# Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 06:05 AM JST

| | | |
|---|---|---|
| PDB ID | : | 5Y81 |
| EMDB ID | : | EMD-6816 |
| Title | : | NuA4 TEEAA sub-complex |
| Authors | : | Wang, X.; Cai, G. |
| Deposited on | : | 2017-08-18 |
| Resolution | : | 4.70 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

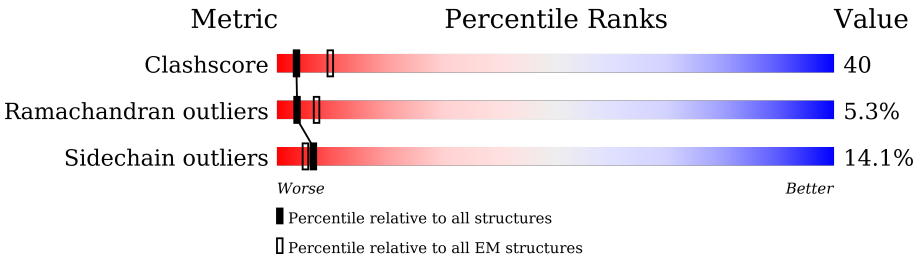
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 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 4.70 Å.

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




| Metric | Whole archive (#Entries) | 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 | B | 1115 | 47% 31% 9% 12% |
| 2 | C | 336 | 24% 11% 7% 58% |
| 3 | D | 500 | 56% 16% 28% |
| 4 | H | 279 | 41% 14% 45% |
| 5 | A | 2627 | 59% 15% 24% |
| 6 | F | 490 | 5% 41% 43% 14% |
| 7 | G | 375 | 9% 38% 52% 6% |
| 8 | E | 41 | 5% 24% 73% |

# 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25723 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 Transcription-associated protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | B | 981 | 5937 | 3675 | 1116 | 1136 | 10 | 0 | 0 |

- Molecule 2 is a protein called Chromatin modification-related protein EAF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | C | 140 | 800 | 489 | 156 | 154 | 1 | 0 | 0 |

- Molecule 3 is a protein called Eaf1-disorder domain.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | D | 360 | 1800 | 1080 | 360 | 360 | 0 | 0 |

- Molecule 4 is a protein called Chromatin modification-related protein EAF5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 4 | H | 154 | 764 | 456 | 154 | 154 | 0 | 0 |

- Molecule 5 is a protein called Transcription-associated protein 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 5 | A | 2007 | 10017 | 5997 | 2008 | 2012 | 0 | 0 |

- Molecule 6 is a protein called Actin-related protein 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 421 | 3334 | 2121 | 553 | 648 | 12 | 1 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 0 | PRO | - | expression tag | UNP P80428 |

- Molecule 7 is a protein called Actin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 351 | Total | C | N | O | S | 0 | 0 |
| | | | 2729 | 1735 | 458 | 519 | 17 | | |

- Molecule 8 is a protein called Chromatin modification-related protein EAF1.

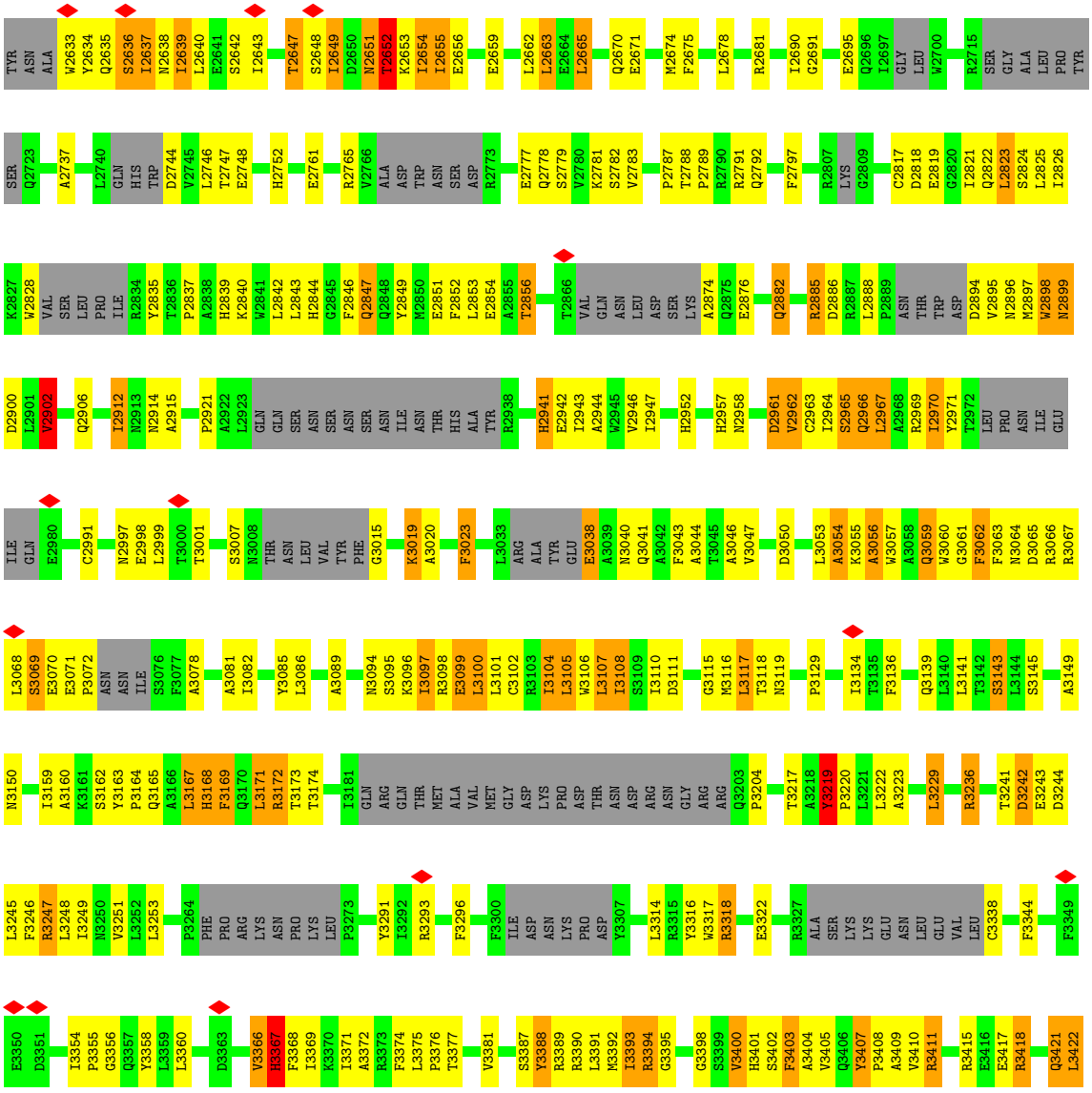
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | E | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 342 | 222 | 56 | 61 | 3 | | |

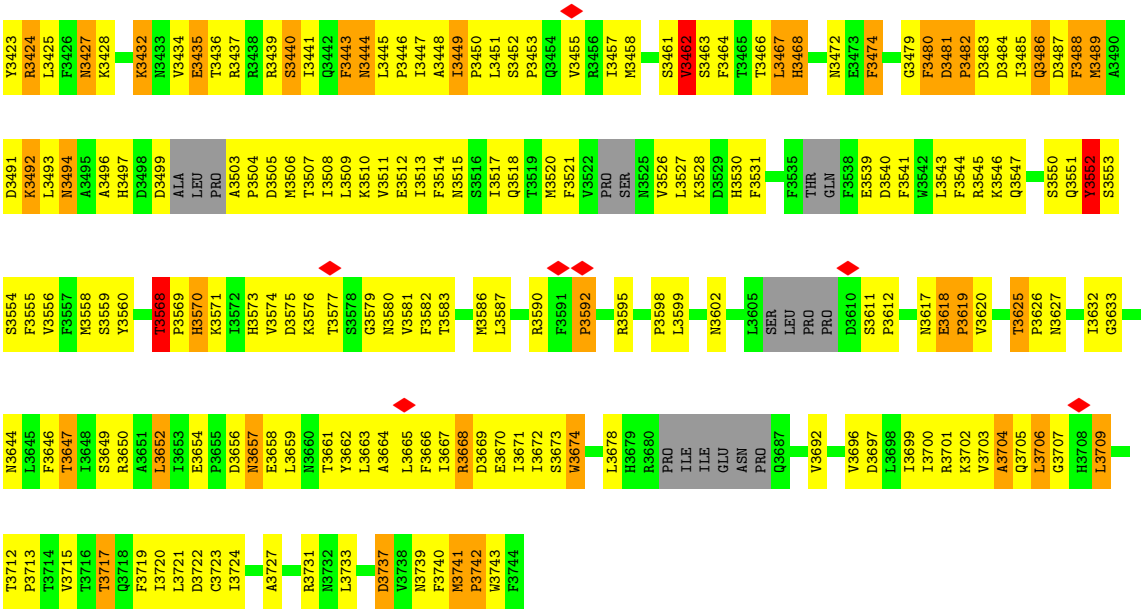
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Transcription-associated protein 1

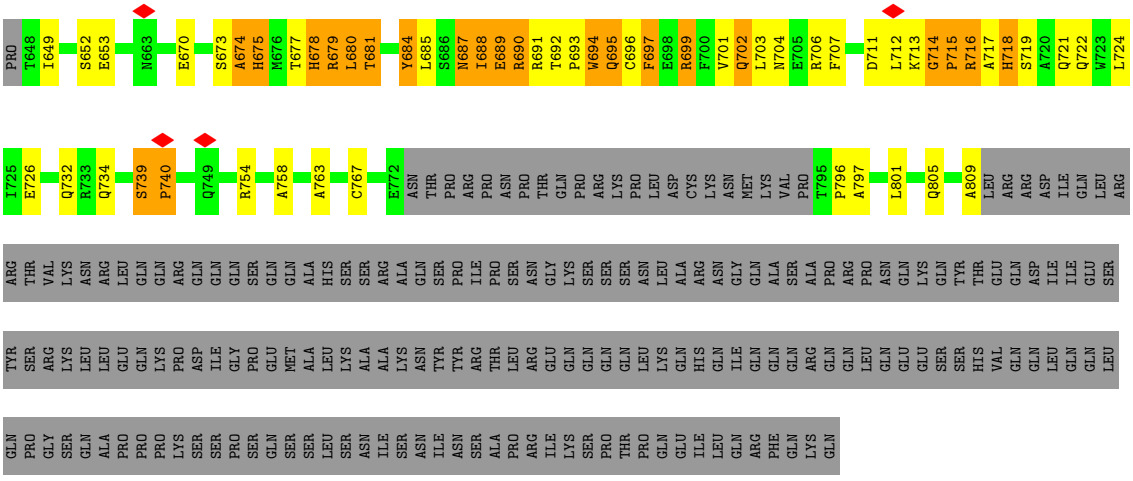
Chain B:



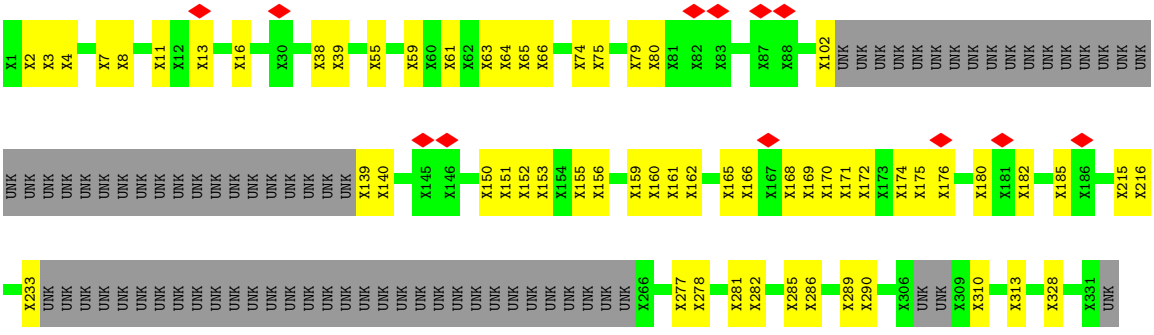
• Molecule 2: Chromatin modification-related protein EAF1

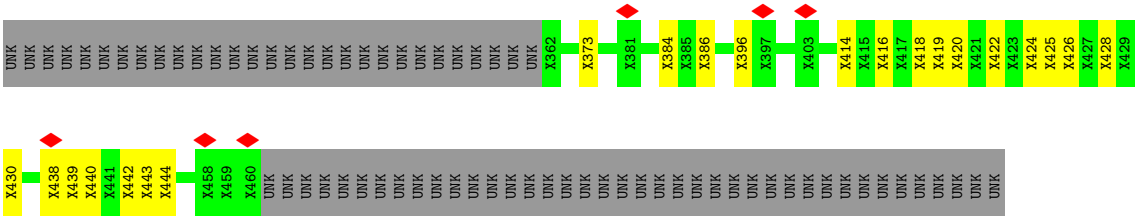
Chain C:

• Molecule 3: Eaf1-disorder domain

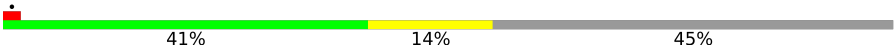
Chain D:

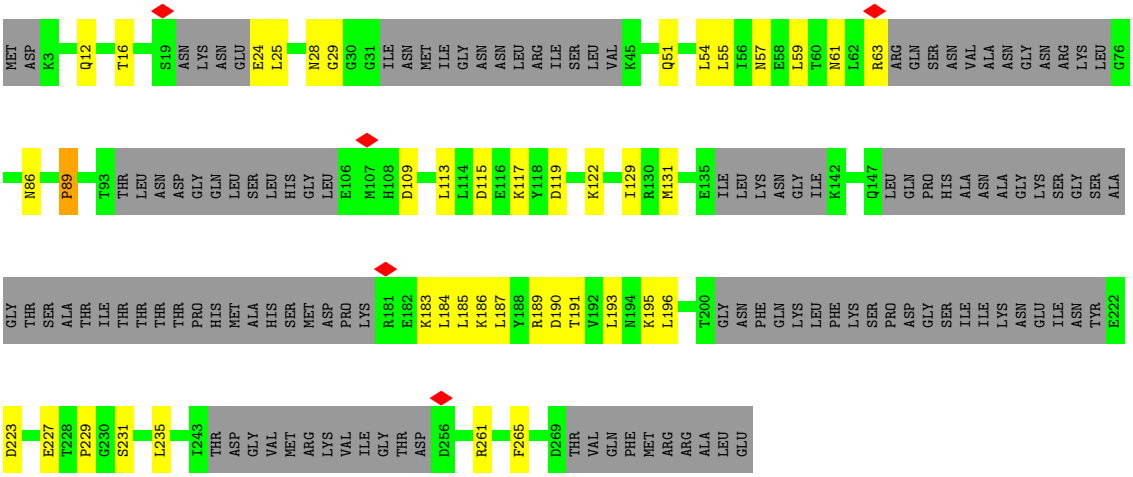





• Molecule 4: Chromatin modification-related protein EAF5

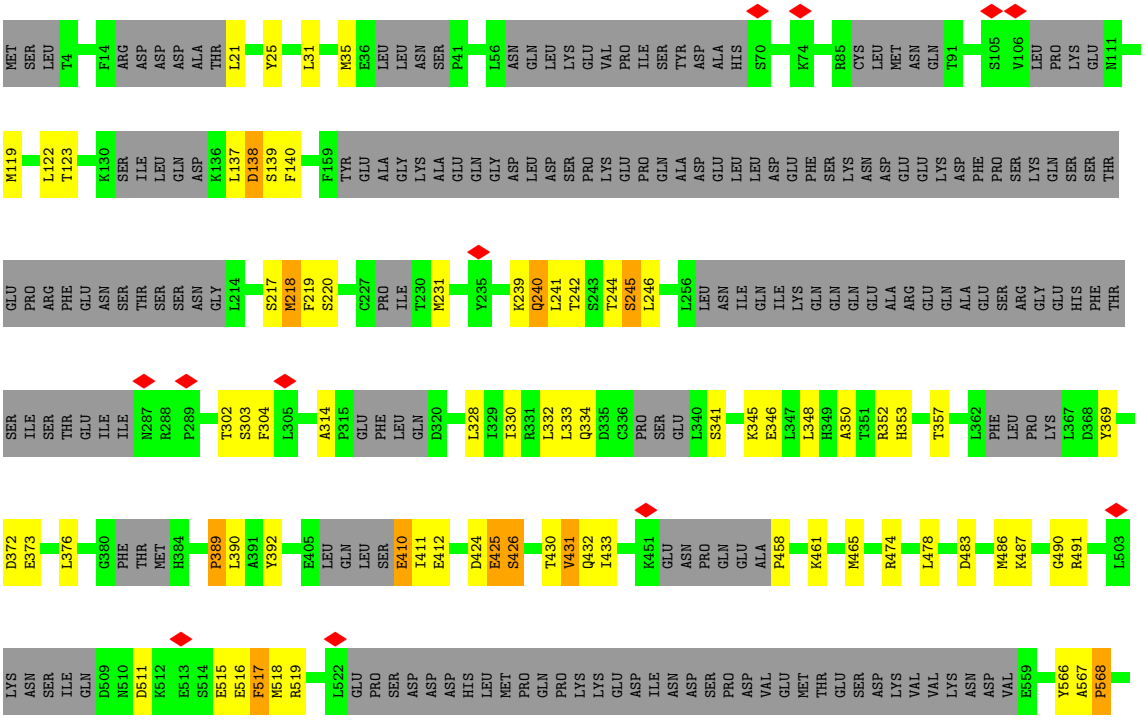
Chain H:

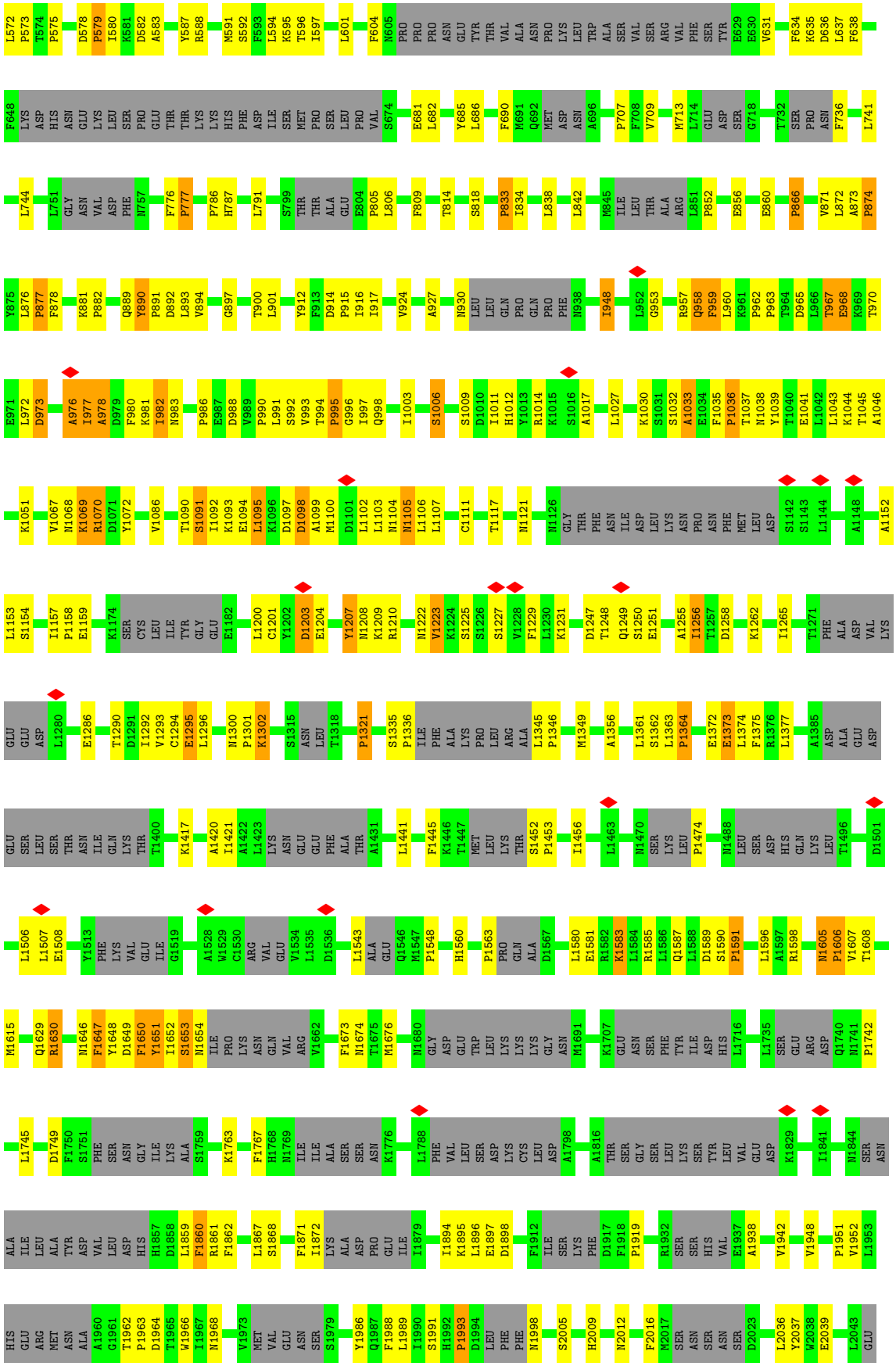


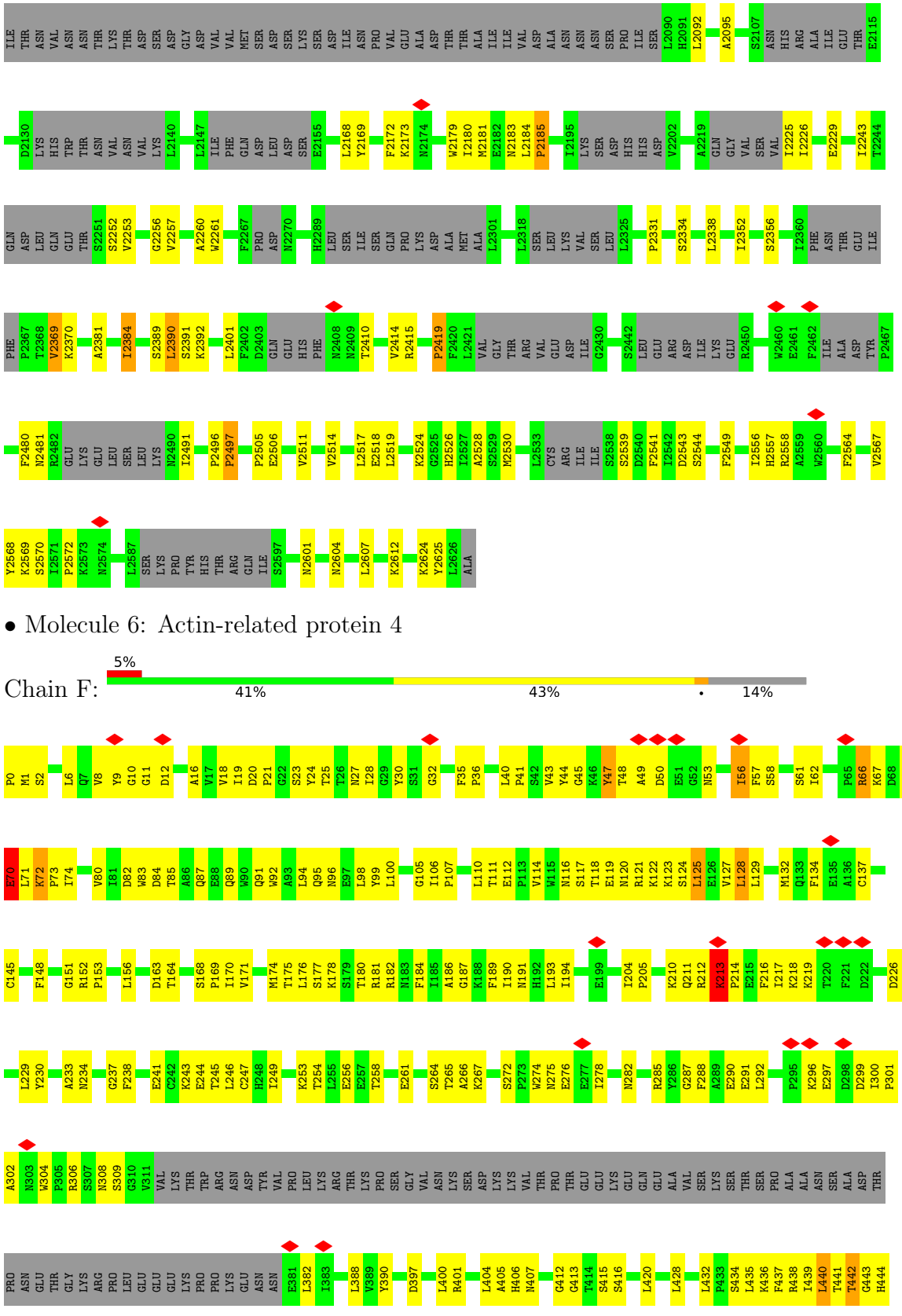



• Molecule 5: Transcription-associated protein 1

Chain A:

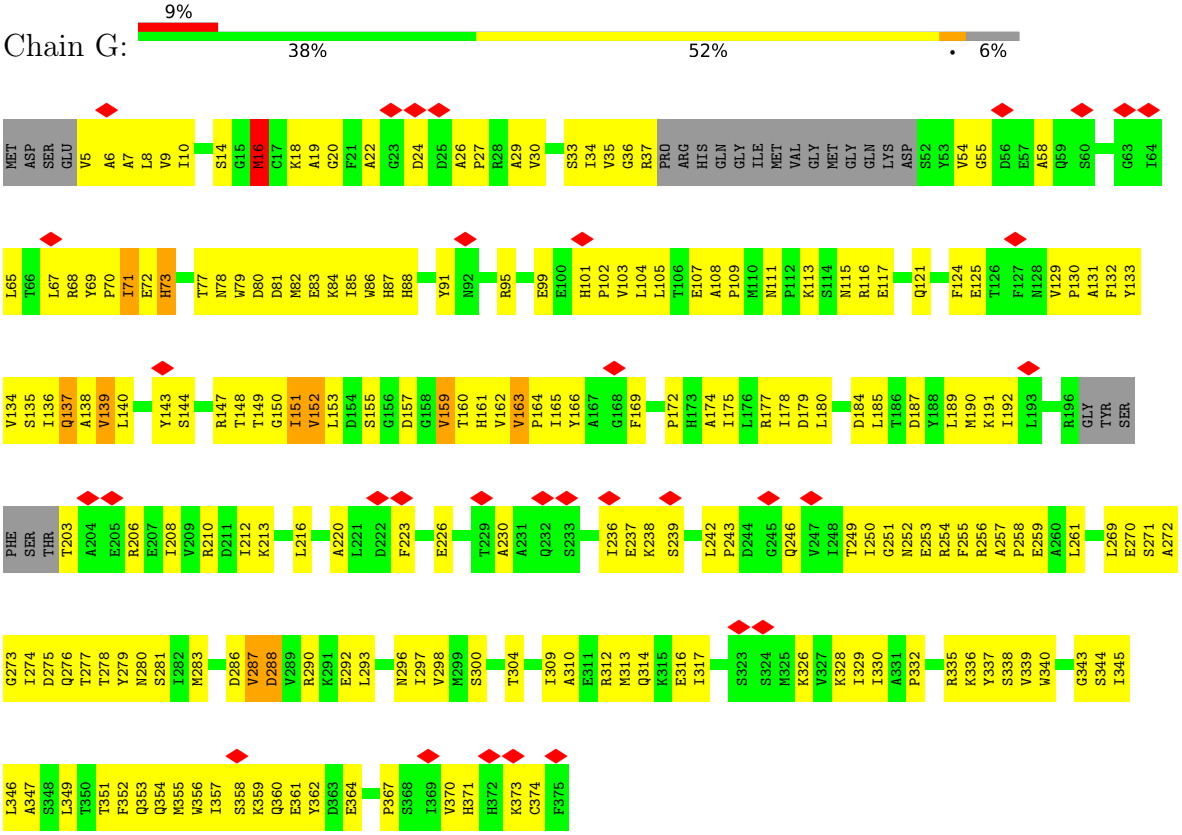




• Molecule 6: Actin-related protein 4

Chain F:


• Molecule 7: Actin




• Molecule 8: Chromatin modification-related protein EAF1

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 63197 | 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 ($e^-/Å^2$) | 30 | 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 | 0.132 | Depositor |
| Minimum map value | -0.063 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.005 | Depositor |
| Recommended contour level | 0.0225 | Depositor |
| Map size (Å) | 374.4, 374.4, 374.4 | wwPDB |
| Map dimensions | 288, 288, 288 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.3, 1.3, 1.3 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | B | 0.36 | 0/5992 | 0.58 | 2/8237 (0.0%) |
| 2 | C | 0.29 | 0/805 | 0.57 | 2/1110 (0.2%) |
| 4 | H | 0.31 | 0/755 | 0.48 | 2/1039 (0.2%) |
| 5 | A | 0.28 | 1/9944 (0.0%) | 0.51 | 32/13772 (0.2%) |
| 6 | F | 0.39 | 0/3406 | 0.56 | 0/4618 |
| 7 | G | 0.40 | 0/2787 | 0.54 | 0/3776 |
| 8 | E | 0.43 | 0/351 | 0.60 | 0/473 |
| All | All | 0.34 | 1/24040 (0.0%) | 0.54 | 38/33025 (0.1%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | A | 410 | GLU | C-N | 9.50 | 1.55 | 1.34 |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 777 | PRO | N-CA-CB | 6.52 | 111.12 | 103.30 |
| 1 | B | 3129 | PRO | N-CA-CB | 6.48 | 111.08 | 103.30 |
| 5 | A | 891 | PRO | N-CA-CB | 6.46 | 111.05 | 103.30 |
| 5 | A | 1919 | PRO | N-CA-CB | 6.36 | 110.93 | 103.30 |
| 4 | H | 89 | PRO | N-CA-CB | 6.30 | 110.86 | 103.30 |
| 5 | A | 707 | PRO | N-CA-CB | 6.24 | 110.78 | 103.30 |
| 5 | A | 2497 | PRO | N-CA-CB | 6.21 | 110.75 | 103.30 |
| 5 | A | 786 | PRO | N-CA-CB | 6.19 | 110.72 | 103.30 |
| 5 | A | 573 | PRO | N-CA-CB | 6.16 | 110.69 | 103.30 |
| 5 | A | 1474 | PRO | N-CA-CB | 6.13 | 110.66 | 103.30 |
| 5 | A | 575 | PRO | N-CA-CB | 6.00 | 110.49 | 103.30 |
| 5 | A | 579 | PRO | N-CA-CB | 5.94 | 110.43 | 103.30 |
| 5 | A | 2331 | PRO | N-CA-CB | 5.87 | 110.34 | 103.30 |
| 2 | C | 796 | PRO | N-CA-CB | 5.86 | 110.33 | 103.30 |
| 5 | A | 1336 | PRO | N-CA-CB | 5.85 | 110.32 | 103.30 |
| 5 | A | 1963 | PRO | N-CA-CB | 5.83 | 110.29 | 103.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 882 | PRO | N-CA-CB | 5.80 | 110.26 | 103.30 |
| 5 | A | 833 | PRO | N-CA-CB | 5.77 | 110.23 | 103.30 |
| 5 | A | 2496 | PRO | N-CA-CB | 5.77 | 110.22 | 103.30 |
| 2 | C | 740 | PRO | N-CA-CB | 5.74 | 110.19 | 103.30 |
| 5 | A | 1993 | PRO | N-CA-CB | 5.74 | 110.18 | 103.30 |
| 5 | A | 1951 | PRO | N-CA-CB | 5.73 | 110.18 | 103.30 |
| 5 | A | 1548 | PRO | N-CA-CB | 5.69 | 110.12 | 103.30 |
| 1 | B | 2921 | PRO | N-CA-CB | 5.68 | 110.11 | 103.30 |
| 5 | A | 877 | PRO | N-CA-CB | 5.67 | 110.10 | 103.30 |
| 5 | A | 2185 | PRO | N-CA-CB | 5.63 | 110.05 | 103.30 |
| 5 | A | 458 | PRO | N-CA-CB | 5.61 | 110.03 | 103.30 |
| 5 | A | 874 | PRO | N-CA-CB | 5.61 | 110.03 | 103.30 |
| 5 | A | 1563 | PRO | N-CA-CB | 5.60 | 110.02 | 103.30 |
| 5 | A | 1321 | PRO | N-CA-CB | 5.55 | 109.96 | 103.30 |
| 5 | A | 1453 | PRO | N-CA-CB | 5.52 | 109.92 | 103.30 |
| 5 | A | 852 | PRO | N-CA-CB | 5.50 | 109.90 | 103.30 |
| 5 | A | 805 | PRO | N-CA-CB | 5.49 | 109.88 | 103.30 |
| 5 | A | 1742 | PRO | N-CA-CB | 5.49 | 109.88 | 103.30 |
| 4 | H | 229 | PRO | N-CA-CB | 5.46 | 109.84 | 103.30 |
| 5 | A | 866 | PRO | N-CA-CB | 5.27 | 109.63 | 103.30 |
| 5 | A | 568 | PRO | N-CA-CB | 5.16 | 109.49 | 103.30 |
| 5 | A | 2505 | PRO | N-CA-CB | 5.15 | 109.48 | 103.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | B | 5937 | 0 | 4061 | 713 | 0 |
| 2 | C | 800 | 0 | 481 | 63 | 0 |
| 3 | D | 1800 | 0 | 405 | 60 | 0 |
| 4 | H | 764 | 0 | 309 | 24 | 0 |
| 5 | A | 10017 | 0 | 4245 | 320 | 0 |
| 6 | F | 3334 | 0 | 3292 | 264 | 0 |
| 7 | G | 2729 | 0 | 2697 | 238 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 8 | E | 342 | 0 | 331 | 40 | 0 |
| All | All | 25723 | 0 | 15821 | 1656 | 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 40.

