23 | 1.84 | 0.57 |
| 2:B:123:PRO:HG3 | 2:B:334:LEU:HD12 | 1.87 | 0.57 |
| 1:C:58:ILE:O | 1:C:58:ILE:HG22 | 2.04 | 0.57 |
| 2:B:533:ILE:O | 2:B:756:PHE:C | 2.18 | 0.57 |
| 1:A:341:ASN:N | 1:A:345:ASP:O | 2.35 | 0.57 |
| 2:B:233:LYS:HA | 2:B:261:VAL:HG13 | 1.87 | 0.57 |
| 1:C:240:MET:HE3 | 1:C:245:TYR:CE1 | 2.39 | 0.56 |
| 2:D:536:MET:CA | 2:D:749:THR:HA | 2.26 | 0.56 |
| 1:A:162:HIS:ND1 | 1:A:192:GLU:OE2 | 2.37 | 0.56 |
| 1:A:436:CYS:O | 1:A:452:PRO:HA | 2.05 | 0.56 |
| 1:C:56:TRP:CB | 1:C:59:GLN:HB2 | 2.34 | 0.56 |
| 1:A:55:SER:H | 1:A:293:HIS:CE1 | 2.23 | 0.56 |
| 2:B:511:SER:HA | 2:B:528:PHE:CG | 2.39 | 0.56 |
| 1:C:519:ILE:HG12 | 1:C:529:PHE:CD1 | 2.40 | 0.56 |
| 1:C:839:ARG:NE | 2:B:582:PRO:O | 2.38 | 0.56 |
| 2:D:407:SER:HG | 2:D:506:VAL:H | 1.52 | 0.56 |
| 2:D:511:SER:HA | 2:D:528:PHE:CG | 2.39 | 0.56 |
| 2:D:643:ALA:CB | 1:A:648:THR:CG2 | 2.79 | 0.56 |
| 1:A:230:THR:HA | 1:A:233:ARG:HD2 | 1.87 | 0.56 |
| 1:C:310:GLY:N | 2:D:78:ASP:OD2 | 2.39 | 0.56 |
| 1:C:521:ASN:HD22 | 2:B:780:LEU:CA | 1.98 | 0.56 |
| 1:A:536:GLN:HE22 | 1:A:734:ALA:HB2 | 1.68 | 0.56 |
| 1:A:693:PHE:HB3 | 1:A:703:TYR:HE1 | 1.71 | 0.56 |
| 2:B:533:ILE:CB | 2:B:757:ALA:N | 2.64 | 0.56 |
| 1:A:355:ASN:HD21 | 1:A:379:ILE:HG12 | 1.71 | 0.56 |
| 1:A:519:ILE:HG12 | 1:A:529:PHE:CD1 | 2.40 | 0.56 |
| 1:C:828:ILE:HD11 | 2:B:572:ILE:CD1 | 2.36 | 0.56 |
| 1:C:155:MET:O | 1:C:159:SER:N | 2.37 | 0.56 |
| 1:C:162:HIS:HB3 | 1:C:216:ALA:HB2 | 1.88 | 0.56 |
| 1:C:633:GLY:HA2 | 1:C:636:TRP:HD1 | 1.71 | 0.56 |
| 2:D:220:LYS:HG3 | 2:B:220:LYS:NZ | 2.21 | 0.56 |
| 2:B:157:VAL:HG21 | 2:B:361:LEU:HD13 | 1.87 | 0.56 |
| 2:B:226:VAL:HG22 | 2:B:254:PHE:HB2 | 1.87 | 0.56 |
| 1:C:317:THR:O | 1:C:321:PHE:N | 2.34 | 0.56 |
| 1:C:341:ASN:N | 1:C:345:ASP:O | 2.35 | 0.56 |
| 1:C:810:PHE:CE2 | 2:B:645:TYR:OH | 1.91 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:169:VAL:HA | 2:D:199:ASP:HB2 | 1.87 | 0.56 |
| 1:A:489:ARG:HA | 1:A:495:LYS:O | 2.05 | 0.56 |
| 1:A:531:LYS:HZ3 | 1:A:777:LEU:CD2 | 2.17 | 0.56 |
| 2:D:416:PHE:HD1 | 2:D:528:PHE:CZ | 2.02 | 0.56 |
| 2:B:407:SER:HG | 2:B:506:VAL:H | 1.52 | 0.56 |
| 1:C:738:PHE:HE1 | 1:C:793:VAL:HG13 | 1.71 | 0.56 |
| 1:A:773:SER:HA | 1:A:776:ILE:CG2 | 2.36 | 0.56 |
| 2:B:169:VAL:HA | 2:B:199:ASP:HB2 | 1.87 | 0.56 |
| 2:B:682:PHE:CE1 | 2:B:727:ALA:HB3 | 2.41 | 0.56 |
| 1:C:162:HIS:ND1 | 1:C:192:GLU:OE2 | 2.37 | 0.55 |
| 1:A:354:MET:HB3 | 1:A:361:LEU:HD22 | 1.88 | 0.55 |
| 1:C:410:TYR:HB3 | 1:C:412:LYS:HE3 | 1.88 | 0.55 |
| 1:C:531:LYS:NZ | 1:C:777:LEU:CD2 | 2.66 | 0.55 |
| 2:D:229:LEU:HB2 | 2:D:257:VAL:HG22 | 1.88 | 0.55 |
| 2:D:643:ALA:HB1 | 1:A:648:THR:CG2 | 2.24 | 0.55 |
| 2:B:102:ASP:HB2 | 2:B:129:GLY:HA3 | 1.86 | 0.55 |
| 1:C:230:THR:HA | 1:C:233:ARG:HD2 | 1.87 | 0.55 |
| 1:C:362:VAL:HG13 | 1:C:377:ARG:HD3 | 1.88 | 0.55 |
| 1:C:489:ARG:HA | 1:C:495:LYS:O | 2.05 | 0.55 |
| 1:C:817:PHE:CZ | 2:B:561:MET:CE | 2.87 | 0.55 |
| 2:D:96:HIS:HE1 | 2:D:315:GLU:HG2 | 1.71 | 0.55 |
| 2:D:310:PHE:HB3 | 2:D:312:TYR:H | 1.72 | 0.55 |
| 2:D:780:LEU:H | 1:A:521:ASN:HD21 | 1.51 | 0.55 |
| 1:A:310:GLY:N | 2:B:78:ASP:OD2 | 2.39 | 0.55 |
| 2:B:510:GLY:O | 2:B:528:PHE:CD1 | 2.60 | 0.55 |
| 1:C:817:PHE:CD1 | 2:B:561:MET:HE2 | 2.40 | 0.55 |
| 2:D:536:MET:C | 2:D:728:PHE:H | 1.98 | 0.55 |
| 1:A:410:TYR:HB3 | 1:A:412:LYS:HE3 | 1.88 | 0.55 |
| 1:A:738:PHE:HE1 | 1:A:793:VAL:HG13 | 1.71 | 0.55 |
| 2:B:96:HIS:HE1 | 2:B:315:GLU:HG2 | 1.71 | 0.55 |
| 1:C:355:ASN:HD21 | 1:C:379:ILE:HG12 | 1.71 | 0.55 |
| 1:C:739:GLU:HA | 1:C:742:GLN:HB2 | 1.88 | 0.55 |
| 2:D:510:GLY:O | 2:D:528:PHE:CD1 | 2.60 | 0.55 |
| 2:B:533:ILE:O | 2:B:756:PHE:HB2 | 2.07 | 0.55 |
| 2:D:233:LYS:HA | 2:D:261:VAL:HG13 | 1.87 | 0.55 |
| 2:D:777:LEU:O | 1:A:521:ASN:OD1 | 2.24 | 0.55 |
| 2:B:229:LEU:HB2 | 2:B:257:VAL:HG22 | 1.88 | 0.55 |
| 1:C:354:MET:HB3 | 1:C:361:LEU:HD22 | 1.88 | 0.55 |
| 1:C:487:GLN:HA | 1:C:497:GLU:O | 2.07 | 0.55 |
| 2:B:310:PHE:HB3 | 2:B:312:TYR:H | 1.72 | 0.55 |
| 1:C:520:ASN:ND2 | 1:C:523:ARG:CG | 2.43 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:693:PHE:HB3 | 1:C:703:TYR:HE1 | 1.71 | 0.55 |
| 2:D:220:LYS:NZ | 2:B:220:LYS:CG | 2.70 | 0.55 |
| 2:D:533:ILE:O | 2:D:756:PHE:HB2 | 2.07 | 0.55 |
| 1:C:396:THR:HB | 1:C:472:PHE:HA | 1.89 | 0.55 |
| 1:A:163:ILE:HB | 1:A:191:ALA:HA | 1.89 | 0.55 |
| 1:A:739:GLU:HA | 1:A:742:GLN:HB2 | 1.88 | 0.55 |
| 1:C:163:ILE:HB | 1:C:191:ALA:HA | 1.89 | 0.55 |
| 1:C:234:ALA:HA | 1:C:237:MET:HB2 | 1.90 | 0.55 |
| 1:C:283:ASP:HB3 | 1:C:338:VAL:HG21 | 1.89 | 0.55 |
| 1:C:521:ASN:N | 1:C:695:ARG:HH22 | 2.05 | 0.55 |
| 1:C:525:GLN:HG3 | 2:B:777:LEU:HD22 | 1.88 | 0.55 |
| 1:C:608:TRP:CZ2 | 2:B:626:THR:HG22 | 2.41 | 0.55 |
| 1:C:773:SER:HA | 1:C:776:ILE:CG2 | 2.36 | 0.55 |
| 1:C:824:ILE:CG1 | 2:B:634:TRP:HZ2 | 1.80 | 0.55 |
| 2:D:409:VAL:HG22 | 2:D:478:TYR:HB2 | 1.88 | 0.55 |
| 1:A:312:THR:HG22 | 2:B:77:THR:H | 1.72 | 0.55 |
| 1:A:633:GLY:HA2 | 1:A:636:TRP:HD1 | 1.71 | 0.55 |
| 2:B:41:GLY:H | 2:B:102:ASP:HA | 1.72 | 0.54 |
| 1:C:26:ILE:HG13 | 1:C:58:ILE:O | 2.07 | 0.54 |
| 1:C:119:LEU:HA | 1:C:138:LEU:O | 2.08 | 0.54 |
| 1:A:162:HIS:HB3 | 1:A:216:ALA:HB2 | 1.88 | 0.54 |
| 1:A:521:ASN:N | 1:A:695:ARG:HH22 | 2.05 | 0.54 |
| 2:B:694:ILE:HA | 2:B:697:ASN:HB2 | 1.89 | 0.54 |
| 1:C:121:LEU:O | 1:C:140:THR:OG1 | 2.25 | 0.54 |
| 1:C:239:ASN:O | 1:C:241:THR:N | 2.40 | 0.54 |
| 1:C:521:ASN:ND2 | 2:B:780:LEU:C | 2.60 | 0.54 |
| 2:D:408:ILE:HD12 | 2:D:475:TYR:HB3 | 1.89 | 0.54 |
| 1:A:121:LEU:O | 1:A:140:THR:OG1 | 2.25 | 0.54 |
| 1:A:362:VAL:HG13 | 1:A:377:ARG:HD3 | 1.88 | 0.54 |
| 2:B:526:VAL:CG1 | 2:B:527:PRO:CD | 2.49 | 0.54 |
| 1:C:513:ILE:HB | 1:C:761:GLY:HA3 | 1.90 | 0.54 |
| 1:C:777:LEU:CB | 2:B:516:GLU:CB | 2.83 | 0.54 |
| 2:D:533:ILE:CB | 2:D:757:ALA:N | 2.64 | 0.54 |
| 2:D:630:MET:C | 2:D:634:TRP:CZ3 | 2.81 | 0.54 |
| 2:D:694:ILE:HA | 2:D:697:ASN:HB2 | 1.89 | 0.54 |
| 2:D:777:LEU:HD22 | 1:A:525:GLN:HG3 | 1.90 | 0.54 |
| 2:B:538:SER:C | 2:B:748:VAL:CG2 | 2.70 | 0.54 |
| 1:C:312:THR:HG22 | 2:D:77:THR:H | 1.72 | 0.54 |
| 2:D:416:PHE:CE2 | 2:D:528:PHE:CE2 | 2.89 | 0.54 |
| 2:D:526:VAL:CG1 | 2:D:527:PRO:CD | 2.49 | 0.54 |
| 2:B:536:MET:O | 2:B:727:ALA:HA | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:41:GLY:H | 2:D:102:ASP:HA | 1.72 | 0.54 |
| 2:D:645:TYR:OH | 1:A:810:PHE:CE2 | 1.96 | 0.54 |
| 2:D:694:ILE:O | 2:D:698:TYR:N | 2.36 | 0.54 |
| 2:D:780:LEU:CA | 1:A:521:ASN:HD22 | 2.03 | 0.54 |
| 1:A:119:LEU:HA | 1:A:138:LEU:O | 2.08 | 0.54 |
| 1:A:234:ALA:HA | 1:A:237:MET:HB2 | 1.90 | 0.54 |
| 1:C:341:ASN:HA | 1:C:347:LYS:HE3 | 1.90 | 0.54 |
| 1:A:487:GLN:HA | 1:A:497:GLU:O | 2.07 | 0.54 |
| 2:B:408:ILE:HD12 | 2:B:475:TYR:HB3 | 1.89 | 0.54 |
| 2:B:409:VAL:HG22 | 2:B:478:TYR:HB2 | 1.88 | 0.54 |
| 1:C:484:PHE:O | 1:C:501:MET:N | 2.41 | 0.54 |
| 2:D:784:GLY:C | 1:A:696:GLN:NE2 | 2.53 | 0.54 |
| 1:A:240:MET:HE3 | 1:A:245:TYR:CE1 | 2.43 | 0.54 |
| 1:C:193:LYS:HE3 | 1:C:214:LEU:HD21 | 1.89 | 0.54 |
| 2:D:582:PRO:O | 1:A:839:ARG:NE | 2.41 | 0.54 |
| 1:A:239:ASN:O | 1:A:241:THR:N | 2.41 | 0.54 |
| 1:A:142:PRO:HB3 | 1:A:345:ASP:HB3 | 1.91 | 0.53 |
| 1:A:484:PHE:O | 1:A:501:MET:N | 2.41 | 0.53 |
| 2:B:630:MET:C | 2:B:634:TRP:CZ3 | 2.81 | 0.53 |
| 1:C:521:ASN:OD1 | 2:B:777:LEU:O | 2.26 | 0.53 |
| 1:A:193:LYS:HE3 | 1:A:214:LEU:HD21 | 1.88 | 0.53 |
| 1:A:396:THR:HB | 1:A:472:PHE:HA | 1.89 | 0.53 |
| 2:B:413:GLU:OE1 | 2:B:511:SER:N | 2.40 | 0.53 |
| 1:C:694:ARG:HH21 | 1:C:707:GLU:HG2 | 1.73 | 0.53 |
| 2:D:516:GLU:CG | 1:A:777:LEU:HB2 | 2.38 | 0.53 |
| 1:C:817:PHE:CZ | 2:B:561:MET:HG3 | 2.40 | 0.53 |
| 1:C:398:LEU:HB3 | 1:C:512:MET:HG3 | 1.90 | 0.53 |
| 1:C:407:PRO:HG2 | 1:C:458:PHE:HE1 | 1.74 | 0.53 |
| 1:C:817:PHE:CE2 | 2:B:561:MET:HG3 | 2.44 | 0.53 |
| 2:D:384:SER:HB2 | 2:D:386:ARG:HE | 1.74 | 0.53 |
| 1:A:694:ARG:HH21 | 1:A:707:GLU:HG2 | 1.73 | 0.53 |
| 1:C:715:ALA:HA | 1:C:718:ILE:HD12 | 1.90 | 0.53 |
| 2:D:645:TYR:HA | 2:D:648:ASN:HB2 | 1.90 | 0.53 |
| 1:A:341:ASN:HA | 1:A:347:LYS:HE3 | 1.90 | 0.53 |
| 1:C:541:LEU:O | 1:C:728:ALA:HA | 2.08 | 0.53 |
| 2:D:413:GLU:OE1 | 2:D:511:SER:N | 2.40 | 0.53 |
| 1:A:283:ASP:HB3 | 1:A:338:VAL:HG21 | 1.89 | 0.53 |
| 1:A:407:PRO:HG2 | 1:A:458:PHE:HE1 | 1.74 | 0.53 |
| 1:A:439:PRO:HG2 | 1:A:442:THR:HG22 | 1.91 | 0.53 |
| 1:C:364:VAL:O | 1:C:375:ASN:N | 2.38 | 0.53 |
| 2:D:295:GLY:HA2 | 2:D:298:ILE:HD12 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:781:GLN:O | 2:D:785:ASP:N | 2.42 | 0.53 |
| 1:A:363:GLN:H | 1:A:377:ARG:HH11 | 1.56 | 0.53 |
| 1:A:541:LEU:O | 1:A:728:ALA:HA | 2.08 | 0.53 |
| 1:A:774:LEU:HA | 1:A:777:LEU:HD12 | 1.91 | 0.53 |
| 2:B:416:PHE:CE2 | 2:B:528:PHE:CE2 | 2.89 | 0.53 |
| 2:B:537:VAL:HA | 2:B:727:ALA:HA | 1.90 | 0.53 |
| 1:C:68:LYS:HZ1 | 1:C:77:SER:H | 1.57 | 0.53 |
| 2:D:42:HIS:HA | 2:D:73:LEU:HB3 | 1.91 | 0.53 |
| 1:A:48:GLN:HA | 1:A:51:LYS:HD2 | 1.91 | 0.53 |
| 2:B:511:SER:HA | 2:B:528:PHE:CD1 | 2.44 | 0.53 |
| 2:B:645:TYR:HA | 2:B:648:ASN:HB2 | 1.90 | 0.53 |
| 2:D:634:TRP:CD1 | 1:A:820:VAL:HG11 | 2.41 | 0.52 |
| 1:A:240:MET:CE | 1:A:245:TYR:CE1 | 2.92 | 0.52 |
| 1:C:817:PHE:CG | 2:B:561:MET:CE | 2.93 | 0.52 |
| 2:D:511:SER:HA | 2:D:528:PHE:CD1 | 2.44 | 0.52 |
| 2:D:535:VAL:HB | 2:D:750:ILE:HA | 1.91 | 0.52 |
| 2:B:211:GLU:HB2 | 2:B:215:THR:HG23 | 1.91 | 0.52 |
| 2:B:384:SER:HB2 | 2:B:386:ARG:HE | 1.74 | 0.52 |
| 1:C:125:MET:O | 1:C:139:ARG:NH2 | 2.42 | 0.52 |
| 1:C:165:LEU:O | 1:C:194:VAL:HA | 2.10 | 0.52 |
| 2:D:777:LEU:C | 1:A:521:ASN:OD1 | 2.48 | 0.52 |
| 1:A:399:LYS:HB2 | 1:A:511:ASP:H | 1.75 | 0.52 |
| 1:C:142:PRO:HB3 | 1:C:345:ASP:HB3 | 1.90 | 0.52 |
| 1:C:240:MET:CE | 1:C:245:TYR:CE1 | 2.92 | 0.52 |
| 1:C:439:PRO:HG2 | 1:C:442:THR:HG22 | 1.91 | 0.52 |
| 2:D:176:ILE:HD12 | 2:D:207:ASP:HA | 1.92 | 0.52 |
| 2:D:626:THR:HG22 | 1:A:608:TRP:CZ2 | 2.44 | 0.52 |
| 1:A:26:ILE:HG13 | 1:A:58:ILE:O | 2.09 | 0.52 |
| 1:A:513:ILE:HB | 1:A:761:GLY:HA3 | 1.90 | 0.52 |
| 1:C:396:THR:HA | 1:C:472:PHE:HD1 | 1.74 | 0.52 |
| 1:C:409:VAL:HA | 1:C:456:TYR:O | 2.10 | 0.52 |
| 1:C:774:LEU:HA | 1:C:777:LEU:HD12 | 1.91 | 0.52 |
| 2:D:211:GLU:HB2 | 2:D:215:THR:HG23 | 1.91 | 0.52 |
| 2:D:561:MET:HE2 | 1:A:817:PHE:CD1 | 2.44 | 0.52 |
| 1:A:396:THR:HA | 1:A:472:PHE:HD1 | 1.74 | 0.52 |