All (1656) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3106:TRP:CZ3 | 1:B:3668:ARG:HD2 | 1.26 | 1.69 |
| 7:G:163:VAL:CG2 | 7:G:175:ILE:HG12 | 1.24 | 1.67 |
| 7:G:163:VAL:HG22 | 7:G:175:ILE:CG1 | 1.28 | 1.64 |
| 7:G:163:VAL:CG2 | 7:G:175:ILE:CG1 | 1.76 | 1.59 |
| 1:B:3139:GLN:CB | 1:B:3418:ARG:HH21 | 1.07 | 1.58 |
| 7:G:163:VAL:CG2 | 7:G:175:ILE:CD1 | 1.81 | 1.57 |
| 1:B:3236:ARG:HG3 | 1:B:3338:CYS:CB | 1.30 | 1.54 |
| 1:B:3474:PHE:CE2 | 1:B:3526:VAL:HG21 | 1.38 | 1.53 |
| 1:B:3427:ASN:CB | 1:B:3443:PHE:HE1 | 1.17 | 1.53 |
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:HD2 | 1.39 | 1.52 |
| 1:B:3171:LEU:HD23 | 1:B:3172:ARG:N | 1.22 | 1.52 |
| 1:B:3474:PHE:CE2 | 1:B:3526:VAL:CG2 | 1.90 | 1.51 |
| 5:A:2243:ILE:HA | 5:A:2252:SER:CB | 1.39 | 1.51 |
| 1:B:3427:ASN:HB2 | 1:B:3443:PHE:CE1 | 1.47 | 1.49 |
| 1:B:3625:THR:CB | 1:B:3727:ALA:HB1 | 1.39 | 1.48 |
| 1:B:3403:PHE:CB | 1:B:3457:ILE:HB | 1.42 | 1.47 |
| 1:B:3043:PHE:CB | 1:B:3060:TRP:NE1 | 1.77 | 1.47 |
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:CD | 1.98 | 1.47 |
| 1:B:3106:TRP:HH2 | 1:B:3668:ARG:CG | 1.24 | 1.46 |
| 1:B:3731:ARG:NH2 | 2:C:694:TRP:CD1 | 1.82 | 1.46 |
| 1:B:2828:TRP:CB | 1:B:2842:LEU:HD21 | 1.45 | 1.45 |
| 1:B:2828:TRP:CB | 1:B:2842:LEU:CD2 | 1.97 | 1.42 |
| 1:B:3427:ASN:CB | 1:B:3443:PHE:CE1 | 2.01 | 1.41 |
| 1:B:3139:GLN:CB | 1:B:3418:ARG:NH2 | 1.83 | 1.39 |
| 1:B:3043:PHE:CB | 1:B:3060:TRP:HE1 | 1.33 | 1.38 |
| 1:B:2633:TRP:CB | 5:A:2624:LYS:CB | 1.99 | 1.38 |
| 1:B:3731:ARG:NH2 | 2:C:694:TRP:HD1 | 1.08 | 1.38 |
| 1:B:3253:LEU:CD2 | 1:B:3314:LEU:CB | 2.00 | 1.37 |
| 1:B:3731:ARG:HD2 | 2:C:694:TRP:NE1 | 1.39 | 1.34 |
| 2:C:721:GLN:O | 2:C:724:LEU:CB | 1.75 | 1.34 |
| 1:B:3244:ASP:HA | 1:B:3247:ARG:CD | 1.57 | 1.33 |
| 1:B:3367:HIS:HE1 | 5:A:912:TYR:O | 1.08 | 1.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3568:THR:HB | 1:B:3569:PRO:CD | 1.56 | 1.32 |
| 1:B:3705:GLN:CB | 1:B:3709:LEU:HA | 1.61 | 1.31 |
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:CG | 2.09 | 1.30 |
| 1:B:3450:PRO:C | 1:B:3451:LEU:HD12 | 1.49 | 1.30 |
| 1:B:3427:ASN:CA | 1:B:3443:PHE:CE1 | 2.11 | 1.30 |
| 1:B:3667:ILE:CD1 | 1:B:3692:VAL:CB | 2.12 | 1.28 |
| 6:F:442:THR:CG2 | 6:F:448:ARG:HE | 1.45 | 1.27 |
| 1:B:3424:ARG:NH1 | 1:B:3447:ILE:HA | 1.50 | 1.26 |
| 1:B:3719:PHE:HA | 1:B:3722:ASP:OD2 | 1.34 | 1.25 |
| 5:A:333:LEU:CB | 5:A:376:LEU:CB | 2.14 | 1.25 |
| 3:D:418:UNK:CB | 6:F:441:THR:H | 1.50 | 1.23 |
| 5:A:1093:LYS:O | 5:A:1095:LEU:N | 1.71 | 1.22 |
| 5:A:430:THR:O | 5:A:432:GLN:N | 1.73 | 1.21 |
| 1:B:3427:ASN:CA | 1:B:3443:PHE:HE1 | 1.45 | 1.21 |
| 1:B:3374:PHE:CB | 1:B:3392:MET:CB | 2.17 | 1.21 |
| 1:B:3100:LEU:HD13 | 1:B:3101:LEU:N | 1.56 | 1.21 |
| 6:F:444:HIS:O | 6:F:446:ILE:N | 1.70 | 1.21 |
| 1:B:3474:PHE:CD2 | 1:B:3526:VAL:HG11 | 1.74 | 1.20 |
| 7:G:163:VAL:HG21 | 7:G:175:ILE:CD1 | 1.50 | 1.20 |
| 1:B:3163:TYR:CB | 1:B:3167:LEU:CD2 | 2.21 | 1.19 |
| 5:A:1372:GLU:O | 5:A:1375:PHE:N | 1.76 | 1.18 |
| 5:A:1043:LEU:O | 5:A:1046:ALA:HB3 | 1.43 | 1.18 |
| 1:B:3450:PRO:O | 1:B:3451:LEU:CD1 | 1.91 | 1.17 |
| 6:F:213:LYS:HB3 | 6:F:214:PRO:CD | 1.70 | 1.17 |
| 5:A:2243:ILE:CB | 5:A:2252:SER:C | 2.14 | 1.17 |
| 1:B:3568:THR:HB | 1:B:3569:PRO:HD2 | 1.18 | 1.17 |
| 5:A:1363:LEU:O | 5:A:1364:PRO:CB | 1.85 | 1.16 |
| 1:B:3474:PHE:CE2 | 1:B:3526:VAL:HG22 | 1.76 | 1.16 |
| 6:F:62:ILE:O | 6:F:71:LEU:HD21 | 1.45 | 1.16 |
| 1:B:3528:LYS:CB | 1:B:3632:ILE:O | 1.93 | 1.16 |
| 1:B:3236:ARG:CG | 1:B:3338:CYS:CB | 2.24 | 1.15 |
| 1:B:3427:ASN:HA | 1:B:3443:PHE:CE1 | 1.78 | 1.15 |
| 5:A:1091:SER:CB | 5:A:1099:ALA:HA | 1.76 | 1.15 |
| 1:B:3360:LEU:CB | 1:B:3424:ARG:HH21 | 1.57 | 1.14 |
| 1:B:3099:GLU:HB2 | 1:B:3425:LEU:HD11 | 1.16 | 1.14 |
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:CB | 2.29 | 1.14 |
| 1:B:3496:ALA:HB1 | 2:C:684:TYR:CE1 | 1.83 | 1.14 |
| 1:B:3106:TRP:HH2 | 1:B:3668:ARG:CD | 1.43 | 1.14 |
| 1:B:3367:HIS:CE1 | 5:A:912:TYR:O | 1.99 | 1.14 |
| 5:A:1091:SER:CA | 5:A:1099:ALA:HB2 | 1.77 | 1.13 |
| 1:B:3450:PRO:O | 1:B:3451:LEU:HD12 | 0.95 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3068:LEU:HD23 | 1:B:3081:ALA:CB | 1.76 | 1.13 |
| 1:B:3625:THR:CB | 1:B:3727:ALA:CB | 2.26 | 1.12 |
| 5:A:2243:ILE:CA | 5:A:2252:SER:CB | 2.26 | 1.12 |
| 5:A:137:LEU:O | 5:A:139:SER:N | 1.82 | 1.12 |
| 5:A:631:VAL:CB | 5:A:1587:GLN:CB | 2.26 | 1.12 |
| 1:B:2690:ILE:HA | 1:B:3715:VAL:CB | 1.80 | 1.11 |
| 6:F:213:LYS:HB3 | 6:F:214:PRO:HD2 | 1.24 | 1.11 |
| 1:B:3360:LEU:CB | 1:B:3424:ARG:NH2 | 2.13 | 1.11 |
| 1:B:2647:THR:CB | 1:B:2651:ASN:OD1 | 1.99 | 1.10 |
| 1:B:2659:GLU:HG3 | 1:B:2681:ARG:CB | 1.80 | 1.10 |
| 1:B:3740:PHE:C | 1:B:3742:PRO:HD3 | 1.68 | 1.10 |
| 1:B:3171:LEU:CD2 | 1:B:3172:ARG:N | 2.12 | 1.10 |
| 1:B:3106:TRP:HB2 | 1:B:3665:LEU:HD13 | 1.16 | 1.10 |
| 1:B:3244:ASP:HA | 1:B:3247:ARG:HD3 | 1.17 | 1.10 |
| 1:B:3253:LEU:HD21 | 1:B:3314:LEU:CB | 1.76 | 1.09 |
| 5:A:239:LYS:O | 5:A:241:LEU:N | 1.83 | 1.09 |
| 1:B:3053:LEU:CB | 1:B:3056:ALA:HB2 | 1.82 | 1.09 |
| 1:B:3496:ALA:HB1 | 2:C:684:TYR:HE1 | 0.98 | 1.09 |
| 1:B:3106:TRP:CZ3 | 1:B:3668:ARG:CD | 2.21 | 1.09 |
| 6:F:87:GLN:O | 6:F:132:MET:HE3 | 1.49 | 1.08 |
| 1:B:3116:MET:O | 1:B:3119:ASN:N | 1.86 | 1.08 |
| 1:B:3427:ASN:HA | 1:B:3443:PHE:CZ | 1.87 | 1.08 |
| 6:F:442:THR:HG21 | 6:F:448:ARG:HE | 1.07 | 1.08 |
| 1:B:3568:THR:CB | 1:B:3569:PRO:CD | 2.28 | 1.08 |
| 5:A:1292:ILE:O | 5:A:1294:CYS:N | 1.86 | 1.08 |
| 7:G:138:ALA:CB | 7:G:165:ILE:HD11 | 1.83 | 1.08 |
| 7:G:163:VAL:HG22 | 7:G:175:ILE:CD1 | 1.58 | 1.07 |
| 1:B:3407:TYR:H | 1:B:3408:PRO:CD | 1.69 | 1.06 |
| 5:A:1091:SER:CB | 5:A:1099:ALA:CB | 2.33 | 1.06 |
| 1:B:3068:LEU:HB2 | 1:B:3078:ALA:CB | 1.86 | 1.06 |
| 1:B:3106:TRP:HH2 | 1:B:3668:ARG:HG3 | 1.17 | 1.06 |
| 1:B:3163:TYR:CB | 1:B:3167:LEU:HD23 | 1.82 | 1.06 |
| 2:C:673:SER:HA | 2:C:681:THR:HG21 | 1.36 | 1.06 |
| 7:G:163:VAL:HG21 | 7:G:175:ILE:HD13 | 1.08 | 1.06 |
| 1:B:2828:TRP:CB | 1:B:2842:LEU:HD23 | 1.78 | 1.05 |
| 1:B:3068:LEU:HD23 | 1:B:3081:ALA:HB3 | 1.33 | 1.05 |
| 1:B:2638:ASN:O | 1:B:2642:SER:N | 1.89 | 1.05 |
| 1:B:3068:LEU:HB2 | 1:B:3078:ALA:HB1 | 1.33 | 1.05 |
| 1:B:3474:PHE:CD2 | 1:B:3526:VAL:HG21 | 1.91 | 1.05 |
| 1:B:3705:GLN:CB | 1:B:3709:LEU:CA | 2.33 | 1.05 |
| 1:B:2670:GLN:CA | 1:B:2837:PRO:HG3 | 1.85 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3163:TYR:CB | 1:B:3167:LEU:HD22 | 1.86 | 1.05 |
| 1:B:3450:PRO:C | 1:B:3451:LEU:CD1 | 2.24 | 1.05 |
| 1:B:3068:LEU:CD2 | 1:B:3081:ALA:HB3 | 1.86 | 1.05 |
| 5:A:1859:LEU:O | 5:A:1861:ARG:N | 1.89 | 1.05 |
| 7:G:163:VAL:HG23 | 7:G:175:ILE:HG12 | 1.11 | 1.05 |
| 1:B:3377:THR:CB | 1:B:3390:ARG:O | 2.05 | 1.04 |
| 1:B:3407:TYR:H | 1:B:3408:PRO:HD2 | 1.22 | 1.04 |
| 5:A:1091:SER:HA | 5:A:1099:ALA:HB2 | 1.37 | 1.04 |
| 1:B:3043:PHE:CB | 1:B:3060:TRP:CD1 | 2.40 | 1.03 |
| 5:A:1097:ASP:O | 5:A:1099:ALA:N | 1.91 | 1.03 |
| 1:B:3618:GLU:O | 1:B:3620:VAL:N | 1.90 | 1.03 |
| 1:B:3244:ASP:HA | 1:B:3247:ARG:HD2 | 1.37 | 1.03 |
| 5:A:1152:ALA:O | 5:A:1154:SER:N | 1.91 | 1.03 |
| 5:A:2243:ILE:CB | 5:A:2253:VAL:N | 2.19 | 1.03 |
| 1:B:3403:PHE:CB | 1:B:3457:ILE:CB | 2.36 | 1.02 |
| 1:B:3719:PHE:O | 1:B:3722:ASP:HB2 | 1.58 | 1.02 |
| 5:A:424:ASP:O | 5:A:426:SER:N | 1.91 | 1.02 |
| 1:B:3404:ALA:H | 1:B:3457:ILE:HG22 | 1.22 | 1.02 |
| 5:A:1441:LEU:O | 5:A:1445:PHE:N | 1.93 | 1.01 |
| 1:B:3171:LEU:O | 1:B:3174:THR:N | 1.93 | 1.01 |
| 7:G:163:VAL:HG23 | 7:G:175:ILE:CG1 | 1.69 | 1.01 |
| 1:B:3427:ASN:HB2 | 1:B:3443:PHE:CD1 | 1.95 | 1.01 |
| 3:D:79:UNK:O | 3:D:80:UNK:O | 1.77 | 1.01 |
| 7:G:163:VAL:CG2 | 7:G:175:ILE:HD11 | 1.87 | 1.01 |
| 5:A:1091:SER:CB | 5:A:1099:ALA:CA | 2.39 | 1.00 |
| 1:B:2670:GLN:N | 1:B:2837:PRO:HG3 | 1.76 | 1.00 |
| 1:B:2638:ASN:O | 1:B:2642:SER:HB3 | 1.62 | 1.00 |
| 1:B:3618:GLU:O | 1:B:3619:PRO:C | 1.96 | 0.99 |
| 5:A:1043:LEU:O | 5:A:1046:ALA:CB | 2.10 | 0.99 |
| 2:C:715:PRO:O | 2:C:717:ALA:N | 1.96 | 0.99 |
| 1:B:3099:GLU:CB | 1:B:3425:LEU:HD11 | 1.91 | 0.99 |
| 2:C:713:LYS:O | 2:C:714:GLY:O | 1.79 | 0.99 |
| 1:B:3703:VAL:O | 1:B:3704:ALA:O | 1.80 | 0.99 |
| 1:B:3427:ASN:CA | 1:B:3443:PHE:CZ | 2.45 | 0.99 |
| 6:F:87:GLN:O | 6:F:132:MET:CE | 2.11 | 0.98 |
| 1:B:3474:PHE:CD2 | 1:B:3526:VAL:CG1 | 2.46 | 0.98 |
| 1:B:3649:SER:OG | 1:B:3705:GLN:HA | 1.63 | 0.98 |
| 6:F:442:THR:HG21 | 6:F:448:ARG:NE | 1.77 | 0.98 |
| 5:A:1292:ILE:C | 5:A:1294:CYS:H | 1.68 | 0.98 |
| 1:B:3244:ASP:CA | 1:B:3247:ARG:HD3 | 1.93 | 0.97 |
| 1:B:3424:ARG:HH12 | 1:B:3447:ILE:HA | 1.07 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3741:MET:N | 1:B:3742:PRO:CD | 2.26 | 0.97 |
| 1:B:3106:TRP:HB2 | 1:B:3665:LEU:CD1 | 1.93 | 0.97 |
| 6:F:71:LEU:HD11 | 6:F:229:LEU:HD13 | 1.45 | 0.97 |
| 6:F:66:ARG:HB3 | 6:F:66:ARG:NH1 | 1.79 | 0.97 |
| 5:A:1372:GLU:O | 5:A:1374:LEU:N | 1.97 | 0.97 |
| 5:A:1157:ILE:O | 5:A:1159:GLU:N | 1.95 | 0.97 |
| 1:B:2659:GLU:CG | 1:B:2681:ARG:CB | 2.42 | 0.97 |
| 1:B:3411:ARG:O | 1:B:3415:ARG:N | 1.97 | 0.96 |
| 5:A:1227:SER:O | 5:A:1231:LYS:CB | 2.12 | 0.96 |
| 6:F:91:GLN:HB2 | 6:F:132:MET:CE | 1.95 | 0.96 |
| 5:A:1300:ASN:O | 5:A:1302:LYS:N | 1.98 | 0.96 |
| 6:F:211:GLN:OE1 | 6:F:217:ILE:HD12 | 1.65 | 0.96 |
| 1:B:3085:TYR:C | 1:B:3104:ILE:CD1 | 2.34 | 0.96 |
| 1:B:3391:LEU:O | 1:B:3402:SER:CB | 2.14 | 0.95 |
| 3:D:418:UNK:CB | 6:F:441:THR:N | 2.28 | 0.95 |
| 1:B:3424:ARG:NE | 1:B:3445:LEU:CB | 2.29 | 0.95 |
| 1:B:3649:SER:CB | 1:B:3705:GLN:HA | 1.96 | 0.95 |
| 1:B:3492:LYS:HA | 1:B:3492:LYS:HE3 | 1.48 | 0.95 |
| 5:A:516:GLU:O | 5:A:518:MET:N | 2.00 | 0.94 |
| 1:B:3422:LEU:HD22 | 1:B:3422:LEU:H | 1.27 | 0.94 |
| 6:F:442:THR:CG2 | 6:F:448:ARG:NE | 2.30 | 0.94 |
| 1:B:2822:GLN:O | 1:B:2825:LEU:N | 1.99 | 0.94 |
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:HB3 | 1.99 | 0.94 |
| 1:B:3253:LEU:HD23 | 1:B:3314:LEU:CB | 1.97 | 0.94 |
| 1:B:3668:ARG:HE | 1:B:3672:ILE:HD13 | 1.32 | 0.94 |
| 1:B:3171:LEU:HD23 | 1:B:3172:ARG:CA | 1.98 | 0.94 |
| 1:B:3247:ARG:HG3 | 1:B:3247:ARG:HH21 | 1.33 | 0.94 |
| 1:B:3171:LEU:CD2 | 1:B:3172:ARG:H | 1.76 | 0.94 |
| 1:B:3649:SER:HB2 | 1:B:3704:ALA:O | 1.68 | 0.93 |
| 1:B:3053:LEU:CB | 1:B:3056:ALA:CB | 2.45 | 0.93 |
| 8:E:391:ILE:HA | 8:E:394:TYR:HB2 | 1.48 | 0.93 |
| 2:C:722:GLN:C | 2:C:724:LEU:H | 1.72 | 0.92 |
| 7:G:138:ALA:HB1 | 7:G:165:ILE:HD11 | 1.47 | 0.92 |
| 1:B:3740:PHE:CB | 1:B:3742:PRO:HD3 | 1.98 | 0.92 |
| 6:F:129:LEU:HD22 | 6:F:129:LEU:H | 1.32 | 0.92 |
| 1:B:2817:CYS:CB | 1:B:2852:PHE:CZ | 2.52 | 0.92 |
| 1:B:3474:PHE:CG | 1:B:3526:VAL:HG11 | 2.04 | 0.92 |
| 1:B:3667:ILE:HD12 | 1:B:3692:VAL:CB | 1.98 | 0.92 |
| 1:B:3644:ASN:HA | 1:B:3647:THR:OG1 | 1.69 | 0.92 |
| 6:F:213:LYS:CB | 6:F:214:PRO:CD | 2.47 | 0.92 |
| 1:B:3244:ASP:O | 1:B:3247:ARG:HG2 | 1.69 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3424:ARG:HE | 1:B:3445:LEU:CB | 1.83 | 0.92 |
| 5:A:244:THR:O | 5:A:245:SER:O | 1.88 | 0.92 |
| 7:G:139:VAL:HG13 | 7:G:165:ILE:HG21 | 1.50 | 0.92 |
| 1:B:2690:ILE:CA | 1:B:3715:VAL:CB | 2.47 | 0.91 |
| 1:B:3244:ASP:CA | 1:B:3247:ARG:CD | 2.46 | 0.91 |
| 1:B:3667:ILE:HD13 | 1:B:3692:VAL:CB | 1.99 | 0.91 |
| 7:G:286:ASP:HB3 | 7:G:288:ASP:OD1 | 1.71 | 0.91 |
| 1:B:3731:ARG:CD | 2:C:694:TRP:HE1 | 1.82 | 0.91 |
| 4:H:51:GLN:O | 4:H:55:LEU:N | 2.04 | 0.91 |
| 7:G:163:VAL:HG22 | 7:G:175:ILE:HD11 | 1.49 | 0.91 |
| 5:A:1091:SER:CA | 5:A:1099:ALA:CB | 2.48 | 0.91 |
| 1:B:3055:LYS:O | 1:B:3059:GLN:N | 2.03 | 0.90 |
| 1:B:3740:PHE:C | 1:B:3742:PRO:CD | 2.39 | 0.90 |
| 1:B:2640:LEU:HD21 | 1:B:2662:LEU:CB | 2.02 | 0.90 |
| 1:B:3085:TYR:C | 1:B:3104:ILE:HD11 | 1.92 | 0.90 |
| 1:B:3219:TYR:N | 1:B:3220:PRO:HD3 | 1.87 | 0.90 |
| 1:B:3731:ARG:CD | 2:C:694:TRP:NE1 | 2.33 | 0.90 |
| 5:A:1506:LEU:O | 5:A:1508:GLU:N | 2.04 | 0.90 |
| 1:B:2638:ASN:O | 1:B:2642:SER:CB | 2.20 | 0.90 |
| 1:B:3253:LEU:HD22 | 1:B:3314:LEU:CB | 2.00 | 0.90 |
| 1:B:3618:GLU:CB | 1:B:3620:VAL:O | 2.20 | 0.89 |
| 6:F:87:GLN:HG3 | 6:F:132:MET:HE2 | 1.54 | 0.89 |
| 1:B:3106:TRP:HZ3 | 1:B:3668:ARG:HD2 | 1.13 | 0.89 |
| 5:A:1069:LYS:O | 5:A:1072:TYR:N | 2.05 | 0.89 |
| 1:B:3568:THR:HG22 | 1:B:3569:PRO:HD3 | 1.55 | 0.89 |
| 5:A:511:ASP:O | 5:A:515:GLU:CB | 2.20 | 0.89 |
| 6:F:442:THR:OG1 | 6:F:443:GLY:N | 2.06 | 0.89 |
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:NH2 | 2.39 | 0.88 |
| 1:B:3107:LEU:HA | 1:B:3110:ILE:HD12 | 1.54 | 0.88 |
| 1:B:3731:ARG:CZ | 2:C:694:TRP:HD1 | 1.85 | 0.88 |
| 1:B:3407:TYR:N | 1:B:3408:PRO:CD | 2.34 | 0.88 |
| 7:G:151:ILE:HG23 | 7:G:297:ILE:HA | 1.54 | 0.88 |
| 1:B:3568:THR:CB | 1:B:3569:PRO:HD3 | 2.03 | 0.88 |
| 7:G:151:ILE:HG21 | 7:G:297:ILE:HG12 | 1.55 | 0.88 |
| 1:B:2748:GLU:HB3 | 1:B:2752:HIS:CD2 | 2.07 | 0.87 |
| 5:A:239:LYS:C | 5:A:241:LEU:H | 1.78 | 0.87 |
| 6:F:428:LEU:HB3 | 6:F:437:PHE:HE2 | 1.37 | 0.87 |
| 1:B:2821:ILE:CB | 1:B:2849:TYR:CE2 | 2.57 | 0.87 |
| 1:B:3474:PHE:CZ | 1:B:3526:VAL:HG22 | 2.09 | 0.87 |
| 5:A:511:ASP:O | 5:A:515:GLU:N | 2.07 | 0.87 |
| 1:B:3354:ILE:HA | 1:B:3371:ILE:H | 1.39 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3219:TYR:H | 1:B:3220:PRO:HD3 | 1.38 | 0.87 |
| 1:B:3418:ARG:O | 1:B:3422:LEU:CD2 | 2.23 | 0.87 |