| 1:A:409:VAL:HA | 1:A:456:TYR:O | 2.10 | 0.52 |
| 2:B:295:GLY:HA2 | 2:B:298:ILE:HD12 | 1.90 | 0.52 |
| 2:D:537:VAL:H | 2:D:749:THR:HA | 1.75 | 0.52 |
| 2:D:692:ARG:HA | 2:D:695:ARG:HD2 | 1.91 | 0.52 |
| 1:A:364:VAL:O | 1:A:375:ASN:N | 2.38 | 0.52 |
| 2:B:537:VAL:H | 2:B:749:THR:HA | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:C:267:LEU:HA | 1:C:354:MET:O | 2.10 | 0.52 |
| 1:A:435:ILE:HG23 | 1:A:452:PRO:HB2 | 1.90 | 0.52 |
| 1:A:559:GLN:NE2 | 2:B:814:ILE:O | 2.42 | 0.52 |
| 1:C:435:ILE:HG23 | 1:C:452:PRO:HB2 | 1.90 | 0.52 |
| 1:C:441:ASP:O | 1:C:446:SER:OG | 2.28 | 0.52 |
| 1:C:608:TRP:CG | 2:B:629:ILE:HD11 | 2.41 | 0.52 |
| 2:D:526:VAL:HG11 | 2:D:779:LEU:HD21 | 1.92 | 0.52 |
| 1:A:267:LEU:HA | 1:A:354:MET:O | 2.10 | 0.52 |
| 1:A:398:LEU:HB3 | 1:A:512:MET:HG3 | 1.90 | 0.52 |
| 1:A:441:ASP:O | 1:A:446:SER:OG | 2.28 | 0.52 |
| 2:D:220:LYS:NZ | 2:B:217:VAL:HA | 2.25 | 0.52 |
| 2:D:220:LYS:NZ | 2:B:216:GLN:C | 2.57 | 0.52 |
| 1:A:356:LEU:HB3 | 1:A:359:ARG:HA | 1.92 | 0.52 |
| 2:B:176:ILE:HD12 | 2:B:207:ASP:HA | 1.92 | 0.52 |
| 1:C:48:GLN:HA | 1:C:51:LYS:HD2 | 1.91 | 0.52 |
| 1:A:165:LEU:O | 1:A:194:VAL:HA | 2.10 | 0.52 |
| 1:A:168:SER:HA | 1:A:197:PHE:HB2 | 1.91 | 0.52 |
| 1:A:520:ASN:HD21 | 1:A:523:ARG:NE | 2.07 | 0.52 |
| 2:B:692:ARG:HA | 2:B:695:ARG:HD2 | 1.91 | 0.52 |
| 1:C:363:GLN:H | 1:C:377:ARG:HH11 | 1.56 | 0.51 |
| 1:A:531:LYS:HZ2 | 1:A:777:LEU:CG | 2.23 | 0.51 |
| 2:B:98:LEU:HB3 | 2:B:100:PHE:HE2 | 1.75 | 0.51 |
| 2:D:98:LEU:HB3 | 2:D:100:PHE:HE2 | 1.75 | 0.51 |
| 2:D:516:GLU:CG | 1:A:777:LEU:CB | 2.88 | 0.51 |
| 2:D:561:MET:HG3 | 1:A:817:PHE:CE2 | 2.45 | 0.51 |
| 1:A:240:MET:CE | 1:A:245:TYR:HE1 | 2.23 | 0.51 |
| 2:B:526:VAL:HG11 | 2:B:779:LEU:HD21 | 1.92 | 0.51 |
| 1:C:467:ALA:HB2 | 1:C:474:TYR:HE2 | 1.75 | 0.51 |
| 1:C:559:GLN:NE2 | 2:D:814:ILE:O | 2.42 | 0.51 |
| 2:D:561:MET:HE2 | 1:A:817:PHE:CE1 | 2.42 | 0.51 |
| 1:A:715:ALA:HA | 1:A:718:ILE:HD12 | 1.90 | 0.51 |
| 2:B:668:LYS:HA | 2:B:671:GLN:HB2 | 1.92 | 0.51 |
| 2:B:781:GLN:O | 2:B:785:ASP:N | 2.42 | 0.51 |
| 1:C:145:SER:OG | 1:C:179:ARG:NH1 | 2.44 | 0.51 |
| 1:C:240:MET:CE | 1:C:245:TYR:HE1 | 2.24 | 0.51 |
| 1:C:483:LYS:HD3 | 1:C:686:GLN:HB2 | 1.93 | 0.51 |
| 2:D:365:VAL:N | 2:D:373:GLU:O | 2.36 | 0.51 |
| 1:C:404:HIS:HE1 | 1:C:478:LEU:HB3 | 1.75 | 0.51 |
| 1:A:414:THR:HG23 | 1:A:453:GLN:HA | 1.93 | 0.51 |
| 2:B:42:HIS:HA | 2:B:73:LEU:HB3 | 1.91 | 0.51 |
| 2:B:630:MET:C | 2:B:634:TRP:CE3 | 2.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:785:ASP:HA | 1:A:696:GLN:NE2 | 2.25 | 0.51 |
| 1:C:410:TYR:O | 1:C:455:CYS:HA | 2.11 | 0.51 |
| 2:D:217:VAL:HA | 2:B:220:LYS:NZ | 2.25 | 0.51 |
| 1:A:410:TYR:O | 1:A:455:CYS:HA | 2.11 | 0.51 |
| 1:C:154:MET:SD | 1:C:367:TYR:OH | 2.62 | 0.51 |
| 1:C:356:LEU:HB3 | 1:C:359:ARG:HA | 1.92 | 0.51 |
| 1:C:540:ILE:HG12 | 1:C:730:ILE:HG12 | 1.93 | 0.51 |
| 2:D:526:VAL:CB | 2:D:527:PRO:HD2 | 2.37 | 0.51 |
| 1:A:145:SER:OG | 1:A:179:ARG:NH1 | 2.44 | 0.51 |
| 1:A:536:GLN:O | 1:A:755:ARG:CA | 2.56 | 0.51 |
| 2:B:286:TYR:OH | 2:B:379:GLU:OE2 | 2.28 | 0.51 |
| 1:C:168:SER:HA | 1:C:197:PHE:HB2 | 1.91 | 0.51 |
| 1:C:221:LEU:HD11 | 1:C:247:TRP:HE3 | 1.76 | 0.51 |
| 1:C:368:ASN:HB2 | 1:C:371:HIS:HD2 | 1.76 | 0.51 |
| 1:C:399:LYS:HB2 | 1:C:511:ASP:H | 1.75 | 0.51 |
| 1:A:154:MET:SD | 1:A:367:TYR:OH | 2.62 | 0.51 |
| 1:C:461:ASP:OD2 | 1:C:792:TRP:NE1 | 2.39 | 0.50 |
| 1:C:678:LYS:O | 1:C:727:HIS:NE2 | 2.44 | 0.50 |
| 1:A:125:MET:O | 1:A:139:ARG:NH2 | 2.42 | 0.50 |
| 2:B:101:GLY:HA2 | 2:B:128:HIS:H | 1.76 | 0.50 |
| 1:C:414:THR:HG23 | 1:C:453:GLN:HA | 1.93 | 0.50 |
| 1:C:536:GLN:O | 1:C:755:ARG:CA | 2.56 | 0.50 |
| 1:C:608:TRP:CZ2 | 2:B:629:ILE:HD11 | 2.30 | 0.50 |
| 2:D:89:LEU:HB3 | 2:D:95:ILE:HD12 | 1.93 | 0.50 |
| 2:D:561:MET:CE | 1:A:817:PHE:CG | 2.94 | 0.50 |
| 2:D:668:LYS:HA | 2:D:671:GLN:HB2 | 1.92 | 0.50 |
| 1:A:221:LEU:HD11 | 1:A:247:TRP:HE3 | 1.76 | 0.50 |
| 1:A:404:HIS:HE1 | 1:A:478:LEU:HB3 | 1.75 | 0.50 |
| 2:B:494:ASN:O | 2:B:498:GLY:N | 2.31 | 0.50 |
| 2:D:171:SER:HA | 2:D:201:GLN:HB2 | 1.93 | 0.50 |
| 2:D:284:TRP:HB3 | 2:D:374:LYS:HE2 | 1.94 | 0.50 |
| 1:A:351:TYR:HB2 | 1:A:367:TYR:HB2 | 1.93 | 0.50 |
| 1:C:525:GLN:HG3 | 2:B:777:LEU:CD2 | 2.42 | 0.50 |
| 2:D:220:LYS:CG | 2:B:220:LYS:NZ | 2.73 | 0.50 |
| 2:D:536:MET:C | 2:D:727:ALA:HB1 | 2.32 | 0.50 |
| 1:A:467:ALA:HB2 | 1:A:474:TYR:HE2 | 1.75 | 0.50 |
| 1:A:483:LYS:HD3 | 1:A:686:GLN:HB2 | 1.93 | 0.50 |
| 1:A:678:LYS:O | 1:A:727:HIS:NE2 | 2.44 | 0.50 |
| 1:C:251:GLU:HG2 | 1:C:254:ILE:HD12 | 1.93 | 0.50 |
| 1:C:553:SER:OG | 1:C:812:ASN:ND2 | 2.45 | 0.50 |
| 2:D:101:GLY:HA2 | 2:D:128:HIS:H | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:365:VAL:N | 2:B:373:GLU:O | 2.36 | 0.50 |
| 2:D:298:ILE:HG23 | 2:D:341:VAL:HG11 | 1.94 | 0.50 |
| 1:A:251:GLU:HG2 | 1:A:254:ILE:HD12 | 1.93 | 0.50 |
| 1:A:308:CYS:HB2 | 2:B:80:LYS:HG3 | 1.94 | 0.50 |
| 1:A:679:PHE:HA | 1:A:727:HIS:CD2 | 2.46 | 0.50 |
| 2:B:89:LEU:HB3 | 2:B:95:ILE:HD12 | 1.93 | 0.50 |
| 2:B:509:VAL:HA | 2:B:763:ILE:HG23 | 1.93 | 0.50 |
| 2:D:509:VAL:HA | 2:D:763:ILE:HG23 | 1.93 | 0.50 |
| 1:A:75:ALA:HB2 | 1:A:110:THR:HG21 | 1.94 | 0.50 |
| 1:A:560:SER:HA | 1:A:563:TRP:HD1 | 1.77 | 0.50 |
| 1:C:75:ALA:HB2 | 1:C:110:THR:HG21 | 1.94 | 0.50 |
| 1:C:401:VAL:HG12 | 1:C:479:VAL:HG22 | 1.94 | 0.50 |
| 1:A:540:ILE:HG12 | 1:A:730:ILE:HG12 | 1.92 | 0.50 |
| 2:B:284:TRP:HB3 | 2:B:374:LYS:HE2 | 1.94 | 0.50 |
| 2:B:360:ARG:HA | 2:B:379:GLU:HG2 | 1.94 | 0.50 |
| 1:C:777:LEU:CB | 2:B:516:GLU:HG3 | 2.40 | 0.50 |
| 2:D:516:GLU:HG3 | 1:A:777:LEU:CB | 2.39 | 0.50 |
| 1:C:679:PHE:HA | 1:C:727:HIS:CD2 | 2.46 | 0.49 |
| 2:D:360:ARG:HA | 2:D:379:GLU:HG2 | 1.94 | 0.49 |
| 2:B:171:SER:HA | 2:B:201:GLN:HB2 | 1.93 | 0.49 |
| 2:B:298:ILE:HG23 | 2:B:341:VAL:HG11 | 1.94 | 0.49 |
| 2:B:701[A]:MET:HA | 2:B:704:TYR:HD2 | 1.77 | 0.49 |
| 1:C:351:TYR:HB2 | 1:C:367:TYR:HB2 | 1.94 | 0.49 |
| 1:C:531:LYS:HZ2 | 1:C:777:LEU:CG | 2.24 | 0.49 |
| 2:D:52:ARG:HA | 2:D:293:ARG:HH21 | 1.78 | 0.49 |
| 2:D:629:ILE:CD1 | 1:A:608:TRP:CG | 2.95 | 0.49 |
| 1:A:368:ASN:HB2 | 1:A:371:HIS:HD2 | 1.76 | 0.49 |
| 2:B:500:VAL:HG13 | 2:B:766:GLN:HG2 | 1.93 | 0.49 |
| 1:C:777:LEU:CB | 2:B:516:GLU:CG | 2.90 | 0.49 |
| 2:D:174:THR:HG22 | 2:D:230:TYR:HB2 | 1.93 | 0.49 |
| 1:A:520:ASN:HD22 | 1:A:523:ARG:NE | 2.06 | 0.49 |
| 1:C:241:THR:HG22 | 1:C:247:TRP:CZ2 | 2.48 | 0.49 |
| 1:C:323:ARG:NH2 | 2:D:209:SER:OG | 2.44 | 0.49 |
| 1:C:403:ILE:HD11 | 1:C:501:MET:HG3 | 1.95 | 0.49 |
| 1:C:531:LYS:O | 1:C:776:ILE:HD12 | 2.11 | 0.49 |
| 1:C:620:GLY:HA2 | 2:D:610:GLY:HA3 | 1.95 | 0.49 |
| 2:D:500:VAL:HA | 2:D:766:GLN:HE21 | 1.78 | 0.49 |
| 1:A:68:LYS:HZ1 | 1:A:76:LEU:HB2 | 1.77 | 0.49 |
| 2:B:125:LEU:HA | 2:B:145:PHE:O | 2.12 | 0.49 |
| 1:C:308:CYS:HB2 | 2:D:80:LYS:HG3 | 1.94 | 0.49 |
| 1:C:560:SER:HA | 1:C:563:TRP:HD1 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:696:GLN:NE2 | 2:B:784:GLY:C | 2.55 | 0.49 |
| 2:D:443:ASN:HB2 | 2:D:446:THR:H | 1.76 | 0.49 |
| 1:A:683:THR:N | 1:A:710:ASN:OD1 | 2.41 | 0.49 |
| 2:D:629:ILE:CD1 | 1:A:608:TRP:CD2 | 2.62 | 0.49 |
| 2:B:256:ILE:HG12 | 2:B:277:ILE:HD12 | 1.94 | 0.49 |
| 2:B:443:ASN:HB2 | 2:B:446:THR:H | 1.76 | 0.49 |
| 2:D:701[A]:MET:HA | 2:D:704:TYR:HD2 | 1.77 | 0.49 |
| 1:A:462:LEU:HD23 | 1:A:465:LYS:HD2 | 1.95 | 0.49 |
| 1:C:608:TRP:CG | 2:B:629:ILE:CD1 | 2.96 | 0.49 |
| 2:D:276:LEU:HD12 | 2:D:366:LEU:HD12 | 1.95 | 0.49 |
| 2:D:375:VAL:HA | 2:D:387:HIS:CD2 | 2.48 | 0.49 |
| 2:B:433:THR:HB | 2:B:456:CYS:H | 1.77 | 0.49 |
| 1:C:146:HIS:CD2 | 1:C:179:ARG:HH12 | 2.31 | 0.49 |
| 1:C:462:LEU:HD23 | 1:C:465:LYS:HD2 | 1.95 | 0.49 |
| 1:C:696:GLN:NE2 | 2:B:785:ASP:HA | 2.28 | 0.49 |
| 1:C:779:SER:HA | 1:C:784:PHE:HD2 | 1.77 | 0.49 |
| 1:A:67:HIS:NE2 | 1:A:93:SER:OG | 2.43 | 0.49 |
| 1:A:234:ALA:HA | 1:A:237:MET:CG | 2.43 | 0.49 |
| 1:A:333:GLY:HA3 | 1:A:338:VAL:HG23 | 1.95 | 0.49 |
| 1:A:531:LYS:O | 1:A:776:ILE:HD12 | 2.11 | 0.49 |
| 1:A:779:SER:HA | 1:A:784:PHE:HD2 | 1.77 | 0.49 |
| 2:B:174:THR:HG22 | 2:B:230:TYR:HB2 | 1.93 | 0.49 |
| 2:B:466:LYS:HA | 2:B:469:ARG:HD2 | 1.94 | 0.49 |
| 1:C:67:HIS:NE2 | 1:C:93:SER:OG | 2.43 | 0.49 |
| 1:C:521:ASN:OD1 | 2:B:777:LEU:C | 2.50 | 0.49 |
| 2:D:99:VAL:HG22 | 2:D:125:LEU:HD12 | 1.95 | 0.49 |
| 2:B:276:LEU:HD12 | 2:B:366:LEU:HD12 | 1.95 | 0.49 |
| 1:C:333:GLY:HA3 | 1:C:338:VAL:HG23 | 1.95 | 0.48 |
| 1:C:423:GLU:H | 1:C:433:LYS:HZ1 | 1.59 | 0.48 |
| 2:B:537:VAL:CB | 2:B:727:ALA:HB2 | 2.31 | 0.48 |
| 1:C:340:PHE:HA | 1:C:346:ARG:HA | 1.95 | 0.48 |
| 1:C:536:GLN:HB2 | 1:C:758:PHE:HE2 | 1.79 | 0.48 |
| 2:D:466:LYS:HA | 2:D:469:ARG:HD2 | 1.94 | 0.48 |
| 2:D:494:ASN:O | 2:D:498:GLY:N | 2.31 | 0.48 |
| 2:D:513:THR:O | 2:D:518:ARG:NH1 | 2.46 | 0.48 |
| 2:D:777:LEU:CD2 | 1:A:525:GLN:HG3 | 2.43 | 0.48 |
| 1:A:68:LYS:HZ1 | 1:A:77:SER:H | 1.59 | 0.48 |
| 1:A:340:PHE:HA | 1:A:346:ARG:HA | 1.95 | 0.48 |
| 1:A:401:VAL:HG12 | 1:A:479:VAL:HG22 | 1.94 | 0.48 |
| 1:A:776:ILE:CG2 | 1:A:777:LEU:HG | 2.43 | 0.48 |
| 2:B:437:ARG:HH21 | 2:B:453:LYS:HE3 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:500:VAL:HA | 2:B:766:GLN:HE21 | 1.78 | 0.48 |
| 2:B:725:LEU:HD12 | 2:B:728:PHE:CZ | 2.49 | 0.48 |
| 1:C:648:THR:CG2 | 2:B:643:ALA:HB1 | 2.25 | 0.48 |
| 2:D:125:LEU:HA | 2:D:145:PHE:O | 2.12 | 0.48 |
| 2:D:256:ILE:HG12 | 2:D:277:ILE:HD12 | 1.94 | 0.48 |
| 2:D:433:THR:HB | 2:D:456:CYS:H | 1.77 | 0.48 |
| 2:D:437:ARG:HH21 | 2:D:453:LYS:HE3 | 1.78 | 0.48 |
| 2:D:523:ASP:OD2 | 2:D:772:LYS:NZ | 2.47 | 0.48 |
| 1:A:146:HIS:CD2 | 1:A:179:ARG:HH12 | 2.31 | 0.48 |
| 1:A:403:ILE:HD11 | 1:A:501:MET:HG3 | 1.95 | 0.48 |
| 2:B:99:VAL:HG22 | 2:B:125:LEU:HD12 | 1.95 | 0.48 |
| 1:C:776:ILE:CG2 | 1:C:777:LEU:HG | 2.43 | 0.48 |
| 1:A:287:VAL:HG22 | 1:A:330:TYR:CG | 2.48 | 0.48 |
| 1:A:731:TRP:HB2 | 1:A:736:LEU:HD21 | 1.96 | 0.48 |
| 2:B:52:ARG:HA | 2:B:293:ARG:HH21 | 1.78 | 0.48 |
| 2:B:534:SER:C | 2:B:729:ILE:HG12 | 2.34 | 0.48 |
| 1:C:114:TYR:HB3 | 1:C:314:ILE:HA | 1.96 | 0.48 |
| 1:C:368:ASN:HD22 | 1:C:371:HIS:CD2 | 2.31 | 0.48 |
| 2:D:165:TYR:OH | 2:D:389:VAL:N | 2.46 | 0.48 |
| 2:D:500:VAL:HG13 | 2:D:766:GLN:HG2 | 1.93 | 0.48 |
| 1:A:520:ASN:HB3 | 1:A:523:ARG:H | 1.79 | 0.48 |
| 2:B:523:ASP:OD2 | 2:B:772:LYS:NZ | 2.47 | 0.48 |
| 1:C:234:ALA:HA | 1:C:237:MET:CG | 2.43 | 0.48 |
| 1:C:242:GLY:C | 1:C:245:TYR:HD2 | 2.13 | 0.48 |
| 1:C:703:TYR:HE2 | 2:D:431:ARG:HH12 | 1.60 | 0.48 |
| 2:B:286:TYR:CE2 | 2:B:360:ARG:HD3 | 2.49 | 0.48 |
| 2:B:513:THR:O | 2:B:518:ARG:NH1 | 2.46 | 0.48 |
| 1:C:520:ASN:HD21 | 1:C:523:ARG:NE | 2.07 | 0.48 |
| 1:C:839:ARG:NH1 | 2:B:582:PRO:CB | 2.68 | 0.48 |
| 2:D:347:ASP:HB2 | 2:D:358:HIS:HD2 | 1.79 | 0.48 |
| 1:C:505:LEU:HD12 | 1:C:527:ILE:HD13 | 1.96 | 0.48 |
| 1:C:683:THR:N | 1:C:710:ASN:OD1 | 2.41 | 0.48 |
| 2:D:45:ASP:HA | 2:D:73:LEU:HD11 | 1.96 | 0.48 |
| 1:A:368:ASN:HD22 | 1:A:371:HIS:CD2 | 2.31 | 0.48 |
| 1:A:536:GLN:HB2 | 1:A:758:PHE:HE2 | 1.78 | 0.48 |
| 2:B:181:ARG:HA | 2:B:184:ILE:HD12 | 1.96 | 0.48 |
| 1:C:68:LYS:HZ1 | 1:C:76:LEU:HB2 | 1.79 | 0.48 |
| 1:C:776:ILE:HG22 | 1:C:777:LEU:HG | 1.96 | 0.48 |
| 2:D:286:TYR:CE2 | 2:D:360:ARG:HD3 | 2.49 | 0.48 |
| 2:D:487:LYS:HD2 | 2:D:494:ASN:HD22 | 1.79 | 0.48 |
| 2:D:582:PRO:CB | 1:A:839:ARG:NH1 | 2.71 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:620:GLY:HA2 | 2:B:610:GLY:HA3 | 1.95 | 0.48 |
| 1:C:287:VAL:HG22 | 1:C:330:TYR:CG | 2.48 | 0.48 |
| 1:C:824:ILE:HG13 | 2:B:634:TRP:CE2 | 2.38 | 0.48 |
| 1:A:461:ASP:OD2 | 1:A:792:TRP:NE1 | 2.39 | 0.48 |
| 1:A:703:TYR:HE2 | 2:B:431:ARG:HH12 | 1.60 | 0.48 |
| 2:B:45:ASP:HA | 2:B:73:LEU:HD11 | 1.96 | 0.48 |
| 2:B:734:VAL:HA | 2:B:737:TYR:HD2 | 1.79 | 0.48 |
| 1:C:731:TRP:HB2 | 1:C:736:LEU:HD21 | 1.96 | 0.47 |
| 2:D:286:TYR:OH | 2:D:379:GLU:OE2 | 2.28 | 0.47 |
| 1:C:150:VAL:O | 1:C:153:GLU:HB2 | 2.13 | 0.47 |
| 1:C:485:GLY:HA2 | 1:C:686:GLN:HB3 | 1.96 | 0.47 |
| 2:D:143:THR:HA | 2:D:335:HIS:CE1 | 2.49 | 0.47 |
| 2:D:486:GLY:HA3 | 2:D:497:ILE:HD12 | 1.96 | 0.47 |
| 1:A:150:VAL:O | 1:A:153:GLU:HB2 | 2.14 | 0.47 |
| 2:D:181:ARG:HA | 2:D:184:ILE:HD12 | 1.96 | 0.47 |
| 2:D:342:THR:HG22 | 2:D:347:ASP:HA | 1.96 | 0.47 |
| 2:B:143:THR:HA | 2:B:335:HIS:CE1 | 2.49 | 0.47 |
| 2:B:273:PRO:HA | 2:B:370:ARG:HE | 1.79 | 0.47 |
| 2:B:347:ASP:HB2 | 2:B:358:HIS:HD2 | 1.79 | 0.47 |
| 2:B:728:PHE:HB3 | 2:B:730:TYR:CE2 | 2.49 | 0.47 |
| 1:C:777:LEU:HB2 | 2:B:516:GLU:CG | 2.39 | 0.47 |
| 1:C:814:ALA:HA | 1:C:817:PHE:HD2 | 1.79 | 0.47 |
| 2:D:273:PRO:HA | 2:D:370:ARG:HE | 1.80 | 0.47 |
| 1:A:241:THR:HG22 | 1:A:247:TRP:CZ2 | 2.48 | 0.47 |
| 1:A:814:ALA:HA | 1:A:817:PHE:HD2 | 1.80 | 0.47 |
| 2:B:701[B]:MET:HA | 2:B:704:TYR:HD2 | 1.79 | 0.47 |
| 2:D:220:LYS:HZ1 | 2:B:217:VAL:HA | 1.80 | 0.47 |
| 2:D:281:TYR:HE1 | 2:D:360:ARG:H | 1.63 | 0.47 |
| 2:D:629:ILE:HD11 | 1:A:608:TRP:CG | 2.42 | 0.47 |
| 1:A:242:GLY:C | 1:A:245:TYR:HD2 | 2.13 | 0.47 |
| 1:A:720:ALA:O | 1:A:725:LYS:N | 2.47 | 0.47 |
| 2:B:375:VAL:HA | 2:B:387:HIS:CD2 | 2.48 | 0.47 |
| 1:C:234:ALA:CA | 1:C:237:MET:HB2 | 2.45 | 0.47 |
| 1:C:705:HIS:HA | 1:C:709:HIS:HD2 | 1.80 | 0.47 |
| 1:C:774:LEU:HD22 | 2:B:516:GLU:OE2 | 2.14 | 0.47 |
| 1:A:693:PHE:O | 1:A:703:TYR:OH | 2.29 | 0.47 |
| 2:B:165:TYR:OH | 2:B:389:VAL:N | 2.46 | 0.47 |
| 1:C:46:VAL:HG13 | 1:C:60:LEU:HD13 | 1.96 | 0.47 |
| 1:C:242:GLY:N | 1:C:245:TYR:CD2 | 2.83 | 0.47 |
| 2:D:533:ILE:CG2 | 2:D:729:ILE:HG22 | 2.28 | 0.47 |
| 2:D:535:VAL:HG13 | 2:D:729:ILE:HG13 | 1.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:579:TYR:HA | 2:D:582:PRO:HD2 | 1.96 | 0.47 |
| 1:A:114:TYR:HB3 | 1:A:314:ILE:HA | 1.96 | 0.47 |
| 1:A:234:ALA:CA | 1:A:237:MET:HB2 | 2.45 | 0.47 |
| 1:A:553:SER:OG | 1:A:812:ASN:ND2 | 2.45 | 0.47 |
| 1:A:560:SER:HA | 1:A:563:TRP:CD1 | 2.50 | 0.47 |
| 1:A:776:ILE:HG22 | 1:A:777:LEU:HG | 1.96 | 0.47 |
| 2:B:487:LYS:HD2 | 2:B:494:ASN:HD22 | 1.79 | 0.47 |
| 2:B:534:SER:C | 2:B:729:ILE:HA | 2.30 | 0.47 |
| 2:B:535:VAL:HG13 | 2:B:729:ILE:HG13 | 1.42 | 0.47 |
| 2:B:790:GLU:O | 2:B:793:THR:OG1 | 2.28 | 0.47 |
| 1:C:479:VAL:HG12 | 1:C:481:ASP:H | 1.80 | 0.47 |
| 1:C:615:LEU:HD13 | 2:B:632:SER:O | 2.15 | 0.47 |
| 1:A:350:ASN:HA | 1:A:367:TYR:O | 2.14 | 0.47 |
| 1:A:505:LEU:HD12 | 1:A:527:ILE:HD13 | 1.96 | 0.47 |
| 2:B:281:TYR:HE1 | 2:B:360:ARG:H | 1.63 | 0.47 |
| 1:C:350:ASN:HA | 1:C:367:TYR:O | 2.14 | 0.47 |
| 1:A:485:GLY:HA2 | 1:A:686:GLN:HB3 | 1.96 | 0.47 |
| 1:C:165:LEU:HB2 | 1:C:194:VAL:HG22 | 1.97 | 0.47 |
| 2:D:516:GLU:HB3 | 1:A:781:GLU:OE2 | 2.15 | 0.47 |
| 2:D:734:VAL:HA | 2:D:737:TYR:HD2 | 1.79 | 0.47 |
| 1:A:242:GLY:N | 1:A:245:TYR:CD2 | 2.83 | 0.47 |
| 2:B:242:GLU:O | 2:B:245:SER:OG | 2.25 | 0.47 |
| 2:D:516:GLU:CB | 1:A:777:LEU:CB | 2.83 | 0.46 |
| 2:D:578:GLU:O | 2:D:581:SER:OG | 2.28 | 0.46 |
| 1:A:447:PRO:HB2 | 1:A:449:HIS:CE1 | 2.50 | 0.46 |
| 2:B:342:THR:HG22 | 2:B:347:ASP:HA | 1.96 | 0.46 |
| 2:B:535:VAL:CA | 2:B:729:ILE:HA | 2.42 | 0.46 |
| 2:D:712:GLY:N | 2:D:715:ASP:OD2 | 2.47 | 0.46 |
| 2:B:486:GLY:HA3 | 2:B:497:ILE:HD12 | 1.96 | 0.46 |
| 2:B:526:VAL:HG23 | 2:B:779:LEU:HD22 | 1.75 | 0.46 |
| 1:A:605:SER:OG | 1:A:606:ALA:N | 2.48 | 0.46 |
| 1:A:705:HIS:HA | 1:A:709:HIS:HD2 | 1.80 | 0.46 |
| 2:B:579:TYR:HA | 2:B:582:PRO:HD2 | 1.96 | 0.46 |
| 2:B:712:GLY:N | 2:B:715:ASP:OD2 | 2.47 | 0.46 |
| 1:C:447:PRO:HB2 | 1:C:449:HIS:CE1 | 2.50 | 0.46 |
| 2:D:751:GLY:C | 2:D:753:GLY:N | 2.69 | 0.46 |
| 2:D:781:GLN:H | 1:A:521:ASN:HD21 | 1.62 | 0.46 |
| 2:B:526:VAL:CB | 2:B:527:PRO:HD2 | 2.37 | 0.46 |
| 2:B:769:SER:HB2 | 2:B:771:TRP:CD1 | 2.45 | 0.46 |
| 2:D:636:PHE:CG | 1:A:615:LEU:HD22 | 2.50 | 0.46 |
| 2:D:673:PRO:HB2 | 2:D:680:PHE:H | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:144:TYR:HE1 | 1:A:251:GLU:HB2 | 1.80 | 0.46 |
| 1:A:423:GLU:H | 1:A:433:LYS:HZ1 | 1.63 | 0.46 |
| 2:B:526:VAL:CG1 | 2:B:779:LEU:HD21 | 2.46 | 0.46 |
| 1:C:521:ASN:HD21 | 2:B:781:GLN:H | 1.61 | 0.46 |
| 2:D:629:ILE:HD12 | 1:A:608:TRP:CZ2 | 2.50 | 0.46 |
| 2:B:153:GLN:NE2 | 2:B:356:GLN:O | 2.41 | 0.46 |
| 2:B:684:THR:O | 2:B:710:GLN:N | 2.45 | 0.46 |
| 1:C:560:SER:HA | 1:C:563:TRP:CD1 | 2.50 | 0.46 |
| 1:C:720:ALA:O | 1:C:725:LYS:N | 2.47 | 0.46 |
| 2:D:334:LEU:HB3 | 2:D:338:MET:HG2 | 1.98 | 0.46 |
| 2:D:526:VAL:HG23 | 2:D:779:LEU:HD22 | 1.75 | 0.46 |
| 2:D:630:MET:C | 2:D:634:TRP:CE3 | 2.77 | 0.46 |
| 2:D:735:LEU:HD13 | 2:D:750:ILE:HG22 | 1.98 | 0.46 |
| 1:A:323:ARG:NH2 | 2:B:209:SER:OG | 2.44 | 0.46 |
| 1:A:543:LYS:HE2 | 1:A:724:ASN:HA | 1.97 | 0.46 |
| 1:A:631:ILE:HG13 | 2:B:606:TRP:HH2 | 1.81 | 0.46 |
| 2:B:751:GLY:C | 2:B:753:GLY:N | 2.69 | 0.46 |
| 1:C:531:LYS:CD | 1:C:777:LEU:HD21 | 2.46 | 0.46 |
| 1:C:543:LYS:HE2 | 1:C:724:ASN:HA | 1.97 | 0.46 |
| 1:C:668:ASN:OD1 | 1:C:673:ARG:NH2 | 2.49 | 0.46 |
| 2:D:632:SER:O | 1:A:615:LEU:HD13 | 2.15 | 0.46 |
| 2:D:634:TRP:HZ2 | 1:A:824:ILE:CG1 | 1.78 | 0.46 |
| 2:D:634:TRP:HA | 2:D:637:PHE:HD2 | 1.81 | 0.46 |
| 1:A:626:SER:OG | 1:A:627:PHE:N | 2.48 | 0.46 |
| 2:B:113:LEU:HD13 | 2:B:124:ILE:HG21 | 1.97 | 0.46 |
| 2:B:725:LEU:HD12 | 2:B:728:PHE:HZ | 1.80 | 0.46 |
| 1:C:627:PHE:HD1 | 2:D:606:TRP:HZ2 | 1.63 | 0.46 |
| 1:C:773:SER:HA | 1:C:776:ILE:HG21 | 1.97 | 0.46 |
| 1:A:46:VAL:HG13 | 1:A:60:LEU:HD13 | 1.98 | 0.46 |
| 1:A:531:LYS:CD | 1:A:777:LEU:HD21 | 2.46 | 0.46 |
| 2:B:537:VAL:HG12 | 2:B:727:ALA:HB2 | 0.46 | 0.46 |
| 2:D:526:VAL:CG1 | 2:D:779:LEU:HD21 | 2.46 | 0.46 |
| 2:D:735:LEU:O | 2:D:739:ALA:CB | 2.64 | 0.46 |
| 2:B:673:PRO:HB3 | 2:B:680:PHE:HB2 | 1.98 | 0.46 |
| 1:C:605:SER:OG | 1:C:606:ALA:N | 2.48 | 0.45 |
| 2:D:277:ILE:HG12 | 2:D:365:VAL:HG22 | 1.98 | 0.45 |
| 2:D:680:PHE:HB3 | 2:D:682:PHE:HE2 | 1.81 | 0.45 |
| 1:A:308:CYS:O | 2:B:78:ASP:HB3 | 2.16 | 0.45 |
| 2:B:533:ILE:HG23 | 2:B:729:ILE:CG2 | 2.30 | 0.45 |
| 1:C:195:LEU:HD13 | 1:C:207:LEU:HB3 | 1.98 | 0.45 |
| 1:A:433:LYS:HE2 | 1:A:456:TYR:HE2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:479:VAL:HG12 | 1:A:481:ASP:H | 1.80 | 0.45 |
| 2:B:334:LEU:O | 2:B:338:MET:N | 2.44 | 0.45 |
| 2:B:691:GLU:O | 2:B:702:HIS:NE2 | 2.48 | 0.45 |
| 1:C:204:VAL:O | 1:C:208:LEU:N | 2.47 | 0.45 |
| 1:C:412:LYS:HB2 | 1:C:456:TYR:HE1 | 1.81 | 0.45 |
| 1:C:508:GLY:HA2 | 1:C:763:ARG:HH22 | 1.82 | 0.45 |
| 1:C:531:LYS:CA | 1:C:776:ILE:CD1 | 2.93 | 0.45 |
| 2:D:164:ASP:HB2 | 2:D:386:ARG:NH1 | 2.31 | 0.45 |
| 1:A:55:SER:C | 1:A:293:HIS:HE1 | 2.20 | 0.45 |
| 2:B:690:THR:HA | 2:B:693:ASN:HD22 | 1.82 | 0.45 |
| 1:C:308:CYS:O | 2:D:78:ASP:HB3 | 2.16 | 0.45 |
| 2:D:273:PRO:HD2 | 2:D:276:LEU:HD11 | 1.99 | 0.45 |
| 2:D:485:HIS:O | 2:D:497:ILE:N | 2.34 | 0.45 |
| 2:D:534:SER:C | 2:D:729:ILE:HG12 | 2.37 | 0.45 |
| 1:A:148:SER:HA | 1:A:151:TRP:HD1 | 1.82 | 0.45 |
| 1:A:165:LEU:HB2 | 1:A:194:VAL:HG22 | 1.97 | 0.45 |
| 1:A:508:GLY:HA2 | 1:A:763:ARG:HH22 | 1.82 | 0.45 |
| 2:B:164:ASP:HB2 | 2:B:386:ARG:NH1 | 2.31 | 0.45 |
| 2:B:634:TRP:HA | 2:B:637:PHE:HD2 | 1.81 | 0.45 |
| 1:A:265:GLY:N | 1:A:356:LEU:O | 2.36 | 0.45 |
| 2:B:673:PRO:HB2 | 2:B:680:PHE:H | 1.81 | 0.45 |
| 1:C:145:SER:HB2 | 1:C:179:ARG:HD2 | 1.99 | 0.45 |
| 1:C:519:ILE:CG2 | 1:C:529:PHE:CD2 | 3.00 | 0.45 |
| 1:A:33:LEU:HD11 | 1:A:42:PHE:HE2 | 1.82 | 0.45 |
| 1:A:489:ARG:HG3 | 2:B:195:PHE:HE2 | 1.82 | 0.45 |
| 2:B:680:PHE:HB3 | 2:B:682:PHE:HE2 | 1.81 | 0.45 |
| 2:B:735:LEU:O | 2:B:739:ALA:CB | 2.64 | 0.45 |
| 1:C:631:ILE:HG13 | 2:D:606:TRP:HH2 | 1.81 | 0.45 |
| 2:D:113:LEU:HD13 | 2:D:124:ILE:HG21 | 1.97 | 0.45 |
| 2:D:673:PRO:HB3 | 2:D:680:PHE:HB2 | 1.98 | 0.45 |
| 1:A:221:LEU:N | 1:A:248:LEU:O | 2.41 | 0.45 |
| 1:A:412:LYS:HB2 | 1:A:456:TYR:HE1 | 1.81 | 0.45 |
| 1:A:519:ILE:O | 1:A:692:TYR:OH | 2.32 | 0.45 |
| 1:A:627:PHE:HD1 | 2:B:606:TRP:HZ2 | 1.64 | 0.45 |
| 1:C:55:SER:C | 1:C:293:HIS:HE1 | 2.20 | 0.45 |
| 1:C:433:LYS:HE2 | 1:C:456:TYR:HE2 | 1.81 | 0.45 |
| 2:D:637:PHE:CZ | 1:A:820:VAL:HG22 | 2.52 | 0.45 |
| 2:D:680:PHE:HB3 | 2:D:682:PHE:CE2 | 2.52 | 0.45 |
| 2:D:690:THR:HA | 2:D:693:ASN:HD22 | 1.82 | 0.45 |
| 2:D:701[B]:MET:HA | 2:D:704:TYR:HD2 | 1.79 | 0.45 |
| 2:D:777:LEU:CD2 | 1:A:521:ASN:O | 2.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:195:LEU:HD13 | 1:A:207:LEU:HB3 | 1.98 | 0.45 |
| 1:A:668:ASN:OD1 | 1:A:673:ARG:NH2 | 2.49 | 0.45 |
| 1:A:779:SER:HA | 1:A:784:PHE:HB2 | 1.99 | 0.45 |
| 2:B:276:LEU:HB2 | 2:B:366:LEU:HD12 | 1.99 | 0.45 |
| 2:B:367:ASN:ND2 | 2:B:373:GLU:OE1 | 2.50 | 0.45 |
| 2:B:534:SER:O | 2:B:729:ILE:CG1 | 2.64 | 0.45 |
| 2:B:718:VAL:O | 2:B:722:THR:N | 2.48 | 0.45 |
| 2:D:153:GLN:NE2 | 2:D:356:GLN:O | 2.41 | 0.45 |
| 2:D:334:LEU:O | 2:D:338:MET:N | 2.44 | 0.45 |