| 1:B:3106:TRP:CZ2 | 1:B:3668:ARG:CB | 2.58 | 0.86 |
| 1:B:3388:TYR:CB | 1:B:3404:ALA:HB1 | 2.04 | 0.86 |
| 1:B:2961:ASP:C | 1:B:2963:CYS:H | 1.78 | 0.86 |
| 1:B:3418:ARG:CB | 1:B:3418:ARG:HH11 | 1.88 | 0.86 |
| 1:B:3551:GLN:O | 1:B:3554:SER:N | 2.08 | 0.86 |
| 6:F:428:LEU:HB3 | 6:F:437:PHE:CE2 | 2.09 | 0.86 |
| 1:B:3474:PHE:HE2 | 1:B:3526:VAL:CG2 | 1.52 | 0.86 |
| 7:G:16:MET:SD | 7:G:16:MET:N | 2.49 | 0.86 |
| 5:A:1650:PHE:O | 5:A:1652:ILE:N | 2.09 | 0.86 |
| 1:B:3055:LYS:CB | 1:B:3059:GLN:HG3 | 2.06 | 0.86 |
| 1:B:3652:LEU:HD22 | 1:B:3652:LEU:O | 1.76 | 0.85 |
| 1:B:3169:PHE:CE1 | 1:B:3451:LEU:HD21 | 2.09 | 0.85 |
| 7:G:138:ALA:HA | 7:G:152:VAL:HG11 | 1.56 | 0.85 |
| 1:B:3526:VAL:O | 1:B:3530:HIS:N | 2.08 | 0.85 |
| 6:F:87:GLN:CG | 6:F:132:MET:CE | 2.54 | 0.85 |
| 1:B:3424:ARG:CD | 1:B:3445:LEU:CB | 2.53 | 0.85 |
| 6:F:87:GLN:HG2 | 6:F:132:MET:HE1 | 1.56 | 0.85 |
| 6:F:62:ILE:O | 6:F:71:LEU:CD2 | 2.24 | 0.85 |
| 1:B:2651:ASN:O | 1:B:2653:LYS:N | 2.09 | 0.85 |
| 6:F:45:GLY:HA3 | 6:F:56:ILE:HG22 | 1.56 | 0.85 |
| 5:A:1993:PRO:O | 5:A:1998:ASN:N | 2.10 | 0.85 |
| 7:G:16:MET:H | 7:G:16:MET:CE | 1.88 | 0.85 |
| 1:B:3062:PHE:HZ | 1:B:3657:ASN:C | 1.79 | 0.85 |
| 7:G:138:ALA:HB3 | 7:G:165:ILE:HD11 | 1.58 | 0.84 |
| 1:B:2821:ILE:HA | 1:B:2849:TYR:OH | 1.76 | 0.84 |
| 1:B:3731:ARG:HD2 | 2:C:694:TRP:CD1 | 2.12 | 0.84 |
| 1:B:3068:LEU:CB | 1:B:3078:ALA:CB | 2.55 | 0.84 |
| 1:B:3703:VAL:O | 1:B:3704:ALA:C | 2.14 | 0.84 |
| 1:B:3427:ASN:N | 1:B:3443:PHE:CZ | 2.45 | 0.84 |
| 6:F:91:GLN:OE1 | 6:F:132:MET:SD | 2.34 | 0.84 |
| 1:B:3576:LYS:H | 1:B:3576:LYS:HD3 | 1.43 | 0.84 |
| 1:B:3618:GLU:O | 1:B:3620:VAL:O | 1.96 | 0.84 |
| 3:D:155:UNK:O | 3:D:159:UNK:N | 2.09 | 0.84 |
| 5:A:302:THR:O | 5:A:304:PHE:N | 2.10 | 0.84 |
| 1:B:3481:ASP:CB | 1:B:3482:PRO:CD | 2.55 | 0.84 |
| 1:B:3568:THR:CG2 | 1:B:3569:PRO:HD3 | 2.07 | 0.83 |
| 5:A:914:ASP:O | 5:A:915:PRO:C | 2.13 | 0.83 |
| 5:A:1859:LEU:O | 5:A:1862:PHE:N | 2.11 | 0.83 |
| 1:B:3418:ARG:HH11 | 1:B:3418:ARG:HB2 | 1.43 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3168:HIS:O | 1:B:3172:ARG:HB3 | 1.78 | 0.83 |
| 6:F:213:LYS:C | 6:F:213:LYS:HE3 | 1.99 | 0.83 |
| 1:B:3168:HIS:HA | 1:B:3171:LEU:HD22 | 1.61 | 0.83 |
| 1:B:3411:ARG:HD2 | 1:B:3587:LEU:CB | 2.08 | 0.83 |
| 6:F:91:GLN:HB2 | 6:F:132:MET:SD | 2.19 | 0.83 |
| 1:B:3106:TRP:CB | 1:B:3665:LEU:HD13 | 2.07 | 0.83 |
| 1:B:3731:ARG:HD2 | 2:C:694:TRP:HE1 | 1.05 | 0.83 |
| 5:A:1097:ASP:O | 5:A:1100:MET:N | 2.10 | 0.83 |
| 5:A:996:GLY:O | 5:A:998:GLN:N | 2.12 | 0.82 |
| 2:C:722:GLN:O | 2:C:726:GLU:CB | 2.27 | 0.82 |
| 7:G:140:LEU:CD1 | 7:G:343:GLY:N | 2.42 | 0.82 |
| 1:B:2744:ASP:O | 1:B:2747:THR:HG23 | 1.78 | 0.82 |
| 6:F:87:GLN:CG | 6:F:132:MET:HE2 | 2.10 | 0.82 |
| 5:A:1006:SER:CB | 5:A:1009:SER:CB | 2.58 | 0.82 |
| 5:A:2567:VAL:C | 5:A:2569:LYS:H | 1.84 | 0.81 |
| 6:F:442:THR:HG21 | 6:F:448:ARG:CG | 2.10 | 0.81 |
| 1:B:3404:ALA:N | 1:B:3457:ILE:HG22 | 1.94 | 0.81 |
| 1:B:3173:THR:CB | 1:B:3451:LEU:HA | 2.10 | 0.81 |
| 5:A:1506:LEU:C | 5:A:1508:GLU:H | 1.84 | 0.81 |
| 1:B:3667:ILE:HD11 | 1:B:3692:VAL:CB | 2.08 | 0.81 |
| 5:A:1629:GLN:O | 5:A:1630:ARG:O | 1.97 | 0.81 |
| 7:G:140:LEU:HD12 | 7:G:343:GLY:N | 1.94 | 0.81 |
| 1:B:3171:LEU:O | 1:B:3174:THR:OG1 | 1.97 | 0.81 |
| 5:A:976:ALA:O | 5:A:977:ILE:CB | 2.28 | 0.81 |
| 7:G:242:LEU:HD12 | 7:G:246:GLN:HB2 | 1.60 | 0.81 |
| 1:B:2633:TRP:CB | 5:A:2624:LYS:C | 2.50 | 0.80 |
| 1:B:3719:PHE:CA | 1:B:3722:ASP:OD2 | 2.25 | 0.80 |
| 5:A:1361:LEU:O | 5:A:1363:LEU:N | 2.14 | 0.80 |
| 7:G:14:SER:HA | 7:G:71:ILE:HB | 1.62 | 0.80 |
| 7:G:18:LYS:HG2 | 7:G:30:VAL:HG13 | 1.63 | 0.80 |
| 1:B:3106:TRP:CE3 | 1:B:3665:LEU:HD12 | 2.17 | 0.80 |
| 1:B:3253:LEU:HD12 | 1:B:3318:ARG:HG3 | 1.64 | 0.80 |
| 5:A:976:ALA:HA | 5:A:992:SER:CB | 2.12 | 0.80 |
| 1:B:3466:THR:HG22 | 1:B:3573:HIS:HB2 | 1.63 | 0.80 |
| 1:B:3493:LEU:O | 1:B:3510:LYS:NZ | 2.14 | 0.80 |
| 7:G:298:VAL:HG22 | 7:G:330:ILE:HB | 1.63 | 0.80 |
| 1:B:3169:PHE:HE1 | 1:B:3451:LEU:CD2 | 1.95 | 0.80 |
| 1:B:3656:ASP:O | 1:B:3658:GLU:N | 2.14 | 0.79 |
| 5:A:430:THR:O | 5:A:431:VAL:C | 2.21 | 0.79 |
| 1:B:3060:TRP:CE3 | 1:B:3064:ASN:ND2 | 2.49 | 0.79 |
| 1:B:3486:GLN:NE2 | 1:B:3486:GLN:O | 2.16 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1200:LEU:O | 5:A:1203:ASP:CB | 2.31 | 0.79 |
| 7:G:178:ILE:HD11 | 7:G:277:THR:HG21 | 1.65 | 0.79 |
| 1:B:3062:PHE:CZ | 1:B:3657:ASN:C | 2.57 | 0.79 |
| 1:B:3705:GLN:CB | 1:B:3709:LEU:CB | 2.61 | 0.78 |
| 6:F:87:GLN:C | 6:F:132:MET:CE | 2.51 | 0.78 |
| 1:B:3100:LEU:CD1 | 1:B:3101:LEU:N | 2.44 | 0.78 |
| 5:A:217:SER:O | 5:A:220:SER:N | 2.14 | 0.78 |
| 5:A:1590:SER:O | 5:A:1591:PRO:CB | 2.31 | 0.78 |
| 1:B:2655:ILE:HG22 | 1:B:2656:GLU:N | 1.97 | 0.78 |
| 1:B:3116:MET:O | 1:B:3118:THR:N | 2.16 | 0.78 |
| 1:B:3247:ARG:HG2 | 1:B:3248:LEU:H | 1.49 | 0.78 |
| 1:B:3555:PHE:O | 1:B:3559:SER:N | 2.13 | 0.78 |
| 5:A:1650:PHE:O | 5:A:1653:SER:N | 2.17 | 0.78 |
| 7:G:286:ASP:CB | 7:G:288:ASP:OD1 | 2.31 | 0.78 |
| 1:B:3068:LEU:CD2 | 1:B:3081:ALA:CB | 2.53 | 0.78 |
| 1:B:3731:ARG:CZ | 2:C:694:TRP:CD1 | 2.63 | 0.78 |
| 5:A:890:TYR:O | 5:A:893:LEU:N | 2.16 | 0.78 |
| 6:F:72:LYS:NZ | 6:F:72:LYS:HB3 | 1.99 | 0.78 |
| 1:B:2853:LEU:O | 1:B:2856:THR:OG1 | 2.02 | 0.78 |
| 1:B:3102:CYS:SG | 1:B:3134:ILE:CB | 2.72 | 0.77 |
| 8:E:390:ALA:O | 8:E:394:TYR:N | 2.16 | 0.77 |
| 1:B:2944:ALA:HA | 1:B:2970:ILE:HD12 | 1.66 | 0.77 |
| 1:B:3068:LEU:HB3 | 1:B:3078:ALA:HA | 1.66 | 0.77 |
| 5:A:1091:SER:CB | 5:A:1099:ALA:HB1 | 2.15 | 0.77 |
| 1:B:3461:SER:CB | 1:B:3464:PHE:CZ | 2.67 | 0.77 |
| 7:G:140:LEU:HD12 | 7:G:343:GLY:H | 1.49 | 0.77 |
| 3:D:140:UNK:O | 6:F:178:LYS:NZ | 2.15 | 0.77 |
| 5:A:2567:VAL:O | 5:A:2569:LYS:N | 2.18 | 0.77 |
| 6:F:71:LEU:HD12 | 6:F:229:LEU:HD22 | 1.66 | 0.77 |
| 1:B:2818:ASP:O | 1:B:2821:ILE:CB | 2.33 | 0.77 |
| 1:B:3496:ALA:CB | 2:C:684:TYR:CE1 | 2.65 | 0.77 |
| 5:A:1032:SER:O | 5:A:1033:ALA:CB | 2.33 | 0.77 |
| 1:B:2967:LEU:HD12 | 1:B:2967:LEU:O | 1.84 | 0.77 |
| 1:B:3047:VAL:O | 1:B:3050:ASP:O | 2.03 | 0.77 |
| 2:C:805:GLN:O | 2:C:809:ALA:N | 2.12 | 0.77 |
| 5:A:1097:ASP:O | 5:A:1098:ASP:C | 2.21 | 0.77 |
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:HG3 | 2.00 | 0.76 |
| 5:A:239:LYS:C | 5:A:241:LEU:N | 2.35 | 0.76 |
| 5:A:1091:SER:HA | 5:A:1099:ALA:CB | 2.14 | 0.76 |
| 5:A:736:PHE:N | 5:A:1543:LEU:C | 2.38 | 0.76 |
| 5:A:328:LEU:O | 5:A:332:LEU:CB | 2.33 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:91:GLN:HB2 | 6:F:132:MET:HE1 | 1.68 | 0.76 |
| 6:F:213:LYS:HB3 | 6:F:214:PRO:HD3 | 1.67 | 0.76 |
| 6:F:66:ARG:HB3 | 6:F:66:ARG:HH11 | 1.47 | 0.76 |
| 7:G:108:ALA:HB1 | 7:G:109:PRO:CD | 2.15 | 0.76 |
| 5:A:1296:LEU:HA | 5:A:1356:ALA:HB2 | 1.68 | 0.76 |
| 1:B:3219:TYR:N | 1:B:3220:PRO:CD | 2.49 | 0.75 |
| 5:A:1605:ASN:O | 5:A:1608:THR:N | 2.19 | 0.75 |
| 3:D:439:UNK:O | 3:D:443:UNK:N | 2.19 | 0.75 |
| 5:A:976:ALA:CA | 5:A:992:SER:CB | 2.65 | 0.75 |
| 7:G:9:VAL:O | 7:G:340:TRP:NE1 | 2.17 | 0.75 |
| 7:G:19:ALA:HB3 | 7:G:29:ALA:HB3 | 1.67 | 0.75 |
| 7:G:150:GLY:O | 7:G:293:LEU:CD2 | 2.33 | 0.75 |
| 6:F:87:GLN:HG3 | 6:F:132:MET:CE | 2.16 | 0.75 |
| 7:G:102:PRO:HB3 | 7:G:131:ALA:HB3 | 1.68 | 0.75 |
| 7:G:237:GLU:HG2 | 7:G:251:GLY:HA2 | 1.68 | 0.75 |
| 6:F:213:LYS:HE3 | 6:F:213:LYS:CA | 2.16 | 0.75 |
| 7:G:163:VAL:HG23 | 7:G:175:ILE:CG2 | 2.16 | 0.75 |
| 7:G:220:ALA:HB1 | 7:G:226:GLU:HG3 | 1.69 | 0.75 |
| 5:A:1300:ASN:C | 5:A:1302:LYS:H | 1.89 | 0.75 |
| 1:B:3457:ILE:HD12 | 1:B:3457:ILE:O | 1.86 | 0.75 |
| 1:B:3247:ARG:HG3 | 1:B:3247:ARG:NH2 | 1.99 | 0.75 |
| 1:B:3435:GLU:OE1 | 1:B:3435:GLU:N | 2.20 | 0.75 |
| 1:B:3100:LEU:HD13 | 1:B:3101:LEU:CA | 2.16 | 0.75 |
| 1:B:3625:THR:N | 1:B:3626:PRO:HD3 | 2.02 | 0.75 |
| 3:D:55:UNK:O | 3:D:59:UNK:N | 2.20 | 0.75 |
| 5:A:1255:ALA:O | 5:A:1258:ASP:N | 2.19 | 0.75 |
| 6:F:211:GLN:OE1 | 6:F:217:ILE:CD1 | 2.34 | 0.75 |
| 2:C:717:ALA:O | 2:C:718:HIS:CB | 2.35 | 0.74 |
| 5:A:900:THR:CB | 5:A:948:ILE:CD1 | 2.64 | 0.74 |
| 1:B:2777:GLU:O | 1:B:2781:LYS:N | 2.16 | 0.74 |
| 1:B:3099:GLU:HB2 | 1:B:3425:LEU:CD1 | 2.08 | 0.74 |
| 1:B:3474:PHE:CD2 | 1:B:3526:VAL:CG2 | 2.58 | 0.74 |
| 1:B:3489:MET:CE | 1:B:3511:VAL:HG23 | 2.16 | 0.74 |
| 1:B:2941:HIS:H | 1:B:2941:HIS:CD2 | 2.04 | 0.74 |
| 1:B:3169:PHE:HE1 | 1:B:3451:LEU:CG | 2.00 | 0.74 |
| 1:B:3404:ALA:H | 1:B:3457:ILE:CG2 | 1.98 | 0.74 |
| 1:B:3740:PHE:CA | 1:B:3742:PRO:HD3 | 2.17 | 0.74 |
| 1:B:3097:ILE:HD13 | 1:B:3097:ILE:N | 2.03 | 0.74 |
| 3:D:419:UNK:CB | 6:F:439:ILE:HD12 | 2.17 | 0.74 |
| 5:A:1068:ASN:O | 5:A:1070:ARG:N | 2.21 | 0.74 |
| 1:B:3171:LEU:HD23 | 1:B:3172:ARG:H | 0.92 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3427:ASN:ND2 | 1:B:3428:LYS:N | 2.36 | 0.74 |
| 1:B:3494:ASN:HA | 1:B:3497:HIS:HB3 | 1.70 | 0.74 |
| 1:B:3062:PHE:HZ | 1:B:3658:GLU:N | 1.85 | 0.74 |
| 1:B:3244:ASP:CA | 1:B:3247:ARG:HD2 | 2.15 | 0.73 |
| 1:B:3659:LEU:O | 1:B:3662:TYR:CB | 2.36 | 0.73 |
| 2:C:721:GLN:O | 2:C:724:LEU:CA | 2.36 | 0.73 |
| 1:B:3057:TRP:O | 1:B:3061:GLY:N | 2.17 | 0.73 |
| 5:A:2005:SER:O | 5:A:2009:HIS:N | 2.18 | 0.73 |
| 1:B:3462:VAL:O | 1:B:3464:PHE:CD2 | 2.41 | 0.73 |
| 7:G:163:VAL:CG2 | 7:G:175:ILE:HD13 | 1.76 | 0.73 |
| 7:G:185:LEU:O | 7:G:189:LEU:N | 2.17 | 0.73 |
| 1:B:3492:LYS:HE3 | 1:B:3492:LYS:CA | 2.18 | 0.73 |
| 6:F:129:LEU:HD22 | 6:F:129:LEU:N | 2.03 | 0.73 |
| 5:A:516:GLU:O | 5:A:519:ARG:N | 2.20 | 0.73 |
| 5:A:578:ASP:O | 5:A:582:ASP:N | 2.21 | 0.73 |
| 5:A:1091:SER:C | 5:A:1099:ALA:HB2 | 2.08 | 0.73 |
| 6:F:455:GLY:HA2 | 6:F:458:ILE:HD12 | 1.69 | 0.73 |
| 7:G:164:PRO:HG2 | 7:G:174:ALA:HB3 | 1.71 | 0.73 |
| 5:A:1650:PHE:O | 5:A:1651:TYR:C | 2.26 | 0.73 |
| 7:G:138:ALA:HB1 | 7:G:165:ILE:CD1 | 2.18 | 0.73 |
| 7:G:287:VAL:HG12 | 7:G:290:ARG:NH1 | 2.04 | 0.73 |
| 1:B:3741:MET:N | 1:B:3742:PRO:HD2 | 2.03 | 0.73 |
| 7:G:236:ILE:O | 7:G:254:ARG:NH1 | 2.21 | 0.73 |
| 1:B:2882:GLN:HA | 1:B:2885:ARG:HG3 | 1.70 | 0.72 |
| 1:B:3625:THR:H | 1:B:3626:PRO:HD3 | 1.52 | 0.72 |
| 1:B:3649:SER:HB2 | 1:B:3705:GLN:HA | 1.70 | 0.72 |
| 5:A:239:LYS:O | 5:A:242:THR:N | 2.22 | 0.72 |
| 5:A:1069:LYS:CB | 5:A:1072:TYR:CB | 2.68 | 0.72 |
| 6:F:129:LEU:H | 6:F:129:LEU:CD2 | 2.01 | 0.72 |
| 6:F:210:LYS:HB2 | 6:F:219:LYS:HA | 1.72 | 0.72 |
| 6:F:415:SER:HA | 6:F:420:LEU:HD23 | 1.71 | 0.72 |
| 1:B:3656:ASP:C | 1:B:3658:GLU:H | 1.92 | 0.72 |
| 5:A:972:LEU:O | 5:A:973:ASP:O | 2.07 | 0.72 |
| 5:A:1090:THR:C | 5:A:1092:ILE:H | 1.92 | 0.72 |
| 1:B:3062:PHE:HZ | 1:B:3658:GLU:CA | 2.03 | 0.72 |
| 2:C:722:GLN:C | 2:C:724:LEU:N | 2.38 | 0.72 |
| 5:A:856:GLU:O | 5:A:860:GLU:N | 2.21 | 0.72 |
| 4:H:57:ASN:O | 4:H:61:ASN:N | 2.16 | 0.72 |
| 6:F:8:VAL:HG22 | 8:E:368:TRP:HB3 | 1.70 | 0.72 |
| 5:A:1032:SER:O | 5:A:1033:ALA:HB3 | 1.89 | 0.71 |
| 1:B:3247:ARG:HG2 | 1:B:3248:LEU:N | 2.05 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3247:ARG:NH1 | 1:B:3407:TYR:CB | 2.53 | 0.71 |
| 1:B:3388:TYR:HA | 1:B:3405:VAL:CB | 2.20 | 0.71 |
| 1:B:3424:ARG:HH12 | 1:B:3447:ILE:CA | 1.96 | 0.71 |
| 6:F:92:TRP:O | 6:F:96:ASN:ND2 | 2.23 | 0.71 |
| 5:A:410:GLU:C | 5:A:412:GLU:H | 1.94 | 0.71 |
| 1:B:3105:LEU:HD12 | 1:B:3105:LEU:O | 1.91 | 0.71 |
| 1:B:3444:ASN:O | 1:B:3446:PRO:HD3 | 1.91 | 0.71 |
| 1:B:3618:GLU:C | 1:B:3620:VAL:N | 2.44 | 0.71 |
| 3:D:426:UNK:O | 3:D:430:UNK:N | 2.22 | 0.71 |
| 3:D:440:UNK:O | 3:D:444:UNK:N | 2.23 | 0.71 |
| 5:A:897:GLY:O | 5:A:901:LEU:N | 2.18 | 0.71 |
| 5:A:1372:GLU:O | 5:A:1373:GLU:C | 2.29 | 0.71 |
| 1:B:3509:LEU:HD11 | 2:C:687:ASN:HD22 | 1.54 | 0.71 |
| 3:D:150:UNK:O | 3:D:153:UNK:N | 2.23 | 0.71 |
| 1:B:2899:ASN:OD1 | 1:B:2899:ASN:N | 2.17 | 0.71 |
| 1:B:3169:PHE:CZ | 1:B:3451:LEU:HD21 | 2.25 | 0.71 |
| 1:B:3424:ARG:HD3 | 1:B:3445:LEU:CB | 2.21 | 0.71 |
| 1:B:3167:LEU:O | 1:B:3167:LEU:HD12 | 1.90 | 0.71 |
| 3:D:151:UNK:O | 3:D:155:UNK:N | 2.24 | 0.71 |
| 1:B:2944:ALA:HA | 1:B:2970:ILE:CD1 | 2.21 | 0.71 |
| 1:B:3644:ASN:CA | 1:B:3647:THR:OG1 | 2.39 | 0.71 |
| 1:B:3106:TRP:CZ2 | 1:B:3668:ARG:HB2 | 2.24 | 0.71 |
| 1:B:3719:PHE:HA | 1:B:3722:ASP:CG | 2.09 | 0.71 |
| 6:F:444:HIS:O | 6:F:445:THR:C | 2.29 | 0.70 |
| 1:B:3375:LEU:CB | 1:B:3376:PRO:CD | 2.68 | 0.70 |
| 5:A:583:ALA:O | 5:A:587:TYR:N | 2.23 | 0.70 |
| 6:F:212:ARG:O | 6:F:275:ASN:ND2 | 2.20 | 0.70 |
| 1:B:3169:PHE:HE1 | 1:B:3451:LEU:HG | 1.56 | 0.70 |
| 1:B:3427:ASN:N | 1:B:3443:PHE:CE1 | 2.58 | 0.70 |
| 6:F:442:THR:HG22 | 6:F:448:ARG:HE | 1.49 | 0.70 |
| 7:G:151:ILE:CG2 | 7:G:297:ILE:HA | 2.21 | 0.70 |
| 1:B:3086:LEU:N | 1:B:3104:ILE:HD13 | 2.07 | 0.70 |
| 5:A:1093:LYS:C | 5:A:1095:LEU:H | 1.92 | 0.70 |
| 1:B:3418:ARG:O | 1:B:3422:LEU:HD21 | 1.90 | 0.70 |
| 5:A:814:THR:O | 5:A:818:SER:N | 2.18 | 0.70 |
| 5:A:2415:ARG:O | 5:A:2419:PRO:N | 2.24 | 0.70 |
| 6:F:87:GLN:HG2 | 6:F:132:MET:CE | 2.21 | 0.70 |
| 5:A:410:GLU:C | 5:A:412:GLU:N | 2.45 | 0.70 |
| 1:B:3618:GLU:O | 1:B:3620:VAL:C | 2.28 | 0.70 |
| 5:A:1090:THR:O | 5:A:1092:ILE:N | 2.25 | 0.70 |
| 5:A:1605:ASN:O | 5:A:1607:VAL:N | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:2243:ILE:CB | 5:A:2253:VAL:CA | 2.69 | 0.70 |
| 7:G:132:PHE:N | 7:G:357:ILE:O | 2.25 | 0.70 |
| 5:A:2389:SER:O | 5:A:2392:LYS:N | 2.25 | 0.70 |