| 2:D:790:GLU:O | 2:D:793:THR:OG1 | 2.28 | 0.45 |
| 1:A:773:SER:HA | 1:A:776:ILE:HG21 | 1.97 | 0.45 |
| 1:C:820:VAL:HG11 | 2:B:634:TRP:HD1 | 1.82 | 0.45 |
| 2:D:276:LEU:HB2 | 2:D:366:LEU:HD12 | 1.99 | 0.45 |
| 2:D:367:ASN:ND2 | 2:D:373:GLU:OE1 | 2.50 | 0.45 |
| 1:A:169:ASP:N | 1:A:197:PHE:O | 2.42 | 0.45 |
| 2:B:714:GLU:HG2 | 2:B:717:LEU:HD12 | 1.99 | 0.45 |
| 1:C:144:TYR:HE1 | 1:C:251:GLU:HB2 | 1.80 | 0.44 |
| 1:C:234:ALA:O | 1:C:238:LEU:N | 2.50 | 0.44 |
| 2:D:529:VAL:HG12 | 2:D:530:GLU:O | 2.17 | 0.44 |
| 2:D:740:GLY:O | 2:D:799:ILE:N | 2.42 | 0.44 |
| 1:A:277:GLU:HA | 1:A:280:HIS:HD2 | 1.82 | 0.44 |
| 1:A:470:MET:HE1 | 1:A:771:ASN:HB2 | 2.00 | 0.44 |
| 1:A:520:ASN:HB2 | 1:A:523:ARG:N | 2.30 | 0.44 |
| 2:B:334:LEU:HB3 | 2:B:338:MET:HG2 | 1.98 | 0.44 |
| 2:B:680:PHE:HB3 | 2:B:682:PHE:CE2 | 2.52 | 0.44 |
| 2:B:693:ASN:HA | 2:B:696:ASN:HD22 | 1.83 | 0.44 |
| 1:A:439:PRO:HB3 | 1:A:448:ARG:HB3 | 1.99 | 0.44 |
| 1:A:522:GLU:H | 1:A:695:ARG:NH2 | 2.15 | 0.44 |
| 2:B:172:LEU:HD23 | 2:B:228:LEU:HB2 | 1.99 | 0.44 |
| 2:B:273:PRO:HD2 | 2:B:276:LEU:HD11 | 1.98 | 0.44 |
| 2:B:277:ILE:HG12 | 2:B:365:VAL:HG22 | 1.98 | 0.44 |
| 2:B:535:VAL:HB | 2:B:750:ILE:HA | 1.98 | 0.44 |
| 1:C:126:SER:O | 1:C:129:SER:OG | 2.25 | 0.44 |
| 1:C:648:THR:HG22 | 2:B:643:ALA:HB2 | 1.94 | 0.44 |
| 1:C:648:THR:CG2 | 2:B:643:ALA:HB2 | 2.47 | 0.44 |
| 2:D:279:VAL:HG22 | 2:D:363:VAL:HG22 | 1.99 | 0.44 |
| 2:B:529:VAL:HG12 | 2:B:530:GLU:O | 2.17 | 0.44 |
| 2:B:819:GLY:O | 2:B:822:TYR:HB2 | 2.18 | 0.44 |
| 1:C:105:THR:O | 1:C:108:SER:OG | 2.27 | 0.44 |
| 1:C:489:ARG:HG3 | 2:D:195:PHE:HE2 | 1.82 | 0.44 |
| 1:C:525:GLN:CG | 2:B:777:LEU:HD22 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:779:SER:HA | 1:C:784:PHE:HB2 | 1.99 | 0.44 |
| 2:D:161:ILE:HA | 2:D:386:ARG:NH1 | 2.31 | 0.44 |
| 2:D:274:SER:HB3 | 2:D:368:LYS:HA | 2.00 | 0.44 |
| 1:A:204:VAL:O | 1:A:208:LEU:N | 2.47 | 0.44 |
| 1:A:272:ILE:HB | 1:A:350:ASN:HB2 | 2.00 | 0.44 |
| 2:B:468:SER:HB3 | 2:B:475:TYR:HE2 | 1.82 | 0.44 |
| 1:C:170:ASP:HB2 | 1:C:173:GLY:H | 1.82 | 0.44 |
| 1:C:277:GLU:HA | 1:C:280:HIS:HD2 | 1.82 | 0.44 |
| 2:D:172:LEU:HD23 | 2:D:228:LEU:HB2 | 2.00 | 0.44 |
| 1:A:170:ASP:HB2 | 1:A:173:GLY:H | 1.82 | 0.44 |
| 1:A:234:ALA:O | 1:A:238:LEU:N | 2.50 | 0.44 |
| 2:B:735:LEU:HD13 | 2:B:750:ILE:HG22 | 1.98 | 0.44 |
| 1:C:44:GLU:HA | 1:C:47:ASN:HD22 | 1.83 | 0.44 |
| 1:C:522:GLU:H | 1:C:695:ARG:NH2 | 2.15 | 0.44 |
| 2:D:217:VAL:HA | 2:B:220:LYS:HZ1 | 1.83 | 0.44 |
| 2:D:691:GLU:O | 2:D:702:HIS:NE2 | 2.48 | 0.44 |
| 2:D:714:GLU:HG2 | 2:D:717:LEU:HD12 | 1.99 | 0.44 |
| 1:A:105:THR:O | 1:A:108:SER:OG | 2.27 | 0.44 |
| 1:A:519:ILE:CG2 | 1:A:529:PHE:CD2 | 3.00 | 0.44 |
| 2:B:740:GLY:O | 2:B:799:ILE:N | 2.42 | 0.44 |
| 1:C:148:SER:HA | 1:C:151:TRP:HD1 | 1.82 | 0.44 |
| 1:C:683:THR:O | 1:C:711:TYR:N | 2.51 | 0.44 |
| 2:D:160:LYS:NZ | 2:D:382:THR:O | 2.51 | 0.44 |
| 2:D:535:VAL:N | 2:D:729:ILE:HG12 | 2.17 | 0.44 |
| 2:B:279:VAL:HG22 | 2:B:363:VAL:HG22 | 1.99 | 0.44 |
| 1:C:439:PRO:HB3 | 1:C:448:ARG:HB3 | 1.99 | 0.44 |
| 1:C:503:GLY:O | 1:C:507:SER:N | 2.50 | 0.44 |
| 1:C:626:SER:OG | 1:C:627:PHE:N | 2.48 | 0.44 |
| 2:D:306:MET:O | 2:D:310:PHE:N | 2.44 | 0.44 |
| 2:D:780:LEU:C | 1:A:521:ASN:ND2 | 2.65 | 0.44 |
| 1:A:402:THR:N | 1:A:477:HIS:O | 2.50 | 0.44 |
| 1:C:520:ASN:HB2 | 1:C:523:ARG:CG | 2.48 | 0.44 |
| 2:D:468:SER:HB3 | 2:D:475:TYR:HE2 | 1.82 | 0.44 |
| 1:A:145:SER:HB2 | 1:A:179:ARG:HD2 | 1.99 | 0.44 |
| 2:B:698:TYR:HB2 | 2:B:701[A]:MET:HB2 | 2.00 | 0.44 |
| 2:B:739:ALA:HB2 | 2:B:749:THR:HG21 | 1.99 | 0.44 |
| 1:C:33:LEU:HD11 | 1:C:42:PHE:HE2 | 1.82 | 0.43 |
| 1:C:115:ARG:HH11 | 1:C:319:PRO:HD3 | 1.83 | 0.43 |
| 1:C:470:MET:HE1 | 1:C:771:ASN:HB2 | 2.00 | 0.43 |
| 1:C:506:LEU:HG | 1:C:527:ILE:HD11 | 2.00 | 0.43 |
| 2:D:681:ARG:NH1 | 2:D:723:GLY:O | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:693:ASN:HA | 2:D:696:ASN:HD22 | 1.83 | 0.43 |
| 1:A:531:LYS:CA | 1:A:776:ILE:CD1 | 2.93 | 0.43 |
| 2:B:274:SER:HB3 | 2:B:368:LYS:HA | 2.00 | 0.43 |
| 1:C:487:GLN:HG3 | 1:C:498:TRP:CE2 | 2.53 | 0.43 |
| 1:C:505:LEU:HA | 1:C:763:ARG:HH21 | 1.83 | 0.43 |
| 1:C:531:LYS:CE | 1:C:777:LEU:HD21 | 2.47 | 0.43 |
| 2:D:819:GLY:O | 2:D:822:TYR:HB2 | 2.18 | 0.43 |
| 1:A:167:VAL:HG21 | 1:A:177:GLN:HE21 | 1.84 | 0.43 |
| 1:A:519:ILE:CG1 | 1:A:529:PHE:CE2 | 2.93 | 0.43 |
| 1:A:539:THR:O | 1:A:730:ILE:HA | 2.18 | 0.43 |
| 1:C:167:VAL:HG21 | 1:C:177:GLN:HE21 | 1.84 | 0.43 |
| 1:C:773:SER:CA | 1:C:776:ILE:CG2 | 2.97 | 0.43 |
| 2:D:526:VAL:HG12 | 2:D:527:PRO:HD2 | 0.68 | 0.43 |
| 1:A:115:ARG:HH11 | 1:A:319:PRO:HD3 | 1.83 | 0.43 |
| 2:B:439:PHE:HB3 | 2:B:449:GLY:HA3 | 1.99 | 0.43 |
| 2:B:526:VAL:HG12 | 2:B:527:PRO:HD2 | 0.68 | 0.43 |
| 1:C:34:SER:HB3 | 1:C:96:PRO:HA | 2.01 | 0.43 |
| 1:C:70:ASN:HD22 | 1:C:73:GLN:NE2 | 2.17 | 0.43 |
| 1:C:272:ILE:HB | 1:C:350:ASN:HB2 | 2.00 | 0.43 |
| 1:C:424:PHE:HB3 | 1:C:428:GLY:HA2 | 2.00 | 0.43 |
| 1:C:608:TRP:CZ2 | 2:B:629:ILE:HD12 | 2.53 | 0.43 |
| 1:C:731:TRP:HB2 | 1:C:736:LEU:HD11 | 2.00 | 0.43 |
| 2:D:739:ALA:HB2 | 2:D:749:THR:HG21 | 1.99 | 0.43 |
| 1:A:312:THR:O | 2:B:106:GLN:NE2 | 2.52 | 0.43 |
| 1:A:506:LEU:HG | 1:A:527:ILE:HD11 | 2.00 | 0.43 |
| 1:C:115:ARG:HD3 | 1:C:319:PRO:HD3 | 2.00 | 0.43 |
| 1:C:205:THR:HA | 1:C:208:LEU:HD12 | 2.00 | 0.43 |
| 1:C:241:THR:HG22 | 1:C:247:TRP:HZ2 | 1.83 | 0.43 |
| 1:C:519:ILE:O | 1:C:692:TYR:OH | 2.32 | 0.43 |
| 1:C:520:ASN:HD22 | 1:C:523:ARG:NE | 2.06 | 0.43 |
| 1:C:539:THR:O | 1:C:730:ILE:HA | 2.18 | 0.43 |
| 1:C:541:LEU:HD22 | 1:C:746:LEU:HD22 | 2.01 | 0.43 |
| 2:D:40:LEU:HB2 | 2:D:73:LEU:HD23 | 2.01 | 0.43 |
| 2:D:439:PHE:HB3 | 2:D:449:GLY:HA3 | 1.99 | 0.43 |
| 1:A:115:ARG:HD3 | 1:A:319:PRO:HD3 | 2.00 | 0.43 |
| 1:A:205:THR:HA | 1:A:208:LEU:HD12 | 2.00 | 0.43 |
| 2:B:160:LYS:NZ | 2:B:382:THR:O | 2.51 | 0.43 |
| 1:C:519:ILE:HA | 1:C:529:PHE:CZ | 2.53 | 0.43 |
| 1:C:820:VAL:HG22 | 2:B:637:PHE:CZ | 2.53 | 0.43 |
| 2:D:419:VAL:HG21 | 2:D:479:LEU:HD11 | 2.00 | 0.43 |
| 2:D:728:PHE:HB3 | 2:D:730:TYR:CE2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:440:ASN:ND2 | 1:A:449:HIS:HB2 | 2.34 | 0.43 |
| 1:A:683:THR:O | 1:A:711:TYR:N | 2.51 | 0.43 |
| 2:B:99:VAL:HA | 2:B:125:LEU:HB2 | 2.01 | 0.43 |
| 2:B:281:TYR:HD1 | 2:B:360:ARG:HB2 | 1.83 | 0.43 |
| 2:D:733:ALA:HA | 2:D:736:ASN:HD22 | 1.83 | 0.43 |
| 1:C:123:THR:OG1 | 1:C:139:ARG:NE | 2.51 | 0.43 |
| 1:C:169:ASP:N | 1:C:197:PHE:O | 2.42 | 0.43 |
| 1:C:408:PHE:HA | 1:C:458:PHE:HD1 | 1.84 | 0.43 |
| 1:C:534:LYS:HB2 | 1:C:758:PHE:CD2 | 2.54 | 0.43 |
| 2:D:99:VAL:HA | 2:D:125:LEU:HB2 | 2.01 | 0.43 |
| 1:A:240:MET:HE1 | 1:A:245:TYR:HE1 | 1.83 | 0.43 |
| 1:A:520:ASN:HB2 | 1:A:523:ARG:CG | 2.48 | 0.43 |
| 1:A:531:LYS:CE | 1:A:777:LEU:HD21 | 2.47 | 0.43 |
| 1:A:731:TRP:HB2 | 1:A:736:LEU:HD11 | 2.00 | 0.43 |
| 2:B:40:LEU:HB2 | 2:B:73:LEU:HD23 | 2.01 | 0.43 |
| 2:B:681:ARG:NH1 | 2:B:723:GLY:O | 2.51 | 0.43 |
| 1:C:265:GLY:N | 1:C:356:LEU:O | 2.36 | 0.43 |
| 1:C:402:THR:N | 1:C:477:HIS:O | 2.50 | 0.43 |
| 2:D:242:GLU:O | 2:D:245:SER:OG | 2.25 | 0.43 |
| 2:D:243:ALA:HA | 2:D:246:LEU:HB2 | 2.01 | 0.43 |
| 2:D:520:GLU:O | 2:D:767:LYS:NZ | 2.51 | 0.43 |
| 2:D:769:SER:HB2 | 2:D:771:TRP:CD1 | 2.45 | 0.43 |
| 1:A:408:PHE:HA | 1:A:458:PHE:HD1 | 1.84 | 0.43 |
| 1:A:519:ILE:HA | 1:A:529:PHE:CZ | 2.53 | 0.43 |
| 1:A:828:ILE:HA | 1:A:831:ILE:HD12 | 2.00 | 0.43 |
| 1:C:520:ASN:HB3 | 1:C:523:ARG:H | 1.79 | 0.43 |
| 2:D:516:GLU:OE2 | 1:A:774:LEU:HD22 | 2.19 | 0.43 |
| 2:D:534:SER:O | 2:D:729:ILE:CG1 | 2.67 | 0.43 |
| 2:D:684:THR:O | 2:D:710:GLN:N | 2.45 | 0.43 |
| 1:A:26:ILE:CG1 | 1:A:58:ILE:CG2 | 2.86 | 0.43 |
| 1:A:272:ILE:HD11 | 1:A:352:SER:HB3 | 2.00 | 0.43 |
| 1:A:773:SER:CA | 1:A:776:ILE:CG2 | 2.97 | 0.43 |
| 2:B:243:ALA:HA | 2:B:246:LEU:HB2 | 2.01 | 0.43 |
| 2:B:698:TYR:HB2 | 2:B:701[B]:MET:HB2 | 2.00 | 0.43 |
| 2:B:733:ALA:HA | 2:B:736:ASN:HD22 | 1.83 | 0.43 |
| 1:C:519:ILE:CG1 | 1:C:529:PHE:CD2 | 2.98 | 0.42 |
| 1:A:487:GLN:HG3 | 1:A:498:TRP:CE2 | 2.53 | 0.42 |
| 2:B:419:VAL:HG21 | 2:B:479:LEU:HD11 | 2.00 | 0.42 |
| 2:B:536:MET:HB2 | 2:B:735:LEU:CD2 | 2.41 | 0.42 |
| 1:C:128:TYR:HA | 1:C:134:HIS:CE1 | 2.54 | 0.42 |
| 1:C:272:ILE:HD11 | 1:C:352:SER:HB3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:312:THR:O | 2:D:106:GLN:NE2 | 2.52 | 0.42 |
| 1:C:440:ASN:ND2 | 1:C:449:HIS:HB2 | 2.34 | 0.42 |
| 1:C:615:LEU:HD22 | 2:B:636:PHE:CG | 2.54 | 0.42 |
| 2:D:66:ASP:O | 2:D:68:ASN:ND2 | 2.52 | 0.42 |
| 2:D:182:GLU:O | 2:D:185:SER:OG | 2.27 | 0.42 |
| 2:D:384:SER:HB2 | 2:D:386:ARG:NE | 2.34 | 0.42 |
| 1:A:44:GLU:HA | 1:A:47:ASN:HD22 | 1.83 | 0.42 |
| 1:A:123:THR:OG1 | 1:A:139:ARG:NE | 2.51 | 0.42 |
| 1:A:424:PHE:HB3 | 1:A:428:GLY:HA2 | 2.00 | 0.42 |
| 2:B:78:ASP:O | 2:B:81:SER:OG | 2.24 | 0.42 |
| 2:B:408:ILE:HG12 | 2:B:507:MET:HB2 | 2.01 | 0.42 |
| 1:C:330:TYR:O | 1:C:338:VAL:N | 2.52 | 0.42 |
| 1:C:439:PRO:HG3 | 1:C:480:ALA:HA | 2.01 | 0.42 |
| 2:D:189:THR:O | 2:D:193:ASN:N | 2.50 | 0.42 |
| 2:D:443:ASN:N | 2:D:446:THR:O | 2.41 | 0.42 |
| 2:D:500:VAL:HG11 | 2:D:522:VAL:HG13 | 2.01 | 0.42 |
| 2:D:634:TRP:NE1 | 1:A:824:ILE:CD1 | 2.77 | 0.42 |
| 1:A:34:SER:HB3 | 1:A:96:PRO:HA | 2.01 | 0.42 |
| 1:A:503:GLY:O | 1:A:507:SER:N | 2.50 | 0.42 |
| 1:A:505:LEU:HA | 1:A:763:ARG:HH21 | 1.83 | 0.42 |
| 1:A:534:LYS:HB2 | 1:A:758:PHE:CD2 | 2.54 | 0.42 |
| 1:A:544:LYS:HG2 | 1:A:747:VAL:HG23 | 2.02 | 0.42 |
| 2:B:533:ILE:O | 2:B:750:ILE:HD11 | 2.20 | 0.42 |
| 1:C:657:LEU:HD11 | 2:D:654:ILE:HG12 | 2.01 | 0.42 |
| 2:D:408:ILE:HG12 | 2:D:507:MET:HB2 | 2.01 | 0.42 |
| 1:A:241:THR:HG22 | 1:A:247:TRP:HZ2 | 1.83 | 0.42 |
| 1:A:330:TYR:O | 1:A:338:VAL:N | 2.52 | 0.42 |
| 1:A:439:PRO:HG3 | 1:A:480:ALA:HA | 2.01 | 0.42 |
| 1:A:657:LEU:HD11 | 2:B:654:ILE:HG12 | 2.01 | 0.42 |
| 2:B:520:GLU:O | 2:B:767:LYS:NZ | 2.51 | 0.42 |
| 1:C:781:GLU:OE2 | 2:B:516:GLU:HB3 | 2.20 | 0.42 |
| 1:C:828:ILE:HA | 1:C:831:ILE:HD12 | 2.00 | 0.42 |
| 2:D:649:LEU:HA | 2:D:652:PHE:HD2 | 1.85 | 0.42 |
| 1:A:128:TYR:HA | 1:A:134:HIS:CE1 | 2.54 | 0.42 |
| 1:A:193:LYS:HD2 | 1:A:214:LEU:HD11 | 2.01 | 0.42 |
| 2:B:420:GLU:HB2 | 2:B:455:CYS:HB2 | 2.01 | 0.42 |
| 1:C:277:GLU:HA | 1:C:280:HIS:CD2 | 2.55 | 0.42 |
| 1:C:521:ASN:O | 2:B:777:LEU:CD2 | 2.67 | 0.42 |