| 6:F:204:ILE:HB | 6:F:274:TRP:CE3 | 2.26 | 0.70 |
| 1:B:3168:HIS:O | 1:B:3172:ARG:N | 2.25 | 0.70 |
| 2:C:754:ARG:O | 2:C:758:ALA:N | 2.24 | 0.70 |
| 5:A:1605:ASN:O | 5:A:1606:PRO:C | 2.27 | 0.70 |
| 1:B:3646:PHE:O | 1:B:3649:SER:OG | 2.08 | 0.70 |
| 1:B:3667:ILE:HD13 | 1:B:3692:VAL:CA | 2.21 | 0.70 |
| 3:D:172:UNK:N | 8:E:357:THR:OG1 | 2.25 | 0.69 |
| 6:F:87:GLN:CG | 6:F:132:MET:HE1 | 2.22 | 0.69 |
| 7:G:124:PHE:CZ | 7:G:132:PHE:HB3 | 2.27 | 0.69 |
| 1:B:3101:LEU:O | 1:B:3101:LEU:HD22 | 1.92 | 0.69 |
| 1:B:3391:LEU:H | 1:B:3402:SER:CB | 2.03 | 0.69 |
| 5:A:1964:ASP:O | 5:A:1968:ASN:N | 2.21 | 0.69 |
| 5:A:1859:LEU:O | 5:A:1860:PHE:C | 2.29 | 0.69 |
| 1:B:3094:ASN:CB | 1:B:3097:ILE:HG12 | 2.22 | 0.69 |
| 1:B:3253:LEU:CD1 | 1:B:3318:ARG:HG3 | 2.22 | 0.69 |
| 2:C:699:ARG:HD2 | 2:C:699:ARG:N | 2.04 | 0.69 |
| 7:G:163:VAL:HG22 | 7:G:175:ILE:HG12 | 0.99 | 0.69 |
| 7:G:9:VAL:HG21 | 7:G:344:SER:HA | 1.75 | 0.69 |
| 1:B:3173:THR:O | 1:B:3452:SER:HB2 | 1.93 | 0.69 |
| 1:B:2914:ASN:OD1 | 1:B:2915:ALA:N | 2.25 | 0.69 |
| 1:B:3737:ASP:OD2 | 1:B:3739:ASN:ND2 | 2.26 | 0.69 |
| 5:A:900:THR:CB | 5:A:948:ILE:HD13 | 2.23 | 0.69 |
| 5:A:2181:MET:O | 5:A:2185:PRO:N | 2.26 | 0.69 |
| 6:F:428:LEU:CB | 6:F:437:PHE:HE2 | 2.05 | 0.69 |
| 1:B:3422:LEU:H | 1:B:3422:LEU:CD2 | 2.06 | 0.69 |
| 1:B:2638:ASN:C | 1:B:2642:SER:HB3 | 2.13 | 0.69 |
| 1:B:2962:VAL:HA | 1:B:2965:SER:HB3 | 1.74 | 0.69 |
| 7:G:297:ILE:HB | 7:G:329:ILE:HG13 | 1.76 | 0.68 |
| 1:B:2670:GLN:N | 1:B:2837:PRO:CG | 2.56 | 0.68 |
| 7:G:212:ILE:HG23 | 7:G:216:LEU:HD12 | 1.74 | 0.68 |
| 1:B:2817:CYS:CB | 1:B:2852:PHE:HZ | 2.07 | 0.68 |
| 1:B:3068:LEU:HD23 | 1:B:3081:ALA:HB1 | 1.71 | 0.68 |
| 1:B:3670:GLU:O | 1:B:3673:SER:OG | 2.12 | 0.68 |
| 4:H:12:GLN:O | 4:H:16:THR:N | 2.27 | 0.68 |
| 5:A:369:TYR:O | 5:A:373:GLU:N | 2.26 | 0.68 |
| 6:F:1:MET:H | 7:G:371:HIS:CG | 2.12 | 0.68 |
| 5:A:1292:ILE:C | 5:A:1294:CYS:N | 2.36 | 0.68 |
| 7:G:121:GLN:O | 7:G:362:TYR:OH | 2.12 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3489:MET:HE1 | 1:B:3511:VAL:HG23 | 1.75 | 0.68 |
| 1:B:3568:THR:CB | 1:B:3569:PRO:HD2 | 2.07 | 0.68 |
| 1:B:3644:ASN:O | 1:B:3647:THR:OG1 | 2.09 | 0.68 |
| 5:A:516:GLU:O | 5:A:517:PHE:C | 2.30 | 0.68 |
| 1:B:3055:LYS:C | 1:B:3059:GLN:HB2 | 2.13 | 0.68 |
| 1:B:3625:THR:N | 1:B:3626:PRO:CD | 2.56 | 0.68 |
| 1:B:3514:PHE:O | 1:B:3518:GLN:N | 2.22 | 0.67 |
| 5:A:967:THR:O | 5:A:968:GLU:O | 2.11 | 0.67 |
| 5:A:976:ALA:C | 5:A:992:SER:CB | 2.62 | 0.67 |
| 7:G:151:ILE:CG2 | 7:G:297:ILE:HG12 | 2.24 | 0.67 |
| 1:B:3468:HIS:HB2 | 1:B:3570:HIS:HA | 1.77 | 0.67 |
| 4:H:261:ARG:O | 4:H:265:PHE:N | 2.28 | 0.67 |
| 5:A:2243:ILE:CB | 5:A:2253:VAL:HA | 2.24 | 0.67 |
| 7:G:24:ASP:HB2 | 7:G:340:TRP:HH2 | 1.60 | 0.67 |
| 8:E:382:ALA:O | 8:E:385:THR:OG1 | 2.11 | 0.67 |
| 2:C:713:LYS:O | 2:C:714:GLY:C | 2.32 | 0.67 |
| 5:A:1249:GLN:O | 5:A:1251:GLU:N | 2.24 | 0.67 |
| 1:B:3481:ASP:CB | 1:B:3482:PRO:HD2 | 2.24 | 0.67 |
| 1:B:3649:SER:CB | 1:B:3704:ALA:O | 2.43 | 0.67 |
| 5:A:2243:ILE:CB | 5:A:2252:SER:CB | 2.72 | 0.67 |
| 1:B:3105:LEU:HD12 | 1:B:3105:LEU:C | 2.15 | 0.67 |
| 2:C:684:TYR:HA | 2:C:687:ASN:HB3 | 1.76 | 0.67 |
| 1:B:2670:GLN:HA | 1:B:2837:PRO:HG3 | 1.72 | 0.67 |
| 1:B:3407:TYR:N | 1:B:3408:PRO:HD2 | 2.04 | 0.67 |
| 6:F:11:GLY:N | 6:F:461:SER:O | 2.26 | 0.67 |
| 6:F:233:ALA:O | 6:F:237:GLY:N | 2.27 | 0.67 |
| 7:G:137:GLN:OE1 | 7:G:137:GLN:N | 2.27 | 0.67 |
| 5:A:1345:LEU:HA | 5:A:1349:MET:CB | 2.25 | 0.67 |
| 7:G:347:ALA:O | 7:G:353:GLN:NE2 | 2.27 | 0.67 |
| 7:G:163:VAL:HG21 | 7:G:175:ILE:HD11 | 1.58 | 0.67 |
| 1:B:3448:ALA:HA | 1:B:3458:MET:HA | 1.77 | 0.67 |
| 1:B:3667:ILE:HD13 | 1:B:3692:VAL:C | 2.14 | 0.67 |
| 1:B:3060:TRP:CZ3 | 1:B:3064:ASN:ND2 | 2.62 | 0.66 |
| 1:B:3169:PHE:CE1 | 1:B:3451:LEU:CD2 | 2.73 | 0.66 |
| 5:A:486:MET:O | 5:A:490:GLY:N | 2.28 | 0.66 |
| 7:G:312:ARG:NE | 7:G:316:GLU:OE2 | 2.18 | 0.66 |
| 3:D:156:UNK:O | 3:D:160:UNK:N | 2.28 | 0.66 |
| 7:G:242:LEU:N | 7:G:246:GLN:O | 2.26 | 0.66 |
| 1:B:3019:LYS:CG | 1:B:3020:ALA:N | 2.58 | 0.66 |
| 1:B:3461:SER:CB | 1:B:3464:PHE:HZ | 2.06 | 0.66 |
| 7:G:275:ASP:OD1 | 7:G:276:GLN:N | 2.24 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2633:TRP:CB | 5:A:2624:LYS:CA | 2.73 | 0.66 |
| 4:H:113:LEU:O | 4:H:117:LYS:N | 2.24 | 0.66 |
| 5:A:353:HIS:O | 5:A:357:THR:N | 2.25 | 0.66 |
| 5:A:1093:LYS:C | 5:A:1095:LEU:N | 2.48 | 0.66 |
| 6:F:47:TYR:O | 6:F:53:ASN:OD1 | 2.13 | 0.66 |
| 6:F:174:MET:HA | 6:F:489[B]:ARG:HB3 | 1.78 | 0.66 |
| 7:G:239:SER:HA | 7:G:249:THR:HA | 1.78 | 0.66 |
| 5:A:588:ARG:O | 5:A:592:SER:N | 2.17 | 0.66 |
| 1:B:3060:TRP:O | 1:B:3063:PHE:N | 2.28 | 0.66 |
| 1:B:3527:LEU:O | 1:B:3531:PHE:N | 2.25 | 0.66 |
| 1:B:3719:PHE:C | 1:B:3722:ASP:HB2 | 2.15 | 0.66 |
| 7:G:99:GLU:HA | 7:G:129:VAL:HA | 1.78 | 0.66 |
| 1:B:3062:PHE:CZ | 1:B:3657:ASN:O | 2.49 | 0.66 |
| 1:B:3253:LEU:HD11 | 1:B:3318:ARG:HB2 | 1.78 | 0.66 |
| 2:C:695:GLN:O | 2:C:699:ARG:HD3 | 1.96 | 0.65 |
| 3:D:64:UNK:O | 6:F:434:SER:OG | 2.06 | 0.65 |
| 3:D:396:UNK:HA | 6:F:436:LYS:HE3 | 1.78 | 0.65 |
| 6:F:72:LYS:HD2 | 6:F:73:PRO:HD2 | 1.77 | 0.65 |
| 1:B:3101:LEU:C | 1:B:3101:LEU:HD13 | 2.15 | 0.65 |
| 1:B:3086:LEU:N | 1:B:3104:ILE:CD1 | 2.58 | 0.65 |
| 1:B:3423:TYR:CB | 1:B:3558:MET:CE | 2.74 | 0.65 |
| 5:A:1296:LEU:HA | 5:A:1356:ALA:CB | 2.26 | 0.65 |
| 6:F:169:PRO:HB2 | 6:F:176:LEU:HB2 | 1.79 | 0.65 |
| 7:G:163:VAL:HG23 | 7:G:175:ILE:HG23 | 1.78 | 0.65 |
| 1:B:3494:ASN:HD22 | 1:B:3497:HIS:HB3 | 1.61 | 0.65 |
| 5:A:1646:ASN:O | 5:A:1649:ASP:N | 2.30 | 0.65 |
| 5:A:1763:LYS:O | 5:A:1767:PHE:N | 2.30 | 0.65 |
| 1:B:3101:LEU:O | 1:B:3101:LEU:HD13 | 1.96 | 0.65 |
| 5:A:1036:PRO:O | 5:A:1038:ASN:N | 2.29 | 0.65 |
| 1:B:3437:ARG:O | 1:B:3440:SER:N | 2.28 | 0.65 |
| 5:A:424:ASP:C | 5:A:426:SER:N | 2.50 | 0.65 |
| 5:A:1201:CYS:HA | 5:A:1209:LYS:HA | 1.79 | 0.65 |
| 5:A:1452:SER:O | 5:A:1456:ILE:N | 2.30 | 0.65 |
| 1:B:2748:GLU:HB3 | 1:B:2752:HIS:HD2 | 1.59 | 0.65 |
| 1:B:3241:THR:O | 1:B:3242:ASP:CB | 2.43 | 0.65 |
| 1:B:3541:PHE:O | 1:B:3544:PHE:N | 2.25 | 0.65 |
| 4:H:115:ASP:O | 4:H:119:ASP:N | 2.24 | 0.65 |
| 4:H:183:LYS:O | 4:H:187:LEU:N | 2.27 | 0.65 |
| 1:B:2998:GLU:O | 1:B:3001:THR:N | 2.30 | 0.64 |
| 1:B:2635:GLN:N | 1:B:2635:GLN:OE1 | 2.28 | 0.64 |
| 6:F:191:ASN:HA | 6:F:194:ILE:HD12 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:254:THR:O | 6:F:258:THR:N | 2.29 | 0.64 |
| 1:B:2821:ILE:CB | 1:B:2849:TYR:HE2 | 2.06 | 0.64 |
| 1:B:3100:LEU:HD13 | 1:B:3100:LEU:C | 2.17 | 0.64 |
| 1:B:3509:LEU:HA | 1:B:3512:GLU:HB3 | 1.79 | 0.64 |
| 1:B:3253:LEU:HD21 | 1:B:3314:LEU:CA | 2.27 | 0.64 |
| 1:B:2967:LEU:HD12 | 1:B:2967:LEU:C | 2.17 | 0.64 |
| 1:B:3062:PHE:CZ | 1:B:3658:GLU:CA | 2.80 | 0.64 |
| 7:G:138:ALA:CB | 7:G:165:ILE:CD1 | 2.69 | 0.64 |
| 5:A:1247:ASP:O | 5:A:1248:THR:CB | 2.44 | 0.64 |
| 1:B:3159:ILE:O | 1:B:3163:TYR:N | 2.31 | 0.64 |
| 5:A:2243:ILE:CB | 5:A:2252:SER:O | 2.46 | 0.64 |
| 1:B:3427:ASN:HD22 | 1:B:3428:LYS:N | 1.94 | 0.64 |
| 1:B:2691:GLY:O | 1:B:2695:GLU:N | 2.31 | 0.64 |
| 1:B:3509:LEU:O | 1:B:3513:ILE:N | 2.27 | 0.64 |
| 1:B:3652:LEU:HD22 | 1:B:3652:LEU:C | 2.17 | 0.64 |
| 5:A:217:SER:O | 5:A:219:PHE:N | 2.30 | 0.64 |
| 5:A:389:PRO:O | 5:A:392:TYR:N | 2.30 | 0.64 |
| 5:A:483:ASP:O | 5:A:487:LYS:N | 2.30 | 0.64 |
| 5:A:1152:ALA:C | 5:A:1154:SER:H | 1.97 | 0.64 |
| 4:H:189:ARG:O | 4:H:193:LEU:N | 2.20 | 0.63 |
| 5:A:122:LEU:CB | 5:A:219:PHE:CB | 2.75 | 0.63 |
| 5:A:579:PRO:O | 5:A:583:ALA:N | 2.31 | 0.63 |
| 7:G:138:ALA:HA | 7:G:152:VAL:CG1 | 2.28 | 0.63 |
| 1:B:3100:LEU:C | 1:B:3100:LEU:HD22 | 2.17 | 0.63 |
| 1:B:3171:LEU:C | 1:B:3174:THR:HG1 | 2.00 | 0.63 |
| 1:B:3474:PHE:HE2 | 1:B:3526:VAL:HG21 | 0.93 | 0.63 |
| 5:A:976:ALA:O | 5:A:992:SER:CB | 2.46 | 0.63 |
| 5:A:1091:SER:O | 5:A:1099:ALA:HB2 | 1.98 | 0.63 |
| 1:B:2651:ASN:O | 1:B:2654:ILE:N | 2.31 | 0.63 |
| 1:B:3646:PHE:CB | 1:B:3720:ILE:HD11 | 2.28 | 0.63 |
| 5:A:1117:THR:O | 5:A:1121:ASN:N | 2.29 | 0.63 |
| 3:D:278:UNK:O | 3:D:282:UNK:N | 2.31 | 0.63 |
| 6:F:16:ALA:HB2 | 6:F:107:PRO:HG2 | 1.80 | 0.63 |
| 6:F:71:LEU:CD1 | 6:F:229:LEU:HD22 | 2.29 | 0.63 |
| 5:A:686:LEU:O | 5:A:690:PHE:N | 2.20 | 0.63 |
| 6:F:107:PRO:HB2 | 6:F:469:TRP:CZ3 | 2.34 | 0.63 |
| 5:A:1580:LEU:O | 5:A:1583:LYS:CB | 2.47 | 0.63 |
| 6:F:213:LYS:HE3 | 6:F:213:LYS:HA | 1.80 | 0.63 |
| 6:F:266:ALA:C | 6:F:282:ASN:HD21 | 2.01 | 0.63 |
| 1:B:2779:SER:O | 1:B:2783:VAL:N | 2.27 | 0.63 |
| 1:B:2651:ASN:O | 1:B:2652:THR:C | 2.37 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3040:ASN:OD1 | 1:B:3060:TRP:CZ2 | 2.52 | 0.62 |
| 1:B:3229:LEU:C | 1:B:3229:LEU:HD12 | 2.18 | 0.62 |
| 1:B:3462:VAL:O | 1:B:3464:PHE:N | 2.32 | 0.62 |
| 1:B:3740:PHE:HB3 | 1:B:3742:PRO:HD3 | 1.80 | 0.62 |
| 3:D:277:UNK:O | 3:D:281:UNK:N | 2.31 | 0.62 |
| 2:C:673:SER:O | 2:C:675:HIS:N | 2.32 | 0.62 |
| 4:H:24:GLU:O | 4:H:28:ASN:N | 2.27 | 0.62 |
| 7:G:73:HIS:HA | 7:G:159:VAL:HG13 | 1.82 | 0.62 |
| 1:B:2961:ASP:C | 1:B:2963:CYS:N | 2.48 | 0.62 |
| 1:B:3493:LEU:HD13 | 1:B:3493:LEU:C | 2.19 | 0.62 |
| 1:B:3703:VAL:C | 1:B:3704:ALA:O | 2.36 | 0.62 |
| 5:A:430:THR:C | 5:A:432:GLN:N | 2.53 | 0.62 |
| 1:B:3244:ASP:O | 1:B:3247:ARG:CG | 2.45 | 0.62 |
| 1:B:3474:PHE:CG | 1:B:3526:VAL:CG1 | 2.75 | 0.62 |
| 7:G:163:VAL:HG23 | 7:G:175:ILE:CB | 2.28 | 0.62 |
| 7:G:273:GLY:O | 7:G:277:THR:N | 2.28 | 0.62 |
| 5:A:487:LYS:O | 5:A:491:ARG:N | 2.17 | 0.62 |
| 5:A:1069:LYS:O | 5:A:1070:ARG:C | 2.37 | 0.62 |
| 7:G:151:ILE:HG23 | 7:G:151:ILE:O | 2.00 | 0.62 |
| 5:A:137:LEU:O | 5:A:138:ASP:C | 2.37 | 0.62 |
| 6:F:413:GLY:HA3 | 6:F:449:GLN:HE21 | 1.64 | 0.62 |
| 1:B:2912:ILE:N | 1:B:2912:ILE:HD13 | 2.14 | 0.62 |
| 1:B:3492:LYS:N | 1:B:3492:LYS:HD2 | 2.14 | 0.62 |
| 5:A:217:SER:O | 5:A:218:MET:C | 2.38 | 0.62 |
| 5:A:424:ASP:C | 5:A:426:SER:H | 2.03 | 0.62 |
| 5:A:2256:GLY:O | 5:A:2260:ALA:N | 2.28 | 0.62 |
| 6:F:112:GLU:OE1 | 6:F:116:ASN:ND2 | 2.24 | 0.62 |
| 6:F:301:PRO:HG2 | 6:F:304:TRP:HB2 | 1.81 | 0.62 |
| 1:B:3055:LYS:CB | 1:B:3059:GLN:CG | 2.78 | 0.62 |
| 1:B:3404:ALA:O | 1:B:3457:ILE:CG2 | 2.48 | 0.62 |
| 4:H:51:GLN:O | 4:H:54:LEU:N | 2.32 | 0.62 |
| 4:H:191:THR:O | 4:H:195:LYS:N | 2.33 | 0.62 |
| 5:A:1506:LEU:C | 5:A:1508:GLU:N | 2.51 | 0.62 |
| 1:B:2822:GLN:O | 1:B:2824:SER:N | 2.32 | 0.62 |
| 5:A:1036:PRO:C | 5:A:1038:ASN:H | 2.02 | 0.62 |
| 3:D:161:UNK:O | 3:D:166:UNK:N | 2.33 | 0.61 |
| 5:A:346:GLU:O | 5:A:350:ALA:N | 2.25 | 0.61 |
| 5:A:1090:THR:C | 5:A:1092:ILE:N | 2.53 | 0.61 |
| 1:B:3116:MET:O | 1:B:3117:LEU:C | 2.38 | 0.61 |
| 5:A:897:GLY:HA2 | 5:A:948:ILE:HD11 | 1.81 | 0.61 |
| 7:G:131:ALA:HA | 7:G:358:SER:HA | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3489:MET:HE1 | 1:B:3511:VAL:CG2 | 2.30 | 0.61 |
| 3:D:74:UNK:O | 3:D:75:UNK:CB | 2.48 | 0.61 |
| 6:F:32:GLY:HA2 | 8:E:373:PHE:HZ | 1.65 | 0.61 |
| 8:E:360:ASN:O | 8:E:364:GLU:HG3 | 1.99 | 0.61 |
| 1:B:3418:ARG:O | 1:B:3422:LEU:HD22 | 1.99 | 0.61 |
| 1:B:3422:LEU:HD22 | 1:B:3422:LEU:N | 2.09 | 0.61 |
| 2:C:739:SER:HA | 3:D:328:UNK:O | 2.01 | 0.61 |
| 1:B:2885:ARG:HD3 | 1:B:2885:ARG:C | 2.20 | 0.61 |
| 1:B:3068:LEU:HD22 | 1:B:3081:ALA:HB3 | 1.79 | 0.61 |
| 1:B:3492:LYS:HA | 1:B:3492:LYS:CE | 2.28 | 0.61 |
| 2:C:721:GLN:O | 2:C:724:LEU:N | 2.32 | 0.61 |
| 3:D:168:UNK:O | 3:D:171:UNK:N | 2.34 | 0.61 |
| 4:H:119:ASP:O | 4:H:122:LYS:N | 2.30 | 0.61 |
| 5:A:1859:LEU:C | 5:A:1861:ARG:N | 2.53 | 0.61 |
| 6:F:80:VAL:HB | 6:F:83:TRP:CZ2 | 2.36 | 0.61 |
| 7:G:150:GLY:HA3 | 7:G:296:ASN:HB2 | 1.81 | 0.61 |
| 1:B:3418:ARG:HH11 | 1:B:3418:ARG:CG | 2.14 | 0.61 |
| 6:F:153:PRO:HB3 | 8:E:363:LEU:HD13 | 1.82 | 0.61 |
| 1:B:2651:ASN:H | 1:B:2651:ASN:ND2 | 1.98 | 0.61 |
| 4:H:25:LEU:O | 4:H:29:GLY:N | 2.27 | 0.61 |
| 6:F:71:LEU:HD11 | 6:F:229:LEU:CD1 | 2.25 | 0.61 |
| 7:G:139:VAL:N | 7:G:165:ILE:HD13 | 2.16 | 0.61 |
| 1:B:3062:PHE:HZ | 1:B:3657:ASN:O | 1.83 | 0.61 |
| 6:F:72:LYS:HB3 | 6:F:72:LYS:HZ3 | 1.63 | 0.61 |
| 1:B:3062:PHE:CZ | 1:B:3658:GLU:N | 2.69 | 0.61 |
| 1:B:3354:ILE:CB | 1:B:3355:PRO:CD | 2.79 | 0.61 |
| 1:B:3427:ASN:HA | 1:B:3443:PHE:HZ | 1.58 | 0.61 |
| 4:H:231:SER:O | 4:H:235:LEU:N | 2.33 | 0.61 |
| 7:G:19:ALA:N | 7:G:29:ALA:O | 2.34 | 0.61 |
| 7:G:149:THR:HG23 | 7:G:166:TYR:HA | 1.83 | 0.61 |
| 6:F:8:VAL:HG21 | 8:E:368:TRP:O | 2.01 | 0.61 |
| 6:F:87:GLN:CA | 6:F:132:MET:HE2 | 2.31 | 0.61 |
| 6:F:272:SER:OG | 6:F:276:GLU:N | 2.33 | 0.61 |
| 6:F:446:ILE:HD12 | 6:F:446:ILE:H | 1.64 | 0.61 |
| 1:B:3101:LEU:HD22 | 1:B:3104:ILE:HB | 1.81 | 0.60 |
| 1:B:3106:TRP:CZ2 | 1:B:3668:ARG:HB3 | 2.32 | 0.60 |
| 7:G:9:VAL:N | 7:G:20:GLY:O | 2.25 | 0.60 |
| 1:B:2895:VAL:HG12 | 1:B:2895:VAL:O | 2.02 | 0.60 |
| 1:B:3489:MET:HE2 | 1:B:3511:VAL:HG23 | 1.83 | 0.60 |
| 1:B:3556:VAL:O | 1:B:3559:SER:OG | 2.11 | 0.60 |
| 7:G:7:ALA:O | 7:G:22:ALA:N | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:107:GLU:HB2 | 7:G:111:ASN:HD22 | 1.65 | 0.60 |
| 1:B:2636:SER:HA | 1:B:2639:ILE:HG13 | 1.83 | 0.60 |
| 1:B:3394:ARG:HA | 1:B:3398:GLY:HA2 | 1.83 | 0.60 |
| 8:E:366:ALA:C | 8:E:368:TRP:H | 2.05 | 0.60 |
| 1:B:3019:LYS:HG3 | 1:B:3020:ALA:N | 2.17 | 0.60 |
| 1:B:3139:GLN:CB | 1:B:3418:ARG:CZ | 2.76 | 0.60 |