| 1:C:553:SER:N | 1:C:812:ASN:H | 2.18 | 0.42 |
| 2:D:115:PHE:O | 2:D:119:HIS:CB | 2.61 | 0.42 |
| 2:D:281:TYR:HD1 | 2:D:360:ARG:HB2 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:506:VAL:HA | 2:D:766:GLN:NE2 | 2.35 | 0.42 |
| 1:A:39:GLU:O | 1:A:43:ARG:HG3 | 2.20 | 0.42 |
| 1:A:70:ASN:HD22 | 1:A:73:GLN:NE2 | 2.17 | 0.42 |
| 1:A:541:LEU:HD22 | 1:A:746:LEU:HD22 | 2.01 | 0.42 |
| 2:B:258:PRO:HA | 2:B:278:SER:HA | 2.00 | 0.42 |
| 1:C:193:LYS:HD2 | 1:C:214:LEU:HD11 | 2.01 | 0.42 |
| 1:C:243:SER:HB3 | 1:C:384:GLY:H | 1.85 | 0.42 |
| 2:D:258:PRO:HA | 2:D:278:SER:HA | 2.00 | 0.42 |
| 1:A:277:GLU:HA | 1:A:280:HIS:CD2 | 2.55 | 0.42 |
| 1:C:400:ILE:O | 1:C:477:HIS:N | 2.52 | 0.42 |
| 1:C:520:ASN:HB2 | 1:C:523:ARG:N | 2.30 | 0.42 |
| 2:D:529:VAL:HG13 | 2:D:530:GLU:N | 2.35 | 0.42 |
| 2:D:582:PRO:HB2 | 1:A:839:ARG:NH2 | 1.91 | 0.42 |
| 2:D:698:TYR:HB2 | 2:D:701[A]:MET:HB2 | 2.00 | 0.42 |
| 1:A:221:LEU:HB2 | 1:A:249:VAL:HA | 2.02 | 0.42 |
| 1:A:400:ILE:O | 1:A:477:HIS:N | 2.53 | 0.42 |
| 2:B:66:ASP:O | 2:B:68:ASN:ND2 | 2.52 | 0.42 |
| 2:B:384:SER:HB2 | 2:B:386:ARG:NE | 2.34 | 0.42 |
| 2:B:649:LEU:HA | 2:B:652:PHE:HD2 | 1.85 | 0.42 |
| 1:C:145:SER:O | 1:C:148:SER:OG | 2.19 | 0.42 |
| 1:C:544:LYS:HG2 | 1:C:747:VAL:HG23 | 2.02 | 0.42 |
| 1:C:39:GLU:O | 1:C:43:ARG:HG3 | 2.20 | 0.42 |
| 2:B:408:ILE:HB | 2:B:477:LEU:HD23 | 2.02 | 0.42 |
| 2:B:536:MET:CA | 2:B:749:THR:HA | 2.40 | 0.42 |
| 2:B:721:LYS:HG3 | 2:B:747:LEU:HD11 | 2.02 | 0.42 |
| 1:C:127:ILE:HG13 | 1:C:172:GLU:HG3 | 2.02 | 0.41 |
| 2:D:216:GLN:HG2 | 2:D:219:LEU:HD12 | 2.01 | 0.41 |
| 2:D:259:SER:HB3 | 2:D:280:SER:HB3 | 2.02 | 0.41 |
| 2:D:459:PHE:HD1 | 2:D:791:LEU:HD13 | 1.85 | 0.41 |
| 2:D:536:MET:O | 2:D:727:ALA:HA | 2.14 | 0.41 |
| 1:A:405:GLN:O | 1:A:409:VAL:N | 2.37 | 0.41 |
| 1:C:221:LEU:HB2 | 1:C:249:VAL:HA | 2.02 | 0.41 |
| 1:C:234:ALA:HA | 1:C:237:MET:HG3 | 2.02 | 0.41 |
| 2:D:537:VAL:HG22 | 2:D:749:THR:O | 2.19 | 0.41 |
| 2:D:538:SER:CA | 2:D:748:VAL:N | 2.83 | 0.41 |
| 2:D:698:TYR:HB2 | 2:D:701[B]:MET:HB2 | 2.00 | 0.41 |
| 1:A:234:ALA:HA | 1:A:237:MET:HG3 | 2.02 | 0.41 |
| 1:A:489:ARG:NH2 | 2:B:195:PHE:H | 2.18 | 0.41 |
| 2:B:216:GLN:HG2 | 2:B:219:LEU:HD12 | 2.01 | 0.41 |
| 2:B:259:SER:HB3 | 2:B:280:SER:HB3 | 2.02 | 0.41 |
| 2:B:506:VAL:HA | 2:B:766:GLN:NE2 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:247:TRP:HB2 | 1:C:266:ILE:HG23 | 2.02 | 0.41 |
| 2:D:191:VAL:O | 2:D:194:SER:OG | 2.32 | 0.41 |
| 2:D:420:GLU:HB2 | 2:D:455:CYS:HB2 | 2.01 | 0.41 |
| 2:D:500:VAL:O | 2:D:766:GLN:NE2 | 2.54 | 0.41 |
| 2:D:721:LYS:HG3 | 2:D:747:LEU:HD11 | 2.02 | 0.41 |
| 1:A:94:HIS:CE1 | 1:A:123:THR:HA | 2.55 | 0.41 |
| 1:A:398:LEU:HD23 | 1:A:398:LEU:HA | 1.89 | 0.41 |
| 1:A:723:ASP:HB2 | 1:A:725:LYS:HG3 | 2.02 | 0.41 |
| 2:B:459:PHE:HD1 | 2:B:791:LEU:HD13 | 1.85 | 0.41 |
| 2:B:536:MET:O | 2:B:727:ALA:HB1 | 2.20 | 0.41 |
| 2:B:537:VAL:HG22 | 2:B:749:THR:O | 2.19 | 0.41 |
| 1:C:723:ASP:HB2 | 1:C:725:LYS:HG3 | 2.02 | 0.41 |
| 2:D:751:GLY:HA3 | 2:D:754:TYR:HD2 | 1.86 | 0.41 |
| 1:A:32:VAL:HA | 1:A:65:VAL:O | 2.21 | 0.41 |
| 1:A:553:SER:N | 1:A:812:ASN:H | 2.18 | 0.41 |
| 1:A:776:ILE:O | 1:A:780:HIS:HD2 | 2.03 | 0.41 |
| 2:B:148:GLY:O | 2:B:150:SER:N | 2.52 | 0.41 |
| 1:C:27:VAL:HB | 1:C:60:LEU:HD23 | 2.02 | 0.41 |
| 1:C:489:ARG:NH2 | 2:D:195:PHE:H | 2.18 | 0.41 |
| 1:C:776:ILE:O | 1:C:780:HIS:HD2 | 2.03 | 0.41 |
| 2:D:78:ASP:O | 2:D:81:SER:OG | 2.24 | 0.41 |
| 2:D:364:ILE:HA | 2:D:374:LYS:HA | 2.02 | 0.41 |
| 2:D:533:ILE:O | 2:D:750:ILE:HD11 | 2.20 | 0.41 |
| 2:D:641:PHE:HZ | 1:A:816:VAL:HG12 | 1.78 | 0.41 |
| 1:A:308:CYS:HB3 | 2:B:79:PRO:HG2 | 2.03 | 0.41 |
| 1:A:519:ILE:CG1 | 1:A:529:PHE:CD2 | 2.98 | 0.41 |
| 2:B:529:VAL:HG13 | 2:B:530:GLU:N | 2.35 | 0.41 |
| 1:C:32:VAL:HA | 1:C:65:VAL:O | 2.21 | 0.41 |
| 2:D:148:GLY:O | 2:D:150:SER:N | 2.52 | 0.41 |
| 2:D:168:HIS:HA | 2:D:198:TRP:CE3 | 2.56 | 0.41 |
| 2:D:522:VAL:HG12 | 2:D:523:ASP:O | 2.20 | 0.41 |
| 2:D:777:LEU:HD22 | 1:A:525:GLN:CG | 2.51 | 0.41 |
| 1:A:340:PHE:HB3 | 1:A:344:GLY:HA2 | 2.03 | 0.41 |
| 1:C:340:PHE:HB3 | 1:C:344:GLY:HA2 | 2.03 | 0.41 |
| 1:C:404:HIS:CE1 | 1:C:478:LEU:HB3 | 2.55 | 0.41 |
| 1:C:520:ASN:HA | 2:B:780:LEU:HD11 | 1.69 | 0.41 |
| 2:D:829:ALA:HA | 2:D:832:LEU:HD12 | 2.02 | 0.41 |
| 1:A:466:LEU:O | 1:A:470:MET:CB | 2.53 | 0.41 |
| 2:B:522:VAL:HG12 | 2:B:523:ASP:O | 2.20 | 0.41 |
| 2:B:529:VAL:O | 2:B:530:GLU:C | 2.53 | 0.41 |
| 1:C:783:GLY:O | 1:C:787:ASP:N | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:27:VAL:HB | 1:A:60:LEU:HD23 | 2.02 | 0.41 |
| 1:A:73:GLN:HE21 | 2:B:321:TYR:HB3 | 1.86 | 0.41 |
| 1:A:109:TYR:HB3 | 2:B:112:MET:SD | 2.60 | 0.41 |
| 1:A:783:GLY:O | 1:A:787:ASP:N | 2.52 | 0.41 |
| 2:B:364:ILE:HA | 2:B:374:LYS:HA | 2.02 | 0.41 |
| 2:B:500:VAL:HG11 | 2:B:522:VAL:HG13 | 2.01 | 0.41 |
| 1:C:26:ILE:CG1 | 1:C:58:ILE:CG2 | 2.85 | 0.41 |
| 1:C:73:GLN:HE21 | 2:D:321:TYR:HB3 | 1.86 | 0.41 |
| 1:C:94:HIS:CE1 | 1:C:123:THR:HA | 2.56 | 0.41 |
| 1:C:351:TYR:HD2 | 1:C:367:TYR:HB2 | 1.86 | 0.41 |
| 1:C:398:LEU:HD23 | 1:C:398:LEU:HA | 1.89 | 0.41 |
| 2:D:76:ARG:HB3 | 2:D:78:ASP:HB2 | 2.02 | 0.41 |
| 2:D:523:ASP:CG | 2:D:767:LYS:HG2 | 2.41 | 0.41 |
| 2:D:634:TRP:CE2 | 1:A:824:ILE:HG13 | 2.38 | 0.41 |
| 1:A:127:ILE:HG13 | 1:A:172:GLU:HG3 | 2.02 | 0.41 |
| 1:A:355:ASN:O | 1:A:362:VAL:N | 2.54 | 0.41 |
| 1:A:740:ALA:HA | 1:A:746:LEU:HB2 | 2.02 | 0.41 |
| 2:B:536:MET:CE | 2:B:735:LEU:HD22 | 2.51 | 0.41 |
| 1:C:139:ARG:HB2 | 1:C:345:ASP:OD1 | 2.21 | 0.41 |
| 1:C:487:GLN:HG3 | 1:C:498:TRP:CD2 | 2.56 | 0.41 |
| 2:D:408:ILE:HB | 2:D:477:LEU:HD23 | 2.02 | 0.41 |
| 1:A:318:GLY:HA2 | 1:A:321:PHE:HD2 | 1.86 | 0.41 |
| 1:A:573:VAL:HG11 | 1:A:614:LEU:HD11 | 2.03 | 0.41 |
| 1:A:741:SER:HB2 | 1:A:796:GLN:O | 2.21 | 0.41 |
| 2:B:162:MET:O | 2:B:167:TRP:N | 2.54 | 0.41 |
| 2:B:168:HIS:HA | 2:B:198:TRP:CE3 | 2.56 | 0.41 |
| 2:B:189:THR:O | 2:B:193:ASN:N | 2.50 | 0.41 |
| 2:B:829:ALA:HA | 2:B:832:LEU:HD12 | 2.02 | 0.41 |
| 1:C:338:VAL:HG13 | 1:C:346:ARG:NE | 2.36 | 0.40 |
| 1:C:519:ILE:CG1 | 1:C:529:PHE:CE2 | 2.93 | 0.40 |
| 1:C:741:SER:HB2 | 1:C:796:GLN:O | 2.21 | 0.40 |
| 2:D:529:VAL:O | 2:D:530:GLU:C | 2.53 | 0.40 |
| 2:D:533:ILE:N | 2:D:757:ALA:CB | 2.80 | 0.40 |
| 2:D:718:VAL:O | 2:D:722:THR:N | 2.47 | 0.40 |
| 2:D:820:VAL:HG12 | 2:D:824:LEU:HG | 2.03 | 0.40 |
| 1:A:247:TRP:HB2 | 1:A:266:ILE:HG23 | 2.02 | 0.40 |
| 2:B:500:VAL:O | 2:B:766:GLN:NE2 | 2.54 | 0.40 |
| 2:B:631:VAL:O | 2:B:635:ALA:N | 2.49 | 0.40 |
| 1:C:109:TYR:HB3 | 2:D:112:MET:SD | 2.60 | 0.40 |
| 1:C:234:ALA:HA | 1:C:237:MET:CB | 2.52 | 0.40 |
| 1:C:318:GLY:HA2 | 1:C:321:PHE:HD2 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:740:ALA:HA | 1:C:746:LEU:HB2 | 2.02 | 0.40 |
| 2:D:732:ALA:HA | 2:D:735:LEU:HD12 | 2.04 | 0.40 |
| 1:A:243:SER:HB3 | 1:A:384:GLY:H | 1.85 | 0.40 |
| 1:A:489:ARG:HH21 | 2:B:194:SER:HA | 1.86 | 0.40 |
| 2:B:161:ILE:HA | 2:B:386:ARG:NH1 | 2.31 | 0.40 |
| 2:B:460:CYS:HG | 2:B:528:PHE:HE1 | 1.63 | 0.40 |
| 2:B:538:SER:CA | 2:B:748:VAL:N | 2.83 | 0.40 |
| 2:D:219:LEU:HB3 | 2:D:246:LEU:HD11 | 2.04 | 0.40 |
| 2:D:739:ALA:HB2 | 2:D:749:THR:CG2 | 2.52 | 0.40 |
| 1:A:351:TYR:HD2 | 1:A:367:TYR:HB2 | 1.86 | 0.40 |
| 1:A:404:HIS:CE1 | 1:A:478:LEU:HB3 | 2.55 | 0.40 |
| 2:B:682:PHE:CE1 | 2:B:727:ALA:O | 2.74 | 0.40 |
| 1:C:165:LEU:HA | 1:C:165:LEU:HD23 | 1.88 | 0.40 |
| 1:C:354:MET:SD | 1:C:363:GLN:HG2 | 2.62 | 0.40 |
| 1:C:489:ARG:HH21 | 2:D:195:PHE:H | 1.68 | 0.40 |
| 1:C:573:VAL:HG11 | 1:C:614:LEU:HD11 | 2.03 | 0.40 |
| 2:D:433:THR:HG21 | 2:D:455:CYS:HB3 | 2.03 | 0.40 |
| 2:D:643:ALA:HB2 | 1:A:648:THR:CG2 | 2.50 | 0.40 |
| 1:A:489:ARG:HH21 | 2:B:195:PHE:H | 1.68 | 0.40 |
| 2:B:180:TYR:HA | 2:B:183:PHE:HD2 | 1.87 | 0.40 |
| 2:B:523:ASP:CG | 2:B:767:LYS:HG2 | 2.41 | 0.40 |
| 2:B:820:VAL:HG12 | 2:B:824:LEU:HG | 2.03 | 0.40 |
| 1:C:308:CYS:HB3 | 2:D:79:PRO:HG2 | 2.03 | 0.40 |
| 1:C:431:VAL:O | 1:C:433:LYS:HG3 | 2.22 | 0.40 |
| 2:D:508:ALA:HB3 | 2:D:764:ALA:HB3 | 2.04 | 0.40 |
| 2:D:532:GLY:HA3 | 2:D:755:ILE:CG2 | 2.52 | 0.40 |
| 2:D:687:ASN:N | 2:D:691:GLU:OE1 | 2.55 | 0.40 |
| 2:B:433:THR:HG21 | 2:B:455:CYS:HB3 | 2.03 | 0.40 |
| 2:B:457:LYS:O | 2:B:461:ILE:HD12 | 2.22 | 0.40 |
| 2:B:485:HIS:O | 2:B:497:ILE:N | 2.34 | 0.40 |
| 2:B:732:ALA:HA | 2:B:735:LEU:HD12 | 2.04 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 771/847 (91%) | 690 (90%) | 75 (10%) | 6 (1%) | 19 | 60 |
| 1 | C | 774/847 (91%) | 691 (89%) | 77 (10%) | 6 (1%) | 19 | 60 |
| 2 | B | 741/841 (88%) | 653 (88%) | 83 (11%) | 5 (1%) | 22 | 63 |
| 2 | D | 741/841 (88%) | 653 (88%) | 83 (11%) | 5 (1%) | 22 | 63 |
| All | All | 3027/3376 (90%) | 2687 (89%) | 318 (10%) | 22 (1%) | 26 | 63 |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 95 | PRO |
| 1 | C | 98 | PRO |
| 1 | C | 240 | MET |
| 1 | C | 243 | SER |
| 2 | D | 329 | VAL |
| 1 | A | 95 | PRO |
| 1 | A | 98 | PRO |
| 1 | A | 240 | MET |
| 1 | A | 243 | SER |
| 2 | B | 329 | VAL |
| 1 | C | 239 | ASN |
| 1 | A | 239 | ASN |
| 2 | D | 752 | SER |
| 2 | B | 752 | SER |
| 1 | C | 754 | PHE |
| 2 | D | 327 | PRO |
| 2 | D | 513 | THR |
| 1 | A | 754 | PHE |
| 2 | B | 327 | PRO |
| 2 | B | 513 | THR |
| 2 | D | 819 | GLY |
| 2 | B | 819 | GLY |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 658/731 (90%) | 658 (100%) | 0 | 100 | 100 |
| 1 | C | 659/731 (90%) | 659 (100%) | 0 | 100 | 100 |
| 2 | B | 612/729 (84%) | 611 (100%) | 1 (0%) | 93 | 96 |
| 2 | D | 612/729 (84%) | 611 (100%) | 1 (0%) | 93 | 96 |
| All | All | 2541/2920 (87%) | 2539 (100%) | 2 (0%) | 93 | 97 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 750 | ILE |
| 2 | B | 750 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 47 | ASN |
| 1 | C | 73 | GLN |
| 1 | C | 86 | GLN |
| 1 | C | 177 | GLN |
| 1 | C | 280 | HIS |
| 1 | C | 293 | HIS |
| 1 | C | 341 | ASN |
| 1 | C | 371 | HIS |
| 1 | C | 449 | HIS |
| 1 | C | 499 | ASN |
| 1 | C | 520 | ASN |
| 1 | C | 521 | ASN |
| 1 | C | 709 | HIS |
| 2 | D | 42 | HIS |
| 2 | D | 44 | HIS |
| 2 | D | 68 | ASN |
| 2 | D | 96 | HIS |
| 2 | D | 106 | GLN |
| 2 | D | 216 | GLN |
| 2 | D | 323 | GLN |
| 2 | D | 358 | HIS |
| 2 | D | 367 | ASN |
| 2 | D | 387 | HIS |
| 2 | D | 443 | ASN |

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W O R L D W I D E
PDB
PROTEIN DATA BANK

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 494 | ASN |
| 2 | D | 693 | ASN |
| 2 | D | 696 | ASN |
| 2 | D | 736 | ASN |
| 2 | D | 766 | GLN |
| 1 | A | 47 | ASN |
| 1 | A | 73 | GLN |
| 1 | A | 86 | GLN |
| 1 | A | 177 | GLN |
| 1 | A | 280 | HIS |
| 1 | A | 293 | HIS |
| 1 | A | 341 | ASN |
| 1 | A | 371 | HIS |
| 1 | A | 449 | HIS |
| 1 | A | 499 | ASN |
| 1 | A | 520 | ASN |
| 1 | A | 521 | ASN |
| 1 | A | 536 | GLN |
| 1 | A | 709 | HIS |
| 2 | B | 42 | HIS |
| 2 | B | 44 | HIS |
| 2 | B | 68 | ASN |
| 2 | B | 96 | HIS |
| 2 | B | 323 | GLN |
| 2 | B | 358 | HIS |
| 2 | B | 367 | ASN |
| 2 | B | 387 | HIS |
| 2 | B | 443 | ASN |
| 2 | B | 494 | ASN |
| 2 | B | 693 | ASN |
| 2 | B | 696 | ASN |
| 2 | B | 736 | ASN |
| 2 | B | 766 | GLN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-9717. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections ⓘ