| 5:A:1938:ALA:O | 5:A:1942:VAL:N | 2.31 | 0.60 |
| 6:F:308:ASN:OD1 | 6:F:309:SER:N | 2.34 | 0.60 |
| 7:G:33:SER:O | 7:G:33:SER:OG | 2.18 | 0.60 |
| 5:A:976:ALA:O | 5:A:992:SER:CA | 2.50 | 0.60 |
| 1:B:3068:LEU:HD12 | 1:B:3069:SER:N | 2.17 | 0.60 |
| 1:B:3423:TYR:CB | 1:B:3558:MET:HE2 | 2.32 | 0.60 |
| 5:A:634:PHE:O | 5:A:638:PHE:N | 2.33 | 0.60 |
| 5:A:872:LEU:O | 5:A:876:LEU:N | 2.28 | 0.60 |
| 1:B:3071:GLU:O | 1:B:3072:PRO:O | 2.19 | 0.60 |
| 2:C:739:SER:CB | 3:D:328:UNK:O | 2.49 | 0.60 |
| 7:G:147:ARG:NE | 7:G:296:ASN:OD1 | 2.34 | 0.60 |
| 1:B:3169:PHE:CE1 | 1:B:3451:LEU:CG | 2.85 | 0.60 |
| 1:B:3577:THR:O | 5:A:965:ASP:N | 2.35 | 0.60 |
| 5:A:878:PHE:O | 5:A:881:LYS:N | 2.34 | 0.60 |
| 5:A:995:PRO:CB | 5:A:2558:ARG:CB | 2.80 | 0.60 |
| 7:G:150:GLY:O | 7:G:293:LEU:HD23 | 2.02 | 0.60 |
| 1:B:2638:ASN:O | 1:B:2642:SER:CA | 2.49 | 0.60 |
| 1:B:2690:ILE:CB | 1:B:3715:VAL:CB | 2.80 | 0.60 |
| 5:A:2389:SER:O | 5:A:2390:LEU:C | 2.39 | 0.60 |
| 1:B:3423:TYR:CB | 1:B:3558:MET:HE1 | 2.32 | 0.59 |
| 1:B:3441:ILE:HG22 | 1:B:3441:ILE:O | 2.01 | 0.59 |
| 5:A:682:LEU:O | 5:A:686:LEU:N | 2.25 | 0.59 |
| 8:E:370:GLN:O | 8:E:374:LYS:N | 2.25 | 0.59 |
| 6:F:66:ARG:HB3 | 6:F:66:ARG:CZ | 2.32 | 0.59 |
| 7:G:34:ILE:HD12 | 7:G:55:GLY:O | 2.02 | 0.59 |
| 1:B:3169:PHE:CE1 | 1:B:3451:LEU:HG | 2.37 | 0.59 |
| 1:B:3544:PHE:HE1 | 1:B:3579:GLY:HA2 | 1.67 | 0.59 |
| 6:F:171:VAL:O | 6:F:174:MET:N | 2.26 | 0.59 |
| 1:B:2970:ILE:HG22 | 1:B:2970:ILE:O | 2.00 | 0.59 |
| 5:A:976:ALA:O | 5:A:992:SER:HA | 2.02 | 0.59 |
| 7:G:353:GLN:HA | 7:G:356:TRP:CD1 | 2.38 | 0.59 |
| 1:B:2643:ILE:HG23 | 1:B:2643:ILE:O | 2.00 | 0.59 |
| 5:A:914:ASP:O | 5:A:917:ILE:N | 2.35 | 0.59 |
| 5:A:1646:ASN:O | 5:A:1647:PHE:C | 2.39 | 0.59 |
| 6:F:91:GLN:H | 6:F:132:MET:HE3 | 1.68 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:99:TYR:OH | 7:G:177:ARG:NH1 | 2.36 | 0.59 |
| 1:B:2670:GLN:C | 1:B:2837:PRO:HG3 | 2.23 | 0.59 |
| 1:B:2835:TYR:O | 1:B:2839:HIS:N | 2.35 | 0.59 |
| 1:B:3085:TYR:CB | 1:B:3104:ILE:CD1 | 2.81 | 0.59 |
| 5:A:430:THR:O | 5:A:433:ILE:N | 2.35 | 0.59 |
| 6:F:442:THR:HG21 | 6:F:448:ARG:CD | 2.33 | 0.59 |
| 7:G:192:ILE:HD12 | 7:G:253:GLU:HG2 | 1.84 | 0.59 |
| 7:G:287:VAL:HG23 | 7:G:287:VAL:O | 2.02 | 0.59 |
| 1:B:3366:VAL:O | 1:B:3366:VAL:HG13 | 2.02 | 0.59 |
| 5:A:982:ILE:CB | 5:A:2481:ASN:CA | 2.80 | 0.59 |
| 5:A:1091:SER:O | 5:A:1099:ALA:CB | 2.51 | 0.59 |
| 6:F:171:VAL:HG11 | 6:F:400:LEU:HD13 | 1.84 | 0.59 |
| 1:B:3664:ALA:O | 1:B:3667:ILE:HG13 | 2.03 | 0.58 |
| 5:A:894:VAL:O | 5:A:897:GLY:N | 2.33 | 0.58 |
| 5:A:474:ARG:O | 5:A:478:LEU:N | 2.35 | 0.58 |
| 5:A:594:LEU:O | 5:A:597:ILE:N | 2.36 | 0.58 |
| 5:A:1107:LEU:O | 5:A:1111:CYS:N | 2.36 | 0.58 |
| 6:F:211:GLN:HB2 | 6:F:217:ILE:HD12 | 1.84 | 0.58 |
| 7:G:172:PRO:HA | 7:G:175:ILE:HD12 | 1.85 | 0.58 |
| 1:B:3097:ILE:HG22 | 1:B:3097:ILE:O | 2.02 | 0.58 |
| 6:F:213:LYS:HA | 6:F:213:LYS:CE | 2.33 | 0.58 |
| 6:F:230:TYR:O | 6:F:234:ASN:ND2 | 2.36 | 0.58 |
| 7:G:5:VAL:HB | 7:G:101:HIS:CE1 | 2.37 | 0.58 |
| 7:G:159:VAL:HB | 7:G:179:ASP:HA | 1.83 | 0.58 |
| 1:B:3547:GLN:O | 1:B:3551:GLN:N | 2.31 | 0.58 |
| 7:G:357:ILE:HA | 7:G:361:GLU:OE1 | 2.04 | 0.58 |
| 1:B:2817:CYS:CB | 1:B:2852:PHE:CE2 | 2.86 | 0.58 |
| 1:B:2851:GLU:HA | 1:B:2854:GLU:HB2 | 1.85 | 0.58 |
| 1:B:3106:TRP:HZ3 | 1:B:3668:ARG:CD | 1.91 | 0.58 |
| 1:B:3483:ASP:OD1 | 1:B:3483:ASP:N | 2.34 | 0.58 |
| 5:A:927:ALA:O | 5:A:930:ASN:OD1 | 2.21 | 0.58 |
| 7:G:144:SER:OG | 7:G:338:SER:HB3 | 2.04 | 0.58 |
| 1:B:3354:ILE:CB | 1:B:3369:ILE:O | 2.51 | 0.58 |
| 4:H:109:ASP:O | 4:H:113:LEU:N | 2.22 | 0.58 |
| 5:A:341:SER:O | 5:A:345:LYS:N | 2.33 | 0.58 |
| 6:F:116:ASN:OD1 | 6:F:117:SER:N | 2.37 | 0.58 |
| 1:B:3644:ASN:C | 1:B:3647:THR:OG1 | 2.42 | 0.58 |
| 5:A:1372:GLU:C | 5:A:1374:LEU:N | 2.57 | 0.58 |
| 6:F:94:LEU:O | 6:F:100:LEU:N | 2.35 | 0.58 |
| 1:B:2844:HIS:HA | 1:B:2847:GLN:HB3 | 1.86 | 0.58 |
| 1:B:3404:ALA:C | 1:B:3457:ILE:HG22 | 2.24 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3421:GLN:OE1 | 1:B:3421:GLN:N | 2.37 | 0.58 |
| 3:D:286:UNK:O | 3:D:290:UNK:N | 2.37 | 0.58 |
| 5:A:2601:ASN:O | 5:A:2604:ASN:N | 2.37 | 0.58 |
| 6:F:87:GLN:HA | 6:F:132:MET:HE2 | 1.86 | 0.58 |
| 7:G:335:ARG:HA | 7:G:338:SER:OG | 2.04 | 0.58 |
| 7:G:139:VAL:HG13 | 7:G:165:ILE:CG2 | 2.29 | 0.57 |
| 6:F:58:SER:HB2 | 6:F:92:TRP:HH2 | 1.69 | 0.57 |
| 7:G:79:TRP:HZ2 | 7:G:115:ASN:OD1 | 1.85 | 0.57 |
| 6:F:444:HIS:O | 6:F:446:ILE:CA | 2.52 | 0.57 |
| 6:F:483:LEU:HG | 6:F:487:ARG:HH12 | 1.70 | 0.57 |
| 1:B:3168:HIS:O | 1:B:3172:ARG:CB | 2.49 | 0.57 |
| 1:B:3515:ASN:ND2 | 1:B:3733:LEU:HD22 | 2.20 | 0.57 |
| 5:A:1373:GLU:O | 5:A:1377:LEU:N | 2.34 | 0.57 |
| 6:F:70:GLU:HG2 | 6:F:70:GLU:O | 2.04 | 0.57 |
| 6:F:261:GLU:O | 6:F:265:THR:HB | 2.05 | 0.57 |
| 1:B:3229:LEU:HD12 | 1:B:3229:LEU:O | 2.02 | 0.57 |
| 5:A:1581:GLU:O | 5:A:1585:ARG:CA | 2.52 | 0.57 |
| 6:F:210:LYS:HB3 | 6:F:217:ILE:HG22 | 1.85 | 0.57 |
| 1:B:2941:HIS:CD2 | 1:B:2941:HIS:N | 2.73 | 0.57 |
| 3:D:172:UNK:O | 3:D:176:UNK:N | 2.38 | 0.57 |
| 5:A:2179:TRP:O | 5:A:2183:ASN:N | 2.28 | 0.57 |
| 5:A:2369:VAL:O | 5:A:2370:LYS:C | 2.42 | 0.57 |
| 5:A:2410:THR:O | 5:A:2414:VAL:N | 2.35 | 0.57 |
| 5:A:1097:ASP:C | 5:A:1099:ALA:N | 2.58 | 0.57 |
| 1:B:3054:ALA:O | 1:B:3055:LYS:C | 2.43 | 0.57 |
| 1:B:3740:PHE:HB2 | 1:B:3742:PRO:HD3 | 1.85 | 0.57 |
| 3:D:185:UNK:O | 6:F:9:TYR:N | 2.38 | 0.57 |
| 6:F:25:THR:HG22 | 6:F:41:PRO:HA | 1.87 | 0.57 |
| 6:F:83:TRP:HB3 | 6:F:127:VAL:HG21 | 1.87 | 0.57 |
| 7:G:137:GLN:HG3 | 7:G:339:VAL:HG11 | 1.87 | 0.57 |
| 7:G:279:TYR:CZ | 7:G:283:MET:HG3 | 2.40 | 0.57 |
| 7:G:349:LEU:HB2 | 7:G:352:PHE:HB3 | 1.86 | 0.57 |
| 1:B:2637:ILE:HG13 | 1:B:2665:LEU:HD12 | 1.86 | 0.57 |
| 1:B:2943:ILE:C | 1:B:2970:ILE:HD11 | 2.25 | 0.57 |
| 7:G:250:ILE:HG22 | 7:G:254:ARG:HG3 | 1.87 | 0.57 |
| 1:B:3576:LYS:H | 1:B:3576:LYS:CD | 2.13 | 0.57 |
| 1:B:3503:ALA:HB1 | 1:B:3506:MET:HB2 | 1.87 | 0.56 |
| 6:F:10:GLY:HA2 | 6:F:463:GLY:H | 1.69 | 0.56 |
| 6:F:87:GLN:CA | 6:F:132:MET:CE | 2.82 | 0.56 |
| 6:F:148:PHE:HD2 | 6:F:459:LEU:HD11 | 1.70 | 0.56 |
| 7:G:34:ILE:HG12 | 7:G:69:TYR:CE1 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:238:LYS:O | 7:G:250:ILE:N | 2.38 | 0.56 |
| 1:B:3055:LYS:O | 1:B:3056:ALA:C | 2.43 | 0.56 |
| 1:B:3489:MET:CE | 1:B:3511:VAL:CG2 | 2.83 | 0.56 |
| 1:B:3555:PHE:HB2 | 1:B:3558:MET:HB3 | 1.87 | 0.56 |
| 2:C:715:PRO:O | 2:C:716:ARG:C | 2.43 | 0.56 |
| 5:A:1295:GLU:O | 5:A:1356:ALA:HB1 | 2.04 | 0.56 |
| 1:B:2964:ILE:HD13 | 1:B:2964:ILE:N | 2.19 | 0.56 |
| 1:B:3171:LEU:CG | 1:B:3172:ARG:N | 2.69 | 0.56 |
| 6:F:120:ASN:HA | 6:F:123:LYS:HB3 | 1.88 | 0.56 |
| 7:G:8:LEU:HD12 | 7:G:103:VAL:HG22 | 1.87 | 0.56 |
| 6:F:170:ILE:HD13 | 6:F:175:THR:HA | 1.87 | 0.56 |
| 1:B:2847:GLN:OE1 | 1:B:2847:GLN:HA | 2.04 | 0.56 |
| 6:F:462:LEU:HD21 | 8:E:369:MET:HB2 | 1.88 | 0.56 |
| 7:G:36:GLY:HA3 | 7:G:67:LEU:HD23 | 1.88 | 0.56 |
| 1:B:3068:LEU:HB3 | 1:B:3078:ALA:CA | 2.36 | 0.56 |
| 3:D:79:UNK:O | 3:D:80:UNK:C | 2.50 | 0.56 |
| 5:A:2524:LYS:O | 5:A:2528:ALA:N | 2.38 | 0.56 |
| 7:G:287:VAL:HG12 | 7:G:290:ARG:CZ | 2.35 | 0.56 |
| 1:B:2651:ASN:H | 1:B:2651:ASN:HD22 | 1.54 | 0.56 |
| 1:B:3085:TYR:CA | 1:B:3104:ILE:HD11 | 2.35 | 0.56 |
| 1:B:3568:THR:CG2 | 1:B:3569:PRO:CD | 2.75 | 0.56 |
| 1:B:2991:CYS:CB | 1:B:2999:LEU:CB | 2.83 | 0.56 |
| 1:B:3089:ALA:HB1 | 1:B:3100:LEU:HD11 | 1.88 | 0.56 |
| 5:A:1152:ALA:C | 5:A:1154:SER:N | 2.57 | 0.56 |
| 7:G:300:SER:N | 7:G:304:THR:HG21 | 2.20 | 0.56 |
| 1:B:2849:TYR:HA | 1:B:2852:PHE:HB3 | 1.87 | 0.56 |
| 1:B:3068:LEU:CB | 1:B:3078:ALA:HB2 | 2.33 | 0.56 |
| 1:B:3106:TRP:CZ3 | 1:B:3668:ARG:NH2 | 2.74 | 0.56 |
| 1:B:3354:ILE:HA | 1:B:3371:ILE:N | 2.15 | 0.56 |
| 1:B:3432:LYS:HB2 | 1:B:3432:LYS:NZ | 2.21 | 0.56 |
| 1:B:3517:ILE:O | 1:B:3521:PHE:N | 2.36 | 0.56 |
| 5:A:1036:PRO:C | 5:A:1038:ASN:N | 2.59 | 0.56 |
| 6:F:213:LYS:HE3 | 6:F:213:LYS:O | 2.05 | 0.56 |
| 1:B:3366:VAL:O | 1:B:3367:HIS:O | 2.24 | 0.55 |
| 1:B:3437:ARG:C | 1:B:3440:SER:H | 2.09 | 0.55 |
| 1:B:3573:HIS:HB3 | 1:B:3582:PHE:HB3 | 1.87 | 0.55 |
| 6:F:44:TYR:HB3 | 6:F:74:ILE:HD11 | 1.88 | 0.55 |
| 7:G:58:ALA:HB1 | 7:G:67:LEU:HD22 | 1.87 | 0.55 |
| 1:B:3055:LYS:O | 1:B:3059:GLN:HB2 | 2.06 | 0.55 |
| 1:B:3085:TYR:CB | 1:B:3104:ILE:HD11 | 2.36 | 0.55 |
| 1:B:3015:GLY:HA2 | 1:B:3019:LYS:HB3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:424:ASP:O | 5:A:425:GLU:C | 2.45 | 0.55 |
| 6:F:245:THR:OG1 | 6:F:246:LEU:HD12 | 2.05 | 0.55 |
| 7:G:187:ASP:O | 7:G:191:LYS:HG3 | 2.07 | 0.55 |
| 2:C:797:ALA:O | 2:C:801:LEU:N | 2.39 | 0.55 |
| 6:F:87:GLN:C | 6:F:132:MET:HE1 | 2.25 | 0.55 |
| 6:F:266:ALA:O | 6:F:282:ASN:ND2 | 2.34 | 0.55 |
| 1:B:3462:VAL:C | 1:B:3464:PHE:H | 2.10 | 0.55 |
| 7:G:6:ALA:O | 7:G:101:HIS:ND1 | 2.34 | 0.55 |
| 5:A:591:MET:O | 5:A:595:LYS:N | 2.23 | 0.55 |
| 7:G:27:PRO:HB3 | 7:G:340:TRP:CE2 | 2.42 | 0.55 |
| 5:A:1103:LEU:C | 5:A:1105:ASN:H | 2.09 | 0.55 |
| 5:A:1372:GLU:O | 5:A:1374:LEU:CA | 2.54 | 0.55 |
| 6:F:308:ASN:HA | 6:F:382:LEU:H | 1.71 | 0.55 |
| 7:G:16:MET:O | 7:G:18:LYS:HG3 | 2.06 | 0.55 |
| 7:G:150:GLY:O | 7:G:293:LEU:HD22 | 2.07 | 0.55 |
| 1:B:3085:TYR:O | 1:B:3104:ILE:HD11 | 2.06 | 0.55 |
| 5:A:681:GLU:O | 5:A:685:TYR:N | 2.26 | 0.55 |
| 7:G:332:PRO:HD2 | 7:G:335:ARG:HB3 | 1.88 | 0.55 |
| 1:B:2822:GLN:O | 1:B:2823:LEU:C | 2.44 | 0.55 |
| 1:B:3023:PHE:HB3 | 1:B:3046:ALA:HB1 | 1.89 | 0.55 |
| 1:B:3375:LEU:CB | 1:B:3376:PRO:HD2 | 2.37 | 0.55 |
| 1:B:3656:ASP:C | 1:B:3658:GLU:N | 2.59 | 0.55 |
| 5:A:2564:PHE:CB | 5:A:2607:LEU:O | 2.55 | 0.55 |
| 1:B:2797:PHE:HA | 1:B:2852:PHE:HE1 | 1.71 | 0.54 |
| 1:B:3217:THR:HA | 1:B:3220:PRO:HG3 | 1.89 | 0.54 |
| 1:B:3717:THR:O | 1:B:3720:ILE:HB | 2.06 | 0.54 |
| 1:B:3741:MET:N | 1:B:3742:PRO:HD3 | 2.00 | 0.54 |
| 5:A:1372:GLU:O | 5:A:1374:LEU:C | 2.44 | 0.54 |
| 5:A:2567:VAL:C | 5:A:2569:LYS:N | 2.52 | 0.54 |
| 7:G:286:ASP:HB2 | 7:G:288:ASP:OD2 | 2.08 | 0.54 |
| 7:G:108:ALA:HB1 | 7:G:109:PRO:HD2 | 1.89 | 0.54 |
| 7:G:330:ILE:HG22 | 7:G:332:PRO:HD3 | 1.89 | 0.54 |
| 1:B:3062:PHE:CZ | 1:B:3658:GLU:CB | 2.91 | 0.54 |
| 7:G:10:ILE:HA | 7:G:19:ALA:HA | 1.88 | 0.54 |
| 7:G:54:VAL:HB | 7:G:88:HIS:CG | 2.42 | 0.54 |
| 7:G:84:LYS:HA | 7:G:87:HIS:HB3 | 1.90 | 0.54 |
| 1:B:2634:TYR:N | 1:B:2634:TYR:CD1 | 2.75 | 0.54 |
| 1:B:3731:ARG:CD | 2:C:694:TRP:CD1 | 2.88 | 0.54 |
| 6:F:458:ILE:HG12 | 8:E:373:PHE:HD2 | 1.72 | 0.54 |
| 1:B:3479:GLY:O | 1:B:3480:PHE:O | 2.26 | 0.54 |
| 1:B:3712:THR:CB | 1:B:3713:PRO:HD2 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:20:ASP:OD2 | 6:F:452:SER:OG | 2.18 | 0.54 |
| 7:G:107:GLU:HB3 | 7:G:134:VAL:HG11 | 1.89 | 0.54 |
| 1:B:3586:MET:SD | 1:B:3586:MET:N | 2.81 | 0.54 |
| 5:A:580:ILE:HA | 5:A:583:ALA:CB | 2.38 | 0.54 |
| 5:A:873:ALA:O | 5:A:877:PRO:N | 2.41 | 0.54 |
| 5:A:1090:THR:O | 5:A:1093:LYS:N | 2.39 | 0.54 |
| 5:A:2225:ILE:HA | 5:A:2229:GLU:CB | 2.38 | 0.54 |
| 6:F:0:PRO:HB3 | 7:G:371:HIS:HB3 | 1.90 | 0.54 |
| 6:F:428:LEU:CB | 6:F:437:PHE:CE2 | 2.85 | 0.54 |
| 8:E:365:GLU:O | 8:E:368:TRP:HB2 | 2.08 | 0.54 |
| 1:B:2635:GLN:NE2 | 1:B:3539:GLU:CB | 2.70 | 0.54 |
| 3:D:168:UNK:O | 3:D:170:UNK:N | 2.41 | 0.54 |
| 6:F:438:ARG:HG2 | 6:F:440:LEU:HD22 | 1.90 | 0.54 |
| 1:B:2635:GLN:HE21 | 1:B:3539:GLU:CB | 2.20 | 0.54 |
| 1:B:3100:LEU:HD22 | 1:B:3100:LEU:O | 2.06 | 0.54 |
| 1:B:3247:ARG:HH12 | 1:B:3407:TYR:CB | 2.21 | 0.54 |
| 6:F:35:PHE:CD1 | 6:F:36:PRO:HD2 | 2.43 | 0.54 |
| 1:B:3044:ALA:HB2 | 1:B:3060:TRP:CH2 | 2.43 | 0.53 |
| 3:D:424:UNK:O | 3:D:428:UNK:N | 2.42 | 0.53 |
| 6:F:66:ARG:HG3 | 6:F:69:TYR:CG | 2.43 | 0.53 |
| 7:G:349:LEU:HD13 | 8:E:394:TYR:CD2 | 2.44 | 0.53 |
| 5:A:601:LEU:O | 5:A:604:PHE:N | 2.41 | 0.53 |
| 7:G:91:TYR:HA | 7:G:95:ARG:HA | 1.90 | 0.53 |
| 1:B:3062:PHE:CE2 | 1:B:3658:GLU:CB | 2.91 | 0.53 |
| 1:B:3171:LEU:O | 1:B:3172:ARG:C | 2.47 | 0.53 |
| 1:B:3644:ASN:C | 1:B:3647:THR:HG1 | 2.09 | 0.53 |
| 3:D:65:UNK:O | 3:D:66:UNK:O | 2.27 | 0.53 |
| 5:A:1044:LYS:C | 5:A:1046:ALA:N | 2.62 | 0.53 |
| 6:F:302:ALA:HA | 6:F:306:ARG:HH21 | 1.73 | 0.53 |
| 6:F:447:GLU:HG2 | 6:F:450:TYR:OH | 2.08 | 0.53 |
| 3:D:285:UNK:O | 3:D:289:UNK:N | 2.42 | 0.53 |
| 1:B:2961:ASP:O | 1:B:2963:CYS:N | 2.41 | 0.53 |
| 7:G:83:GLU:O | 7:G:87:HIS:N | 2.38 | 0.53 |
| 1:B:3568:THR:HG21 | 1:B:3739:ASN:HB3 | 1.91 | 0.53 |
| 2:C:694:TRP:HA | 2:C:697:PHE:HD2 | 1.74 | 0.53 |
| 3:D:171:UNK:O | 3:D:175:UNK:N | 2.42 | 0.53 |
| 6:F:465:PHE:CE1 | 6:F:468:LEU:HD22 | 2.43 | 0.53 |
| 6:F:466:HIS:HA | 6:F:469:TRP:CD1 | 2.44 | 0.53 |
| 1:B:3099:GLU:O | 1:B:3099:GLU:HG2 | 2.08 | 0.53 |
| 1:B:3493:LEU:HD13 | 1:B:3497:HIS:HB2 | 1.89 | 0.53 |
| 2:C:677:THR:O | 2:C:678:HIS:O | 2.26 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1045:THR:CB | 5:A:2511:VAL:CB | 2.87 | 0.53 |
| 5:A:2036:LEU:O | 5:A:2039:GLU:N | 2.42 | 0.53 |
| 6:F:84:ASP:O | 6:F:87:GLN:HB3 | 2.08 | 0.53 |
| 6:F:211:GLN:HB2 | 6:F:217:ILE:HB | 1.90 | 0.53 |
| 6:F:444:HIS:C | 6:F:446:ILE:N | 2.52 | 0.53 |
| 1:B:3020:ALA:HB1 | 1:B:3050:ASP:CB | 2.39 | 0.53 |
| 1:B:3354:ILE:CB | 1:B:3355:PRO:HD2 | 2.38 | 0.53 |
| 3:D:170:UNK:O | 3:D:174:UNK:N | 2.42 | 0.53 |