### 6.1.1 Primary map



X          Y          Z
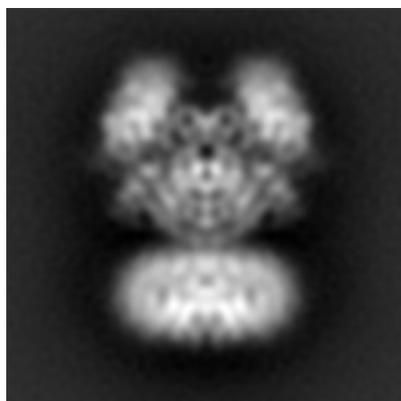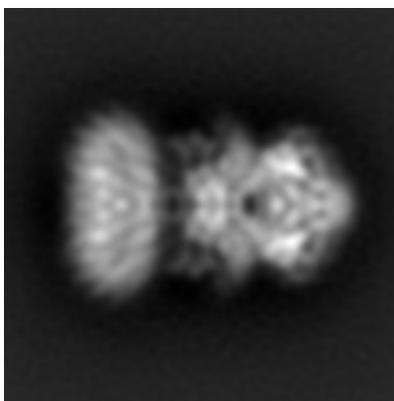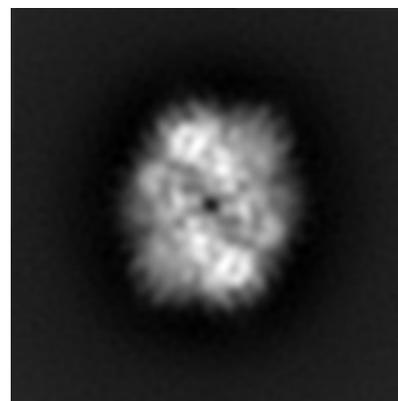
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices ⓘ
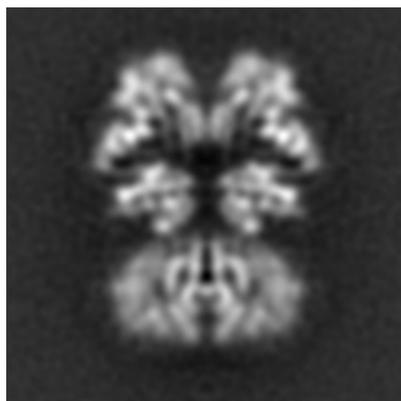
### 6.2.1 Primary map
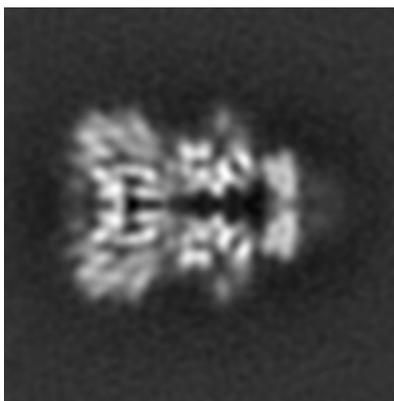


X Index: 120        Y Index: 120        Z Index: 120
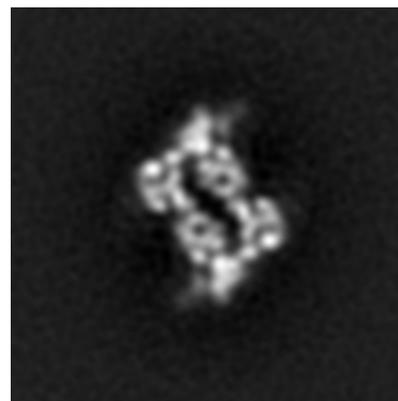
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices ⓘ
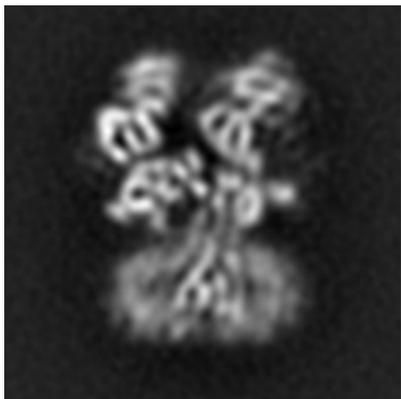
### 6.3.1 Primary map
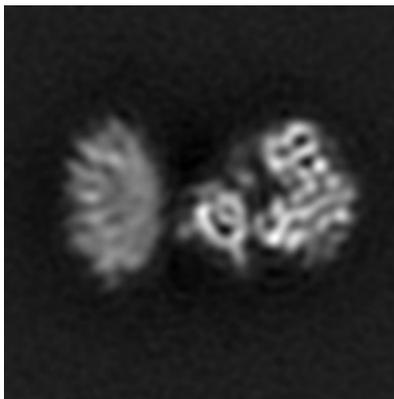


| X Index: 129 | Y Index: 156 | Z Index: 172 |
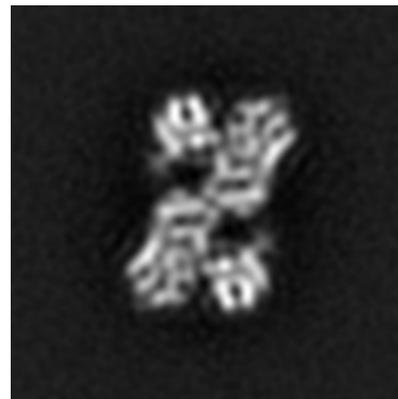
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views ⓘ

### 6.4.1 Primary map



| X | Y | Z |
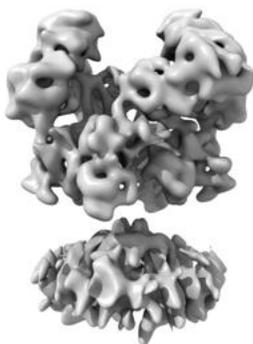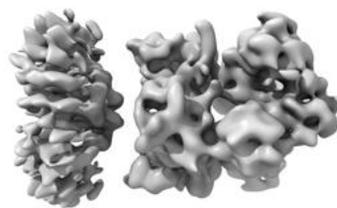
The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7　Map analysis ⓘ

This section contains the results of statistical analysis of the map.

## 7.1　Map-value distribution ⓘ
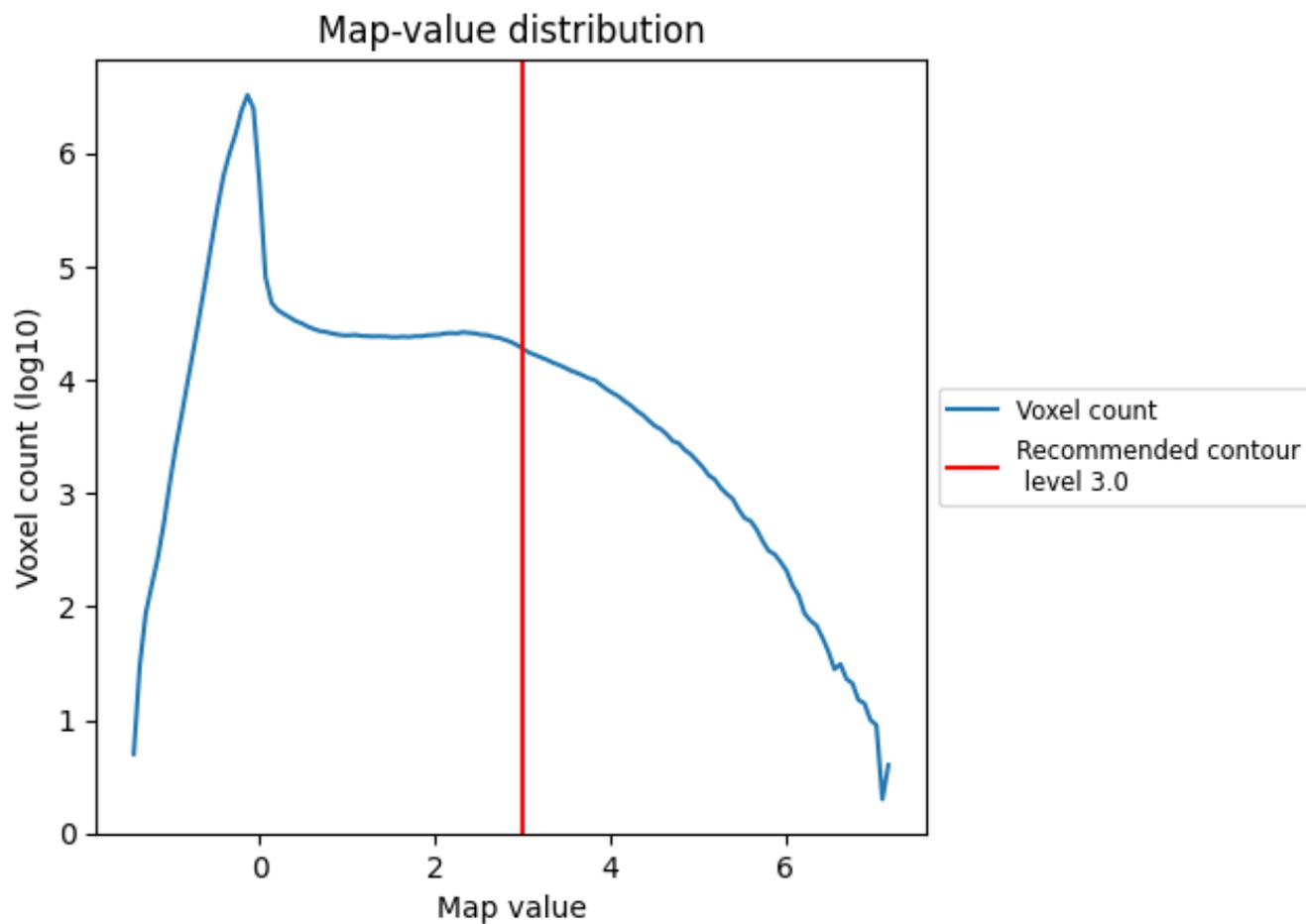


The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate ⓘ
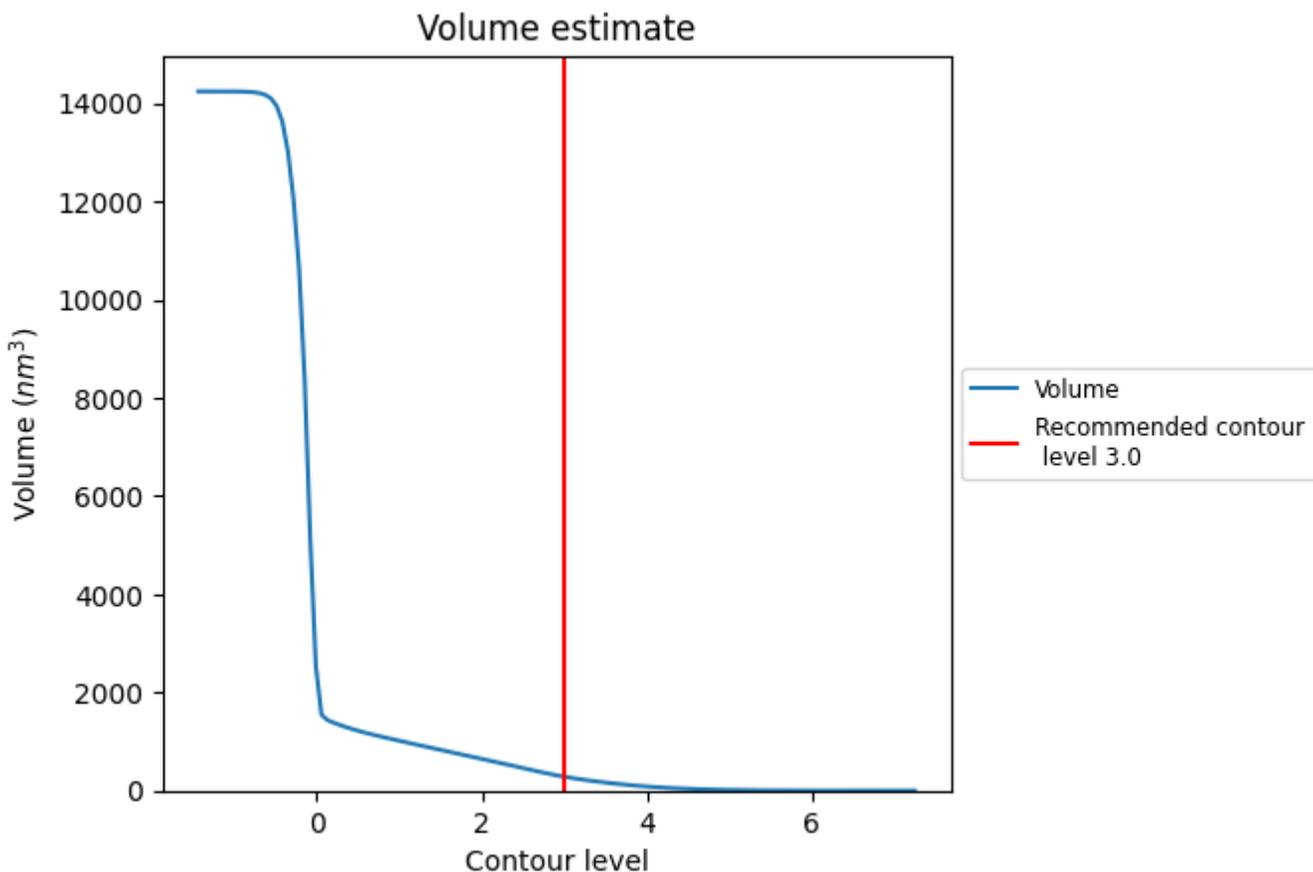