| 5:A:1652:ILE:O | 5:A:1654:ASN:N | 2.41 | 0.53 |
| 5:A:410:GLU:O | 5:A:412:GLU:N | 2.42 | 0.53 |
| 1:B:2822:GLN:C | 1:B:2824:SER:N | 2.61 | 0.53 |
| 3:D:180:UNK:C | 3:D:182:UNK:H | 2.21 | 0.53 |
| 6:F:151:GLY:H | 8:E:370:GLN:HE22 | 1.57 | 0.53 |
| 1:B:3107:LEU:HD12 | 1:B:3110:ILE:HD12 | 1.90 | 0.52 |
| 1:B:3389:ARG:O | 1:B:3404:ALA:HA | 2.10 | 0.52 |
| 5:A:982:ILE:CB | 5:A:2480:PHE:C | 2.78 | 0.52 |
| 1:B:3505:ASP:HA | 1:B:3508:ILE:HB | 1.91 | 0.52 |
| 6:F:249:ILE:HD12 | 6:F:420:LEU:HB2 | 1.91 | 0.52 |
| 1:B:3517:ILE:O | 1:B:3520:MET:N | 2.43 | 0.52 |
| 6:F:190:ILE:O | 6:F:194:ILE:HG13 | 2.09 | 0.52 |
| 7:G:80:ASP:O | 7:G:83:GLU:HB3 | 2.08 | 0.52 |
| 1:B:3246:PHE:HE2 | 1:B:3322:GLU:HA | 1.75 | 0.52 |
| 2:C:689:GLU:C | 2:C:691:ARG:H | 2.12 | 0.52 |
| 1:B:2944:ALA:N | 1:B:2970:ILE:CD1 | 2.73 | 0.52 |
| 1:B:3541:PHE:HE2 | 1:B:3545:ARG:NE | 2.07 | 0.52 |
| 6:F:8:VAL:CG2 | 8:E:368:TRP:HB3 | 2.38 | 0.52 |
| 6:F:442:THR:HG1 | 6:F:443:GLY:H | 1.52 | 0.52 |
| 1:B:3085:TYR:O | 1:B:3104:ILE:CD1 | 2.56 | 0.52 |
| 1:B:3436:THR:O | 1:B:3440:SER:N | 2.43 | 0.52 |
| 6:F:19:ILE:HG22 | 6:F:21:PRO:HD3 | 1.91 | 0.52 |
| 6:F:80:VAL:HB | 6:F:83:TRP:CH2 | 2.43 | 0.52 |
| 1:B:3576:LYS:CD | 1:B:3576:LYS:N | 2.73 | 0.52 |
| 5:A:516:GLU:C | 5:A:518:MET:N | 2.62 | 0.52 |
| 6:F:119:GLU:O | 6:F:123:LYS:N | 2.24 | 0.52 |
| 2:C:692:THR:N | 2:C:693:PRO:CD | 2.73 | 0.52 |
| 5:A:430:THR:O | 5:A:432:GLN:CA | 2.56 | 0.52 |
| 5:A:787:HIS:O | 5:A:791:LEU:N | 2.28 | 0.52 |
| 6:F:62:ILE:HG12 | 6:F:71:LEU:HD23 | 1.91 | 0.52 |
| 7:G:86:TRP:NE1 | 7:G:105:LEU:HD21 | 2.24 | 0.52 |
| 1:B:3160:ALA:HA | 1:B:3167:LEU:CD2 | 2.39 | 0.52 |
| 1:B:3387:SER:O | 1:B:3388:TYR:O | 2.27 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3553:SER:O | 1:B:3556:VAL:HG22 | 2.10 | 0.52 |
| 6:F:114:VAL:HG11 | 6:F:180:THR:HG21 | 1.92 | 0.52 |
| 6:F:442:THR:HG21 | 6:F:448:ARG:HG2 | 1.91 | 0.52 |
| 6:F:447:GLU:HG2 | 6:F:450:TYR:CZ | 2.45 | 0.52 |
| 1:B:3432:LYS:HB2 | 1:B:3432:LYS:HZ2 | 1.74 | 0.52 |
| 1:B:3432:LYS:NZ | 1:B:3432:LYS:CB | 2.73 | 0.52 |
| 1:B:3721:LEU:HA | 1:B:3724:ILE:HD12 | 1.91 | 0.52 |
| 2:C:722:GLN:O | 2:C:724:LEU:N | 2.42 | 0.52 |
| 6:F:151:GLY:H | 8:E:370:GLN:NE2 | 2.07 | 0.52 |
| 7:G:169:PHE:CE1 | 8:E:381:VAL:HG22 | 2.45 | 0.52 |
| 1:B:3246:PHE:CE2 | 1:B:3322:GLU:HA | 2.45 | 0.51 |
| 1:B:3706:LEU:CB | 1:B:3720:ILE:HG13 | 2.40 | 0.51 |
| 5:A:1027:LEU:O | 5:A:1030:LYS:N | 2.37 | 0.51 |
| 6:F:291:GLU:HG3 | 6:F:296:LYS:H | 1.75 | 0.51 |
| 7:G:208:ILE:HD12 | 7:G:208:ILE:H | 1.75 | 0.51 |
| 3:D:438:UNK:O | 6:F:266:ALA:N | 2.42 | 0.51 |
| 1:B:2659:GLU:HG2 | 1:B:2681:ARG:CB | 2.36 | 0.51 |
| 1:B:3020:ALA:CB | 1:B:3050:ASP:CB | 2.89 | 0.51 |
| 1:B:3418:ARG:CG | 1:B:3418:ARG:NH1 | 2.73 | 0.51 |
| 1:B:3492:LYS:N | 1:B:3492:LYS:CD | 2.73 | 0.51 |
| 1:B:3492:LYS:HD2 | 1:B:3492:LYS:H | 1.75 | 0.51 |
| 5:A:389:PRO:O | 5:A:390:LEU:C | 2.48 | 0.51 |
| 6:F:20:ASP:OD2 | 6:F:453:TRP:N | 2.43 | 0.51 |
| 6:F:151:GLY:O | 8:E:367:LYS:HE2 | 2.11 | 0.51 |
| 1:B:3551:GLN:O | 1:B:3553:SER:N | 2.43 | 0.51 |
| 2:C:739:SER:CA | 3:D:328:UNK:O | 2.58 | 0.51 |
| 3:D:414:UNK:C | 3:D:416:UNK:H | 2.22 | 0.51 |
| 5:A:958:GLN:O | 5:A:960:LEU:N | 2.43 | 0.51 |
| 1:B:2998:GLU:O | 1:B:2999:LEU:C | 2.48 | 0.51 |
| 5:A:348:LEU:O | 5:A:352:ARG:N | 2.36 | 0.51 |
| 5:A:1157:ILE:C | 5:A:1159:GLU:N | 2.60 | 0.51 |
| 5:A:2012:ASN:O | 5:A:2016:PHE:N | 2.43 | 0.51 |
| 6:F:48:THR:O | 6:F:50:ASP:N | 2.44 | 0.51 |
| 7:G:37:ARG:C | 7:G:65:LEU:HB3 | 2.31 | 0.51 |
| 1:B:2898:TRP:HE3 | 1:B:2898:TRP:C | 2.13 | 0.51 |
| 1:B:3171:LEU:O | 1:B:3174:THR:CB | 2.59 | 0.51 |
| 1:B:3464:PHE:HA | 1:B:3576:LYS:NZ | 2.26 | 0.51 |
| 1:B:3666:PHE:HA | 1:B:3669:ASP:OD2 | 2.10 | 0.51 |
| 5:A:972:LEU:O | 5:A:973:ASP:C | 2.47 | 0.51 |
| 5:A:1103:LEU:O | 5:A:1105:ASN:N | 2.40 | 0.51 |
| 7:G:9:VAL:HG13 | 7:G:104:LEU:HD23 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3097:ILE:N | 1:B:3097:ILE:CD1 | 2.73 | 0.51 |
| 1:B:3555:PHE:CD1 | 1:B:3581:VAL:HG11 | 2.45 | 0.51 |
| 5:A:957:ARG:O | 5:A:959:PHE:N | 2.44 | 0.51 |
| 5:A:2541:PHE:O | 5:A:2544:SER:N | 2.44 | 0.51 |
| 6:F:241:GLU:HA | 6:F:244:GLU:HG3 | 1.92 | 0.51 |
| 1:B:3444:ASN:ND2 | 1:B:3580:ASN:HD22 | 2.08 | 0.51 |
| 1:B:3461:SER:CB | 1:B:3464:PHE:CE2 | 2.94 | 0.51 |
| 1:B:3551:GLN:CD | 1:B:3580:ASN:HA | 2.31 | 0.51 |
| 5:A:978:ALA:O | 5:A:990:PRO:HA | 2.11 | 0.51 |
| 5:A:1867:LEU:O | 5:A:1871:PHE:N | 2.41 | 0.51 |
| 1:B:3071:GLU:O | 1:B:3072:PRO:C | 2.48 | 0.51 |
| 1:B:3242:ASP:O | 1:B:3245:LEU:N | 2.44 | 0.51 |
| 1:B:3504:PRO:O | 1:B:3507:THR:OG1 | 2.24 | 0.51 |
| 1:B:3576:LYS:HD3 | 1:B:3576:LYS:N | 2.20 | 0.51 |
| 6:F:24:TYR:CD2 | 6:F:25:THR:HG23 | 2.46 | 0.50 |
| 7:G:109:PRO:HD2 | 7:G:161:HIS:CD2 | 2.46 | 0.50 |
| 7:G:132:PHE:CG | 7:G:133:TYR:N | 2.78 | 0.50 |
| 7:G:313:MET:O | 7:G:317:ILE:HG12 | 2.11 | 0.50 |
| 1:B:3247:ARG:CG | 1:B:3248:LEU:N | 2.74 | 0.50 |
| 1:B:3474:PHE:CD2 | 1:B:3526:VAL:CB | 2.94 | 0.50 |
| 5:A:137:LEU:C | 5:A:139:SER:N | 2.63 | 0.50 |
| 5:A:328:LEU:O | 5:A:332:LEU:N | 2.39 | 0.50 |
| 6:F:48:THR:C | 6:F:50:ASP:H | 2.14 | 0.50 |
| 1:B:2639:ILE:O | 1:B:2643:ILE:N | 2.43 | 0.50 |
| 1:B:3462:VAL:C | 1:B:3464:PHE:N | 2.65 | 0.50 |
| 5:A:871:VAL:O | 5:A:874:PRO:N | 2.45 | 0.50 |
| 6:F:27:ASN:ND2 | 6:F:450:TYR:HA | 2.26 | 0.50 |
| 7:G:78:ASN:ND2 | 7:G:81:ASP:OD2 | 2.44 | 0.50 |
| 7:G:109:PRO:HG2 | 7:G:161:HIS:CD2 | 2.46 | 0.50 |
| 1:B:2633:TRP:CB | 5:A:2625:TYR:N | 2.75 | 0.50 |
| 1:B:2651:ASN:C | 1:B:2653:LYS:N | 2.64 | 0.50 |
| 5:A:425:GLU:O | 5:A:426:SER:CB | 2.60 | 0.50 |
| 6:F:187:GLY:O | 6:F:243:LYS:NZ | 2.44 | 0.50 |
| 5:A:511:ASP:O | 5:A:515:GLU:CA | 2.60 | 0.50 |
| 5:A:1441:LEU:O | 5:A:1445:PHE:CB | 2.59 | 0.50 |
| 1:B:2888:LEU:HA | 5:A:953:GLY:HA2 | 1.94 | 0.50 |
| 1:B:3668:ARG:HG2 | 1:B:3672:ILE:HG23 | 1.93 | 0.50 |
| 5:A:982:ILE:CB | 5:A:2481:ASN:N | 2.75 | 0.50 |
| 5:A:1038:ASN:O | 5:A:1039:TYR:C | 2.50 | 0.50 |
| 7:G:138:ALA:C | 7:G:165:ILE:CD1 | 2.80 | 0.50 |
| 7:G:208:ILE:HG12 | 7:G:243:PRO:HG3 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3068:LEU:HB2 | 1:B:3078:ALA:HB2 | 1.83 | 0.50 |
| 1:B:3106:TRP:HE3 | 1:B:3665:LEU:HD12 | 1.73 | 0.50 |
| 1:B:3574:VAL:HA | 1:B:3580:ASN:O | 2.12 | 0.50 |
| 1:B:3618:GLU:O | 1:B:3620:VAL:CA | 2.60 | 0.50 |
| 2:C:695:GLN:O | 2:C:699:ARG:HG2 | 2.11 | 0.50 |
| 3:D:11:UNK:O | 3:D:13:UNK:N | 2.44 | 0.50 |
| 5:A:2381:ALA:O | 5:A:2384:ILE:CB | 2.60 | 0.50 |
| 1:B:3171:LEU:O | 1:B:3174:THR:CA | 2.60 | 0.49 |
| 1:B:3474:PHE:CD1 | 1:B:3474:PHE:C | 2.85 | 0.49 |
| 6:F:412:GLY:O | 6:F:415:SER:OG | 2.28 | 0.49 |
| 7:G:345:ILE:O | 7:G:349:LEU:HG | 2.12 | 0.49 |
| 5:A:2260:ALA:O | 5:A:2261:TRP:C | 2.50 | 0.49 |
| 7:G:139:VAL:N | 7:G:165:ILE:CD1 | 2.75 | 0.49 |
| 7:G:155:SER:HA | 7:G:160:THR:HG23 | 1.93 | 0.49 |
| 1:B:2737:ALA:CB | 1:B:2746:LEU:HD11 | 2.42 | 0.49 |
| 1:B:2912:ILE:N | 1:B:2912:ILE:CD1 | 2.74 | 0.49 |
| 6:F:128:LEU:HD13 | 6:F:134:PHE:CE2 | 2.48 | 0.49 |
| 6:F:182:ARG:N | 6:F:388:LEU:HD11 | 2.26 | 0.49 |
| 7:G:275:ASP:OD2 | 7:G:316:GLU:HB3 | 2.12 | 0.49 |
| 7:G:360:GLN:O | 7:G:364:GLU:N | 2.45 | 0.49 |
| 2:C:690:ARG:HH12 | 2:C:763:ALA:HB1 | 1.78 | 0.49 |
| 4:H:185:LEU:O | 4:H:189:ARG:N | 2.32 | 0.49 |
| 7:G:125:GLU:HG3 | 7:G:362:TYR:OH | 2.13 | 0.49 |
| 1:B:3040:ASN:OD1 | 1:B:3060:TRP:HZ2 | 1.93 | 0.49 |
| 1:B:3424:ARG:NH2 | 1:B:3424:ARG:HG2 | 2.27 | 0.49 |
| 6:F:148:PHE:CD2 | 6:F:459:LEU:HD11 | 2.47 | 0.49 |
| 7:G:10:ILE:HG12 | 7:G:19:ALA:HB1 | 1.94 | 0.49 |
| 7:G:312:ARG:O | 7:G:316:GLU:HG2 | 2.12 | 0.49 |
| 1:B:2944:ALA:CA | 1:B:2970:ILE:CD1 | 2.88 | 0.49 |
| 1:B:3570:HIS:C | 1:B:3570:HIS:CD2 | 2.85 | 0.49 |
| 5:A:736:PHE:N | 5:A:1543:LEU:O | 2.46 | 0.49 |
| 5:A:1652:ILE:C | 5:A:1654:ASN:H | 2.15 | 0.49 |
| 6:F:58:SER:HB2 | 6:F:92:TRP:CH2 | 2.47 | 0.49 |
| 7:G:138:ALA:HB1 | 7:G:163:VAL:HG12 | 1.95 | 0.49 |
| 7:G:286:ASP:HB2 | 7:G:288:ASP:OD1 | 2.11 | 0.49 |
| 1:B:3393:ILE:CB | 1:B:3400:VAL:HA | 2.43 | 0.49 |
| 1:B:3407:TYR:N | 1:B:3408:PRO:HD3 | 2.20 | 0.49 |
| 1:B:3450:PRO:C | 1:B:3451:LEU:HD13 | 2.27 | 0.49 |
| 3:D:3:UNK:O | 3:D:7:UNK:N | 2.45 | 0.49 |
| 5:A:1745:LEU:O | 5:A:1749:ASP:N | 2.32 | 0.49 |
| 6:F:72:LYS:CD | 6:F:73:PRO:HD2 | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:122:LYS:HG2 | 6:F:484:LEU:HD11 | 1.94 | 0.49 |
| 1:B:2670:GLN:O | 1:B:2837:PRO:HB3 | 2.11 | 0.49 |
| 5:A:741:LEU:O | 5:A:744:LEU:N | 2.46 | 0.49 |
| 1:B:3474:PHE:CE2 | 1:B:3526:VAL:CB | 2.88 | 0.49 |
| 2:C:697:PHE:CD1 | 2:C:697:PHE:C | 2.85 | 0.49 |
| 6:F:118:THR:HA | 6:F:121:ARG:HD2 | 1.95 | 0.49 |
| 6:F:132:MET:HB2 | 6:F:134:PHE:CZ | 2.47 | 0.49 |
| 6:F:193:LEU:HD21 | 6:F:299:ASP:HB3 | 1.95 | 0.49 |
| 5:A:806:LEU:O | 5:A:809:PHE:N | 2.46 | 0.49 |
| 5:A:2169:TYR:O | 5:A:2173:LYS:N | 2.46 | 0.49 |
| 5:A:2539:SER:O | 5:A:2543:ASP:N | 2.30 | 0.49 |
| 6:F:205:PRO:HG3 | 6:F:230:TYR:CD1 | 2.48 | 0.49 |
| 7:G:349:LEU:HD13 | 8:E:394:TYR:CE2 | 2.48 | 0.49 |
| 1:B:3086:LEU:HA | 1:B:3104:ILE:HD12 | 1.94 | 0.48 |
| 1:B:3246:PHE:CD1 | 1:B:3246:PHE:C | 2.85 | 0.48 |
| 1:B:3559:SER:HG | 1:B:3560:TYR:N | 2.11 | 0.48 |
| 6:F:70:GLU:HB2 | 6:F:226:ASP:OD2 | 2.11 | 0.48 |
| 6:F:466:HIS:HA | 6:F:469:TRP:HD1 | 1.76 | 0.48 |
| 7:G:139:VAL:CA | 7:G:165:ILE:HD13 | 2.43 | 0.48 |
| 1:B:3697:ASP:O | 1:B:3701:ARG:HG3 | 2.13 | 0.48 |
| 3:D:215:UNK:O | 3:D:216:UNK:CB | 2.59 | 0.48 |
| 1:B:3143:SER:OG | 1:B:3204:PRO:CB | 2.61 | 0.48 |
| 2:C:763:ALA:O | 2:C:767:CYS:N | 2.42 | 0.48 |
| 6:F:297:GLU:O | 6:F:300:ILE:N | 2.44 | 0.48 |
| 1:B:3040:ASN:O | 1:B:3060:TRP:HZ2 | 1.95 | 0.48 |
| 1:B:3098:ARG:O | 1:B:3134:ILE:CB | 2.61 | 0.48 |
| 1:B:3360:LEU:CB | 1:B:3424:ARG:HH22 | 2.18 | 0.48 |
| 1:B:3372:ALA:HB3 | 1:B:3395:GLY:HA2 | 1.95 | 0.48 |
| 5:A:1012:HIS:C | 5:A:1014:ARG:N | 2.67 | 0.48 |
| 1:B:3503:ALA:O | 1:B:3506:MET:HB3 | 2.13 | 0.48 |
| 1:B:3674:TRP:CZ3 | 1:B:3678:LEU:HB2 | 2.48 | 0.48 |
| 6:F:145:CYS:O | 6:F:455:GLY:HA3 | 2.14 | 0.48 |
| 1:B:3068:LEU:CB | 1:B:3078:ALA:HA | 2.40 | 0.48 |
| 1:B:3649:SER:HB2 | 1:B:3704:ALA:C | 2.33 | 0.48 |
| 5:A:1962:THR:O | 5:A:1966:TRP:N | 2.31 | 0.48 |
| 7:G:124:PHE:HB2 | 7:G:362:TYR:CD2 | 2.48 | 0.48 |
| 7:G:336:LYS:HG2 | 7:G:337:TYR:CE1 | 2.48 | 0.48 |
| 1:B:3468:HIS:ND1 | 1:B:3569:PRO:HB2 | 2.28 | 0.48 |
| 5:A:1012:HIS:C | 5:A:1014:ARG:H | 2.15 | 0.48 |
| 7:G:101:HIS:O | 7:G:103:VAL:HG23 | 2.13 | 0.48 |
| 7:G:310:ALA:O | 7:G:313:MET:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2791:ARG:O | 1:B:2792:GLN:C | 2.51 | 0.48 |
| 1:B:3236:ARG:NE | 1:B:3338:CYS:CB | 2.76 | 0.48 |
| 1:B:3646:PHE:CB | 1:B:3720:ILE:CD1 | 2.92 | 0.48 |
| 7:G:312:ARG:O | 7:G:316:GLU:N | 2.28 | 0.48 |
| 8:E:357:THR:N | 8:E:361:ILE:HD12 | 2.29 | 0.48 |
| 1:B:3062:PHE:HZ | 1:B:3658:GLU:HA | 1.77 | 0.48 |
| 1:B:3650:ARG:O | 1:B:3654:GLU:N | 2.45 | 0.48 |
| 7:G:190:MET:SD | 7:G:203:THR:HG22 | 2.53 | 0.48 |
| 1:B:2663:LEU:HD13 | 1:B:2663:LEU:HA | 1.72 | 0.48 |
| 1:B:3509:LEU:HD12 | 1:B:3510:LYS:N | 2.28 | 0.48 |
| 3:D:2:UNK:CB | 3:D:16:UNK:HA | 2.44 | 0.48 |
| 3:D:162:UNK:O | 3:D:165:UNK:N | 2.47 | 0.48 |
| 6:F:118:THR:O | 6:F:121:ARG:HB2 | 2.13 | 0.48 |
| 5:A:2257:VAL:O | 5:A:2261:TRP:N | 2.41 | 0.47 |
| 6:F:190:ILE:HD11 | 6:F:292:LEU:HD11 | 1.96 | 0.47 |
| 6:F:444:HIS:O | 6:F:447:GLU:N | 2.47 | 0.47 |
| 6:F:447:GLU:HA | 6:F:450:TYR:CE1 | 2.49 | 0.47 |
| 7:G:355:MET:HA | 7:G:373:LYS:HZ1 | 1.80 | 0.47 |
| 7:G:371:HIS:O | 8:E:380:LYS:NZ | 2.33 | 0.47 |
| 1:B:2748:GLU:HB3 | 1:B:2752:HIS:NE2 | 2.29 | 0.47 |
| 5:A:1560:HIS:CB | 5:A:1598:ARG:CB | 2.92 | 0.47 |
| 5:A:1646:ASN:O | 5:A:1648:TYR:N | 2.47 | 0.47 |
| 7:G:261:LEU:HB3 | 7:G:274:ILE:HD13 | 1.96 | 0.47 |
| 1:B:3085:TYR:C | 1:B:3104:ILE:HD13 | 2.24 | 0.47 |
| 3:D:168:UNK:O | 3:D:169:UNK:C | 2.62 | 0.47 |
| 5:A:834:ILE:O | 5:A:838:LEU:N | 2.27 | 0.47 |
| 6:F:213:LYS:CB | 6:F:214:PRO:HD3 | 2.35 | 0.47 |
| 6:F:241:GLU:O | 6:F:244:GLU:HB2 | 2.14 | 0.47 |
| 6:F:244:GLU:HB3 | 7:G:287:VAL:CG1 | 2.44 | 0.47 |
| 1:B:3449:ILE:HG22 | 1:B:3451:LEU:HD11 | 1.97 | 0.47 |
| 2:C:695:GLN:O | 2:C:699:ARG:CD | 2.61 | 0.47 |
| 2:C:702:GLN:HA | 2:C:702:GLN:OE1 | 2.14 | 0.47 |
| 5:A:982:ILE:CB | 5:A:2481:ASN:HA | 2.42 | 0.47 |
| 6:F:36:PRO:HB3 | 6:F:453:TRP:CE2 | 2.48 | 0.47 |
| 6:F:174:MET:HA | 6:F:489[A]:ARG:HB3 | 1.95 | 0.47 |
| 6:F:432:LEU:HD21 | 6:F:435:LEU:HD22 | 1.96 | 0.47 |
| 7:G:72:GLU:HB2 | 7:G:77:THR:HG21 | 1.97 | 0.47 |
| 7:G:124:PHE:HB2 | 7:G:362:TYR:CE2 | 2.49 | 0.47 |
| 1:B:2898:TRP:C | 1:B:2898:TRP:CE3 | 2.88 | 0.47 |
| 1:B:2941:HIS:C | 1:B:2943:ILE:H | 2.18 | 0.47 |
| 1:B:3427:ASN:CA | 1:B:3443:PHE:HZ | 2.17 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3427:ASN:HD22 | 1:B:3428:LYS:H | 1.61 | 0.47 |
| 6:F:107:PRO:HB2 | 6:F:469:TRP:CH2 | 2.49 | 0.47 |
| 1:B:3491:ASP:HB3 | 1:B:3492:LYS:NZ | 2.30 | 0.47 |
| 1:B:3545:ARG:NH1 | 1:B:3633:GLY:HA2 | 2.29 | 0.47 |
| 5:A:1091:SER:HA | 5:A:1099:ALA:CA | 2.44 | 0.47 |
| 5:A:1417:LYS:HA | 5:A:1420:ALA:HB3 | 1.97 | 0.47 |
| 5:A:1581:GLU:O | 5:A:1585:ARG:CB | 2.63 | 0.47 |
| 7:G:351:THR:O | 7:G:354:GLN:HG2 | 2.15 | 0.47 |
| 8:E:392:LYS:O | 8:E:396:THR:HG23 | 2.15 | 0.47 |
| 1:B:2637:ILE:HA | 1:B:2640:LEU:HB3 | 1.95 | 0.47 |
| 1:B:2839:HIS:O | 1:B:2843:LEU:HG | 2.15 | 0.47 |