The volume at the recommended contour level is 283 nm$^3$; this corresponds to an approximate mass of 256 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum ⓘ
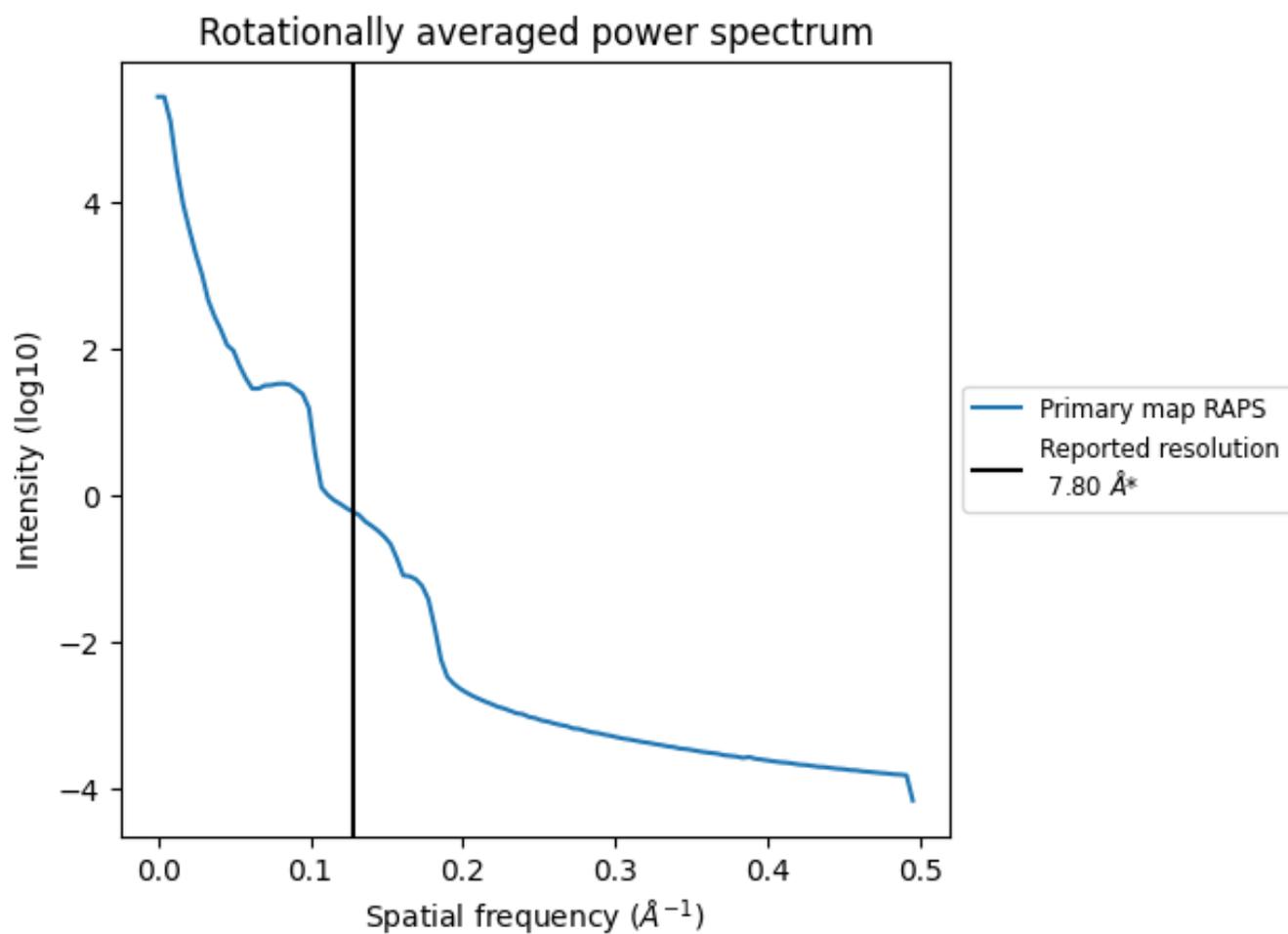


*Reported resolution corresponds to spatial frequency of 0.128 Å$^{-1}$

# 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9717 and PDB model 6IRH. Per-residue inclusion information can be found in section 3 on page 4.

## 9.1 Map-model overlay ⓘ



X　　　　　　　　　　　Y　　　　　　　　　　　Z
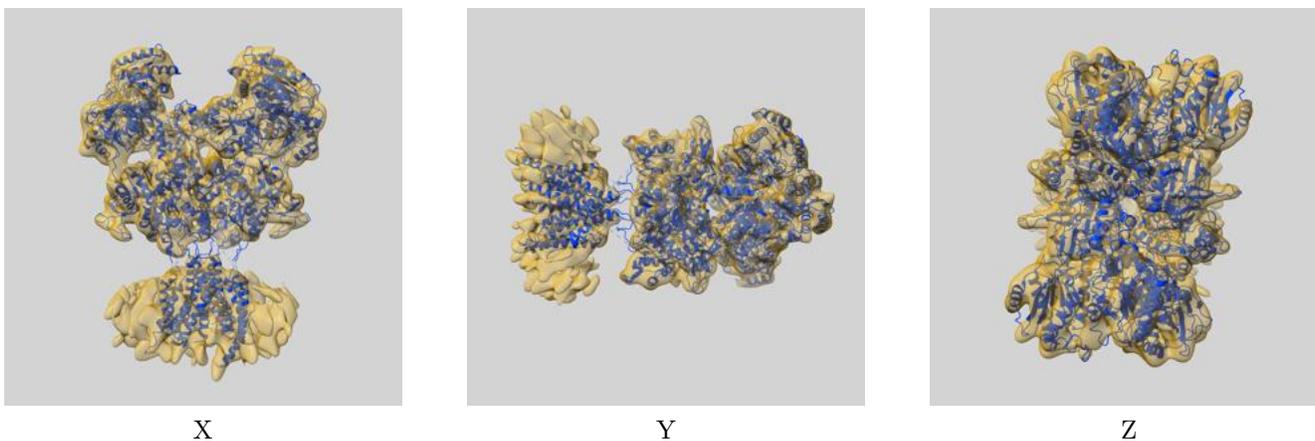
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2　Q-score mapped to coordinate model ⓘ



X　　　　　　　　　Y　　　　　　　　　Z
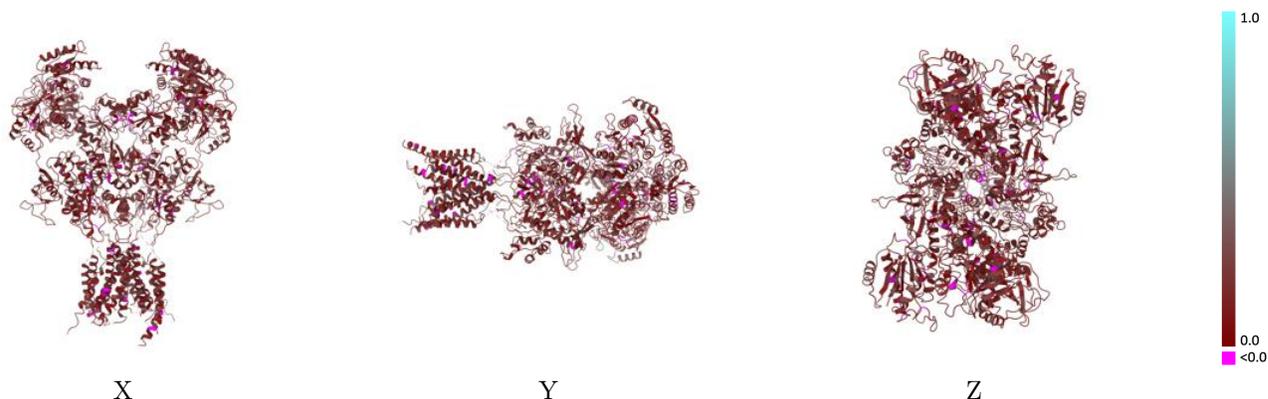
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3　Atom inclusion mapped to coordinate model ⓘ



X　　　　　　　　　Y　　　　　　　　　Z
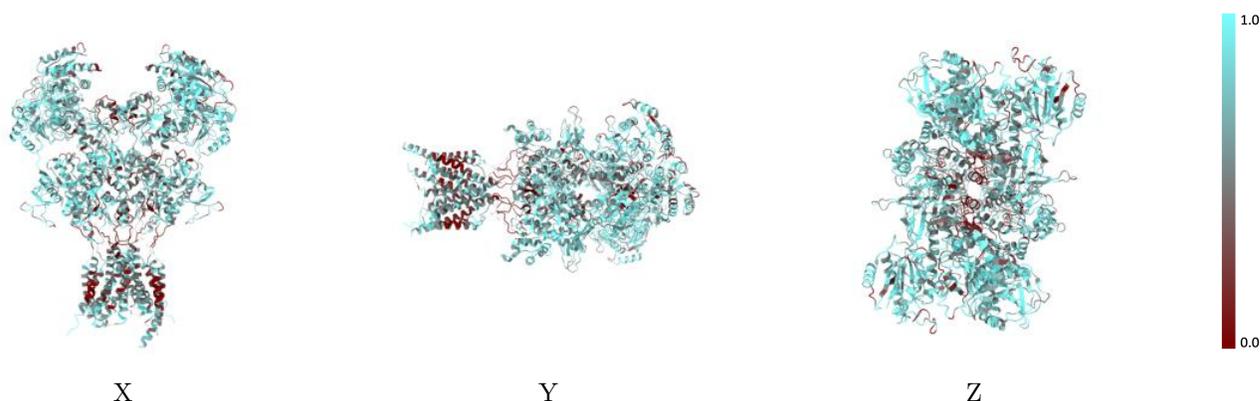
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).

## 9.4　Atom inclusion　ⓘ
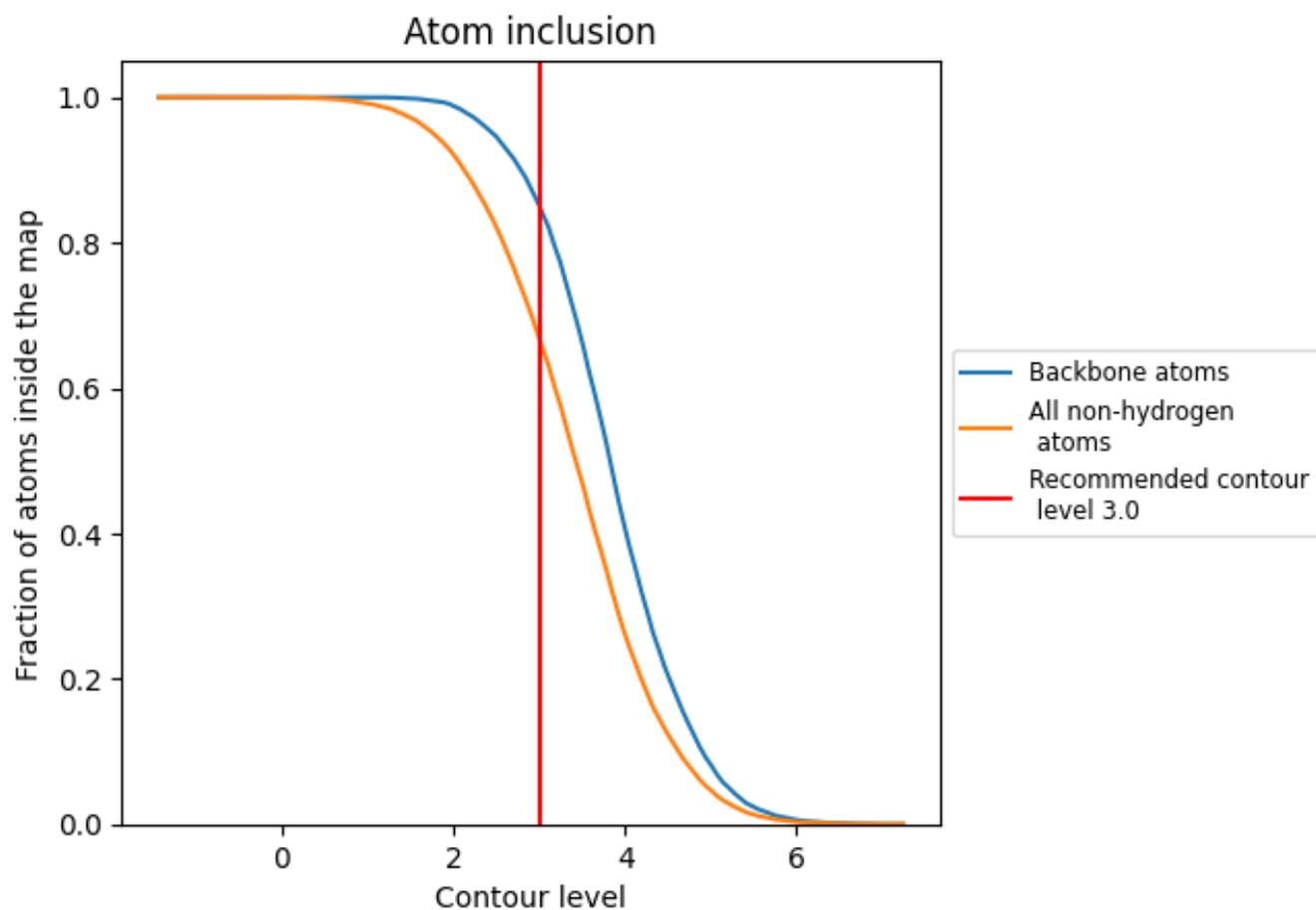


At the recommended contour level, 85% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

## 9.5    Map-model fit summary  (i)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for
the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.6693 | 0.1710 |
| A | 0.6907 | 0.1700 |
| B | 0.6512 | 0.1740 |
| C | 0.6909 | 0.1680 |
| D | 0.6423 | 0.1730 |

1.0

0.0
<0.0