| 1:B:3481:ASP:CB | 1:B:3482:PRO:HD3 | 2.42 | 0.47 |
| 1:B:3658:GLU:O | 1:B:3662:TYR:N | 2.38 | 0.47 |
| 1:B:3699:ILE:O | 1:B:3702:LYS:N | 2.48 | 0.47 |
| 1:B:3721:LEU:HG | 1:B:3724:ILE:HD12 | 1.96 | 0.47 |
| 5:A:461:LYS:O | 5:A:465:MET:N | 2.32 | 0.47 |
| 5:A:1086:VAL:O | 5:A:1090:THR:N | 2.38 | 0.47 |
| 5:A:2352:ILE:O | 5:A:2356:SER:N | 2.46 | 0.47 |
| 6:F:442:THR:HG21 | 6:F:448:ARG:HG3 | 1.92 | 0.47 |
| 7:G:9:VAL:O | 7:G:20:GLY:N | 2.48 | 0.47 |
| 1:B:3065:ASP:O | 1:B:3068:LEU:HG | 2.14 | 0.47 |
| 1:B:3493:LEU:O | 1:B:3493:LEU:HD13 | 2.14 | 0.47 |
| 3:D:4:UNK:O | 3:D:8:UNK:N | 2.47 | 0.47 |
| 4:H:86:ASN:O | 4:H:89:PRO:N | 2.47 | 0.47 |
| 5:A:1201:CYS:C | 5:A:1203:ASP:H | 2.18 | 0.47 |
| 1:B:2969:ARG:O | 1:B:2969:ARG:HD3 | 2.15 | 0.47 |
| 1:B:3100:LEU:HD13 | 1:B:3101:LEU:HA | 1.97 | 0.47 |
| 1:B:3731:ARG:HB3 | 2:C:694:TRP:HE1 | 1.80 | 0.47 |
| 3:D:420:UNK:C | 3:D:422:UNK:N | 2.77 | 0.47 |
| 7:G:180:LEU:HD23 | 7:G:184:ASP:OD2 | 2.14 | 0.47 |
| 7:G:359:LYS:O | 7:G:362:TYR:HB3 | 2.15 | 0.47 |
| 1:B:3163:TYR:CB | 1:B:3167:LEU:HB3 | 2.45 | 0.47 |
| 5:A:31:LEU:O | 5:A:35:MET:N | 2.48 | 0.47 |
| 5:A:330:ILE:O | 5:A:334:GLN:CB | 2.63 | 0.47 |
| 8:E:391:ILE:CA | 8:E:394:TYR:HB2 | 2.32 | 0.47 |
| 1:B:2837:PRO:O | 1:B:2840:LYS:N | 2.47 | 0.46 |
| 1:B:3366:VAL:O | 1:B:3367:HIS:C | 2.51 | 0.46 |
| 1:B:3649:SER:HB2 | 1:B:3705:GLN:CA | 2.42 | 0.46 |
| 1:B:3668:ARG:NE | 1:B:3672:ILE:HD13 | 2.15 | 0.46 |
| 5:A:1043:LEU:O | 5:A:1046:ALA:N | 2.46 | 0.46 |
| 6:F:264:SER:O | 6:F:265:THR:OG1 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:82:MET:HG3 | 7:G:86:TRP:CZ2 | 2.50 | 0.46 |
| 1:B:3244:ASP:O | 1:B:3247:ARG:CD | 2.63 | 0.46 |
| 1:B:3740:PHE:CB | 1:B:3742:PRO:CD | 2.84 | 0.46 |
| 3:D:61:UNK:C | 3:D:63:UNK:N | 2.78 | 0.46 |
| 5:A:1036:PRO:O | 5:A:1039:TYR:N | 2.33 | 0.46 |
| 5:A:1345:LEU:CA | 5:A:1349:MET:CB | 2.92 | 0.46 |
| 5:A:2092:LEU:O | 5:A:2095:ALA:HB3 | 2.14 | 0.46 |
| 7:G:255:PHE:C | 7:G:258:PRO:HD2 | 2.35 | 0.46 |
| 1:B:2651:ASN:ND2 | 1:B:2651:ASN:N | 2.60 | 0.46 |
| 1:B:3496:ALA:CB | 2:C:684:TYR:CD1 | 2.98 | 0.46 |
| 1:B:3668:ARG:NE | 1:B:3672:ILE:HG21 | 2.29 | 0.46 |
| 6:F:152:ARG:HD3 | 6:F:407:ASN:OD1 | 2.15 | 0.46 |
| 4:H:183:LYS:O | 4:H:186:LYS:N | 2.49 | 0.46 |
| 5:A:981:LYS:CB | 5:A:988:ASP:HA | 2.44 | 0.46 |
| 5:A:1581:GLU:C | 5:A:1583:LYS:H | 2.17 | 0.46 |
| 1:B:3427:ASN:N | 1:B:3443:PHE:HZ | 2.09 | 0.46 |
| 1:B:3464:PHE:HA | 1:B:3576:LYS:HZ1 | 1.81 | 0.46 |
| 5:A:1003:ILE:CB | 5:A:1017:ALA:HB2 | 2.45 | 0.46 |
| 5:A:1948:VAL:O | 5:A:1952:VAL:N | 2.31 | 0.46 |
| 6:F:72:LYS:NZ | 6:F:72:LYS:CB | 2.73 | 0.46 |
| 6:F:110:LEU:HD23 | 6:F:111:THR:N | 2.31 | 0.46 |
| 6:F:285:ARG:HA | 6:F:288:PHE:CE2 | 2.50 | 0.46 |
| 7:G:14:SER:HB2 | 7:G:157:ASP:CB | 2.45 | 0.46 |
| 7:G:286:ASP:HB2 | 7:G:288:ASP:CG | 2.35 | 0.46 |
| 1:B:3107:LEU:HD12 | 1:B:3110:ILE:CD1 | 2.45 | 0.46 |
| 3:D:139:UNK:O | 6:F:178:LYS:HE3 | 2.16 | 0.46 |
| 5:A:1102:LEU:O | 5:A:1106:LEU:N | 2.38 | 0.46 |
| 6:F:241:GLU:HG3 | 6:F:244:GLU:OE1 | 2.15 | 0.46 |
| 7:G:101:HIS:O | 7:G:130:PRO:HD2 | 2.15 | 0.46 |
| 8:E:358:HIS:CG | 8:E:359:GLN:H | 2.34 | 0.46 |
| 3:D:102:UNK:C | 3:D:233:UNK:HA | 2.45 | 0.46 |
| 6:F:47:TYR:CD1 | 6:F:50:ASP:OD2 | 2.68 | 0.46 |
| 6:F:95:GLN:O | 6:F:99:TYR:HA | 2.16 | 0.46 |
| 7:G:277:THR:HA | 7:G:280:ASN:HD22 | 1.81 | 0.46 |
| 7:G:286:ASP:O | 7:G:290:ARG:NE | 2.49 | 0.46 |
| 1:B:2737:ALA:HB3 | 1:B:2746:LEU:HD11 | 1.98 | 0.46 |
| 1:B:3082:ILE:CB | 1:B:3108:ILE:HD11 | 2.46 | 0.46 |
| 5:A:1868:SER:O | 5:A:1872:ILE:N | 2.48 | 0.46 |
| 6:F:43:VAL:HG22 | 6:F:73:PRO:HA | 1.97 | 0.46 |
| 1:B:3242:ASP:O | 1:B:3243:GLU:C | 2.52 | 0.46 |
| 5:A:914:ASP:O | 5:A:916:ILE:N | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:1589:ASP:O | 5:A:1590:SER:C | 2.54 | 0.46 |
| 6:F:390:TYR:HD1 | 6:F:432:LEU:HD12 | 1.80 | 0.46 |
| 6:F:444:HIS:CE1 | 8:E:377:HIS:HE1 | 2.34 | 0.46 |
| 1:B:3505:ASP:HA | 1:B:3508:ILE:HD12 | 1.97 | 0.46 |
| 5:A:709:VAL:O | 5:A:713:MET:N | 2.49 | 0.46 |
| 5:A:1041:GLU:HA | 5:A:2514:VAL:CB | 2.46 | 0.46 |
| 7:G:33:SER:CB | 7:G:71:ILE:HG13 | 2.46 | 0.46 |
| 7:G:162:VAL:HG11 | 7:G:278:THR:HA | 1.98 | 0.46 |
| 8:E:378:LYS:O | 8:E:382:ALA:N | 2.42 | 0.46 |
| 1:B:2639:ILE:HA | 1:B:2642:SER:HB3 | 1.98 | 0.45 |
| 1:B:3404:ALA:CA | 1:B:3457:ILE:HG22 | 2.46 | 0.45 |
| 1:B:3555:PHE:CE1 | 1:B:3581:VAL:HG11 | 2.51 | 0.45 |
| 2:C:699:ARG:N | 2:C:699:ARG:CD | 2.73 | 0.45 |
| 5:A:2334:SER:O | 5:A:2338:LEU:N | 2.42 | 0.45 |
| 7:G:140:LEU:HD11 | 7:G:343:GLY:CA | 2.45 | 0.45 |
| 7:G:180:LEU:HD21 | 7:G:269:LEU:HD21 | 1.97 | 0.45 |
| 1:B:2957:HIS:HA | 1:B:3434:VAL:CB | 2.46 | 0.45 |
| 1:B:3068:LEU:CB | 1:B:3078:ALA:CA | 2.94 | 0.45 |
| 1:B:3496:ALA:HB3 | 1:B:3510:LYS:HZ2 | 1.81 | 0.45 |
| 7:G:99:GLU:C | 7:G:130:PRO:HD3 | 2.37 | 0.45 |
| 7:G:108:ALA:HB1 | 7:G:109:PRO:HD3 | 1.96 | 0.45 |
| 7:G:309:ILE:O | 7:G:313:MET:HG2 | 2.16 | 0.45 |
| 1:B:2675:PHE:O | 1:B:2675:PHE:CG | 2.69 | 0.45 |
| 6:F:10:GLY:C | 6:F:12:ASP:H | 2.19 | 0.45 |
| 6:F:443:GLY:O | 6:F:444:HIS:HD2 | 1.99 | 0.45 |
| 7:G:273:GLY:N | 7:G:276:GLN:HB3 | 2.31 | 0.45 |
| 6:F:122:LYS:HA | 6:F:125:LEU:HD12 | 1.98 | 0.45 |
| 7:G:360:GLN:O | 7:G:364:GLU:HG3 | 2.17 | 0.45 |
| 1:B:3060:TRP:O | 1:B:3061:GLY:C | 2.53 | 0.45 |
| 5:A:967:THR:O | 5:A:968:GLU:C | 2.55 | 0.45 |
| 5:A:1091:SER:CA | 5:A:1099:ALA:CA | 2.90 | 0.45 |
| 6:F:156:LEU:HD12 | 6:F:168:SER:O | 2.17 | 0.45 |
| 7:G:24:ASP:HB2 | 7:G:340:TRP:CH2 | 2.46 | 0.45 |
| 1:B:3731:ARG:CB | 2:C:694:TRP:HE1 | 2.29 | 0.45 |
| 1:B:3096:LYS:C | 1:B:3097:ILE:HD13 | 2.35 | 0.45 |
| 1:B:3236:ARG:HD2 | 1:B:3236:ARG:HA | 1.48 | 0.45 |
| 1:B:3296:PHE:O | 1:B:3296:PHE:CD1 | 2.70 | 0.45 |
| 1:B:3437:ARG:O | 1:B:3439:ARG:N | 2.50 | 0.45 |
| 1:B:3555:PHE:CZ | 1:B:3583:THR:HG21 | 2.52 | 0.45 |
| 3:D:310:UNK:O | 3:D:313:UNK:N | 2.49 | 0.45 |
| 5:A:1207:TYR:O | 5:A:1208:ASN:C | 2.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:272:SER:HB3 | 6:F:278:ILE:HG12 | 1.99 | 0.45 |
| 6:F:291:GLU:OE2 | 6:F:296:LYS:HB2 | 2.17 | 0.45 |
| 1:B:2874:ALA:C | 1:B:2876:GLU:H | 2.18 | 0.45 |
| 1:B:3467:LEU:C | 1:B:3467:LEU:CD1 | 2.86 | 0.45 |
| 1:B:3699:ILE:O | 1:B:3700:ILE:C | 2.55 | 0.45 |
| 5:A:580:ILE:C | 5:A:583:ALA:H | 2.19 | 0.45 |
| 6:F:216:PHE:CE2 | 6:F:218:LYS:HG3 | 2.52 | 0.45 |
| 7:G:124:PHE:HD1 | 7:G:359:LYS:HG2 | 1.82 | 0.45 |
| 7:G:143:TYR:CG | 8:E:391:ILE:HG21 | 2.51 | 0.45 |
| 8:E:366:ALA:C | 8:E:368:TRP:N | 2.70 | 0.45 |
| 1:B:3424:ARG:HH21 | 1:B:3424:ARG:CG | 2.30 | 0.45 |
| 1:B:3474:PHE:CE2 | 1:B:3526:VAL:CG1 | 2.92 | 0.45 |
| 2:C:704:ASN:CB | 2:C:711:ASP:HA | 2.46 | 0.45 |
| 3:D:420:UNK:O | 3:D:422:UNK:N | 2.50 | 0.45 |
| 5:A:239:LYS:O | 5:A:240:GLN:C | 2.47 | 0.45 |
| 5:A:1650:PHE:C | 5:A:1652:ILE:N | 2.70 | 0.45 |
| 5:A:1673:PHE:O | 5:A:1676:MET:N | 2.50 | 0.45 |
| 6:F:175:THR:N | 6:F:489[B]:ARG:HG2 | 2.31 | 0.45 |
| 6:F:406:HIS:CD2 | 6:F:406:HIS:O | 2.70 | 0.45 |
| 7:G:138:ALA:CA | 7:G:152:VAL:HG11 | 2.40 | 0.45 |
| 7:G:148:THR:HB | 8:E:388:ALA:HB1 | 1.99 | 0.45 |
| 7:G:346:LEU:HG | 7:G:352:PHE:CE2 | 2.52 | 0.45 |
| 1:B:2885:ARG:C | 1:B:2885:ARG:CD | 2.85 | 0.45 |
| 5:A:592:SER:O | 5:A:596:THR:N | 2.38 | 0.45 |
| 7:G:216:LEU:HD22 | 7:G:238:LYS:HD2 | 1.99 | 0.45 |
| 7:G:271:SER:OG | 7:G:272:ALA:N | 2.50 | 0.45 |
| 1:B:2821:ILE:HA | 1:B:2849:TYR:CZ | 2.52 | 0.44 |
| 1:B:3015:GLY:C | 1:B:3019:LYS:HB3 | 2.38 | 0.44 |
| 1:B:3159:ILE:O | 1:B:3163:TYR:CB | 2.65 | 0.44 |
| 1:B:3358:TYR:CG | 1:B:3358:TYR:O | 2.70 | 0.44 |
| 1:B:3100:LEU:HD13 | 1:B:3101:LEU:H | 1.67 | 0.44 |
| 1:B:3316:TYR:O | 1:B:3316:TYR:CD1 | 2.70 | 0.44 |
| 1:B:3592:PRO:CB | 1:B:3671:ILE:HB | 2.47 | 0.44 |
| 1:B:3649:SER:CB | 1:B:3705:GLN:CA | 2.82 | 0.44 |
| 3:D:38:UNK:O | 3:D:39:UNK:C | 2.65 | 0.44 |
| 3:D:373:UNK:H | 8:E:379:TYR:HE1 | 1.57 | 0.44 |
| 6:F:204:ILE:HD12 | 6:F:274:TRP:CD2 | 2.52 | 0.44 |
| 6:F:253:LYS:HB3 | 6:F:256:GLU:HG2 | 1.98 | 0.44 |
| 7:G:73:HIS:ND1 | 7:G:73:HIS:N | 2.64 | 0.44 |
| 7:G:81:ASP:O | 7:G:84:LYS:N | 2.51 | 0.44 |
| 1:B:2874:ALA:C | 1:B:2876:GLU:N | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2898:TRP:CE3 | 1:B:2898:TRP:O | 2.70 | 0.44 |
| 3:D:384:UNK:O | 3:D:386:UNK:N | 2.50 | 0.44 |
| 5:A:119:MET:O | 5:A:123:THR:N | 2.46 | 0.44 |
| 5:A:302:THR:C | 5:A:304:PHE:N | 2.71 | 0.44 |
| 6:F:127:VAL:HG12 | 6:F:128:LEU:HD23 | 1.99 | 0.44 |
| 1:B:2844:HIS:C | 1:B:2846:PHE:N | 2.70 | 0.44 |
| 1:B:3504:PRO:O | 1:B:3508:ILE:HG13 | 2.18 | 0.44 |
| 1:B:3617:ASN:O | 1:B:3618:GLU:C | 2.55 | 0.44 |
| 6:F:475:TYR:CD1 | 6:F:475:TYR:C | 2.85 | 0.44 |
| 1:B:2651:ASN:HD22 | 1:B:2651:ASN:N | 2.13 | 0.44 |
| 1:B:3424:ARG:HH11 | 1:B:3447:ILE:HA | 1.65 | 0.44 |
| 1:B:3439:ARG:HG3 | 1:B:3441:ILE:HG12 | 2.00 | 0.44 |
| 1:B:3570:HIS:O | 1:B:3570:HIS:CG | 2.70 | 0.44 |
| 4:H:183:LYS:O | 4:H:184:LEU:C | 2.56 | 0.44 |
| 5:A:2549:PHE:HZ | 5:A:2556:ILE:HA | 1.82 | 0.44 |
| 6:F:258:THR:HA | 6:F:261:GLU:HG2 | 1.99 | 0.44 |
| 7:G:187:ASP:OD1 | 7:G:206:ARG:NH1 | 2.51 | 0.44 |
| 7:G:210:ARG:O | 7:G:213:LYS:HB3 | 2.17 | 0.44 |
| 1:B:3106:TRP:CB | 1:B:3665:LEU:CD1 | 2.81 | 0.44 |
| 1:B:3172:ARG:NH2 | 1:B:3173:THR:HA | 2.32 | 0.44 |
| 5:A:1207:TYR:O | 5:A:1210:ARG:N | 2.51 | 0.44 |
| 6:F:57:PHE:CE1 | 6:F:89:GLN:HB2 | 2.53 | 0.44 |
| 6:F:400:LEU:O | 6:F:404:LEU:HG | 2.18 | 0.44 |
| 7:G:117:GLU:HG2 | 7:G:367:PRO:O | 2.17 | 0.44 |
| 7:G:230:ALA:CB | 7:G:252:ASN:HB3 | 2.47 | 0.44 |
| 2:C:688:ILE:HA | 2:C:691:ARG:HE | 1.82 | 0.44 |
| 5:A:1605:ASN:C | 5:A:1607:VAL:N | 2.71 | 0.44 |
| 5:A:1859:LEU:C | 5:A:1861:ARG:H | 2.20 | 0.44 |
| 6:F:18:VAL:O | 6:F:28:ILE:HG23 | 2.18 | 0.44 |
| 6:F:406:HIS:O | 6:F:406:HIS:CG | 2.70 | 0.44 |
| 7:G:16:MET:H | 7:G:16:MET:HE1 | 1.74 | 0.44 |
| 7:G:24:ASP:HB3 | 7:G:26:ALA:H | 1.83 | 0.44 |
| 1:B:2675:PHE:O | 1:B:2675:PHE:CD1 | 2.71 | 0.44 |
| 1:B:2843:LEU:O | 1:B:2846:PHE:N | 2.39 | 0.44 |
| 2:C:732:GLN:O | 2:C:734:GLN:N | 2.50 | 0.44 |
| 1:B:3068:LEU:HD12 | 1:B:3068:LEU:C | 2.39 | 0.44 |
| 1:B:3247:ARG:HH11 | 1:B:3407:TYR:CB | 2.29 | 0.44 |
| 1:B:3358:TYR:O | 1:B:3358:TYR:CD2 | 2.71 | 0.44 |
| 2:C:691:ARG:HG3 | 2:C:692:THR:N | 2.33 | 0.44 |
| 5:A:2389:SER:O | 5:A:2391:SER:N | 2.50 | 0.44 |
| 6:F:186:ALA:O | 6:F:189:PHE:N | 2.49 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:484:LEU:HA | 6:F:487:ARG:HH11 | 1.82 | 0.44 |
| 7:G:35:VAL:N | 7:G:68:ARG:O | 2.43 | 0.44 |
| 8:E:364:GLU:O | 8:E:368:TRP:HD1 | 2.01 | 0.44 |
| 1:B:3015:GLY:CA | 1:B:3019:LYS:HB3 | 2.48 | 0.43 |
| 1:B:3570:HIS:CD2 | 1:B:3570:HIS:O | 2.70 | 0.43 |
| 5:A:1038:ASN:O | 5:A:1041:GLU:N | 2.52 | 0.43 |
| 5:A:1653:SER:O | 5:A:1654:ASN:C | 2.56 | 0.43 |
| 6:F:267:LYS:HA | 6:F:282:ASN:HD21 | 1.83 | 0.43 |
| 8:E:375:GLU:O | 8:E:378:LYS:N | 2.51 | 0.43 |
| 4:H:193:LEU:O | 4:H:196:LEU:N | 2.46 | 0.43 |
| 5:A:2243:ILE:CB | 5:A:2252:SER:CA | 2.94 | 0.43 |
| 6:F:390:TYR:CD1 | 6:F:432:LEU:HD12 | 2.53 | 0.43 |
| 7:G:257:ALA:HB3 | 7:G:258:PRO:HD3 | 2.00 | 0.43 |
| 1:B:3552:TYR:O | 1:B:3552:TYR:CD1 | 2.70 | 0.43 |
| 2:C:712:LEU:O | 2:C:716:ARG:CB | 2.66 | 0.43 |
| 5:A:838:LEU:O | 5:A:842:LEU:N | 2.49 | 0.43 |
| 7:G:253:GLU:HG2 | 7:G:256:ARG:HD3 | 2.00 | 0.43 |
| 7:G:326:LYS:HE3 | 7:G:328:LYS:HD2 | 2.01 | 0.43 |
| 1:B:3070:GLU:OE1 | 1:B:3070:GLU:HA | 2.18 | 0.43 |
| 1:B:3451:LEU:CD1 | 1:B:3451:LEU:N | 2.73 | 0.43 |
| 2:C:670:GLU:O | 2:C:674:ALA:N | 2.37 | 0.43 |
| 3:D:150:UNK:O | 3:D:152:UNK:N | 2.51 | 0.43 |
| 6:F:177:SER:HA | 6:F:180:THR:HG23 | 2.00 | 0.43 |
| 6:F:244:GLU:HB3 | 7:G:287:VAL:HG11 | 1.99 | 0.43 |
| 7:G:18:LYS:HE3 | 7:G:337:TYR:CD1 | 2.53 | 0.43 |
| 7:G:130:PRO:HA | 7:G:359:LYS:HZ3 | 1.83 | 0.43 |
| 7:G:140:LEU:CD1 | 7:G:343:GLY:CA | 2.96 | 0.43 |
| 1:B:3085:TYR:CB | 1:B:3104:ILE:HD13 | 2.48 | 0.43 |
| 1:B:3253:LEU:CD1 | 1:B:3318:ARG:HB2 | 2.45 | 0.43 |
| 1:B:3411:ARG:O | 1:B:3415:ARG:CB | 2.66 | 0.43 |
| 1:B:3546:LYS:NZ | 1:B:3550:SER:HB2 | 2.34 | 0.43 |
| 2:C:649:ILE:O | 2:C:652:SER:N | 2.51 | 0.43 |
| 3:D:79:UNK:C | 3:D:80:UNK:O | 2.59 | 0.43 |
| 5:A:1044:LYS:C | 5:A:1046:ALA:H | 2.22 | 0.43 |
| 5:A:1044:LYS:O | 5:A:1046:ALA:N | 2.52 | 0.43 |
| 5:A:1255:ALA:O | 5:A:1256:ILE:C | 2.56 | 0.43 |
| 6:F:82:ASP:OD2 | 6:F:85:THR:OG1 | 2.34 | 0.43 |
| 7:G:137:GLN:HG3 | 7:G:339:VAL:CG1 | 2.48 | 0.43 |
| 7:G:223:PHE:HD1 | 7:G:259:GLU:HG3 | 1.84 | 0.43 |
| 3:D:11:UNK:C | 3:D:13:UNK:N | 2.82 | 0.43 |
| 5:A:2526:HIS:O | 5:A:2530:MET:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:180:THR:O | 6:F:181:ARG:NH1 | 2.42 | 0.43 |
| 8:E:377:HIS:O | 8:E:381:VAL:HG23 | 2.19 | 0.43 |
| 1:B:2898:TRP:CZ3 | 1:B:2902:VAL:HG21 | 2.53 | 0.43 |
| 1:B:3108:ILE:HD12 | 1:B:3108:ILE:HA | 1.74 | 0.43 |
| 1:B:3443:PHE:CD1 | 1:B:3443:PHE:N | 2.73 | 0.43 |
| 1:B:3733:LEU:HD21 | 1:B:3742:PRO:HG2 | 2.00 | 0.43 |
| 6:F:94:LEU:O | 6:F:99:TYR:N | 2.52 | 0.43 |
| 7:G:253:GLU:HA | 7:G:256:ARG:HB2 | 2.00 | 0.43 |
| 1:B:3488:PHE:CE1 | 1:B:3492:LYS:HG2 | 2.54 | 0.43 |
| 1:B:3493:LEU:C | 1:B:3493:LEU:CD1 | 2.86 | 0.43 |
| 2:C:679:ARG:C | 2:C:681:THR:H | 2.22 | 0.43 |
| 6:F:48:THR:C | 6:F:50:ASP:N | 2.71 | 0.43 |
| 6:F:413:GLY:HA3 | 6:F:449:GLN:NE2 | 2.33 | 0.43 |
| 7:G:107:GLU:HB2 | 7:G:111:ASN:ND2 | 2.32 | 0.43 |
| 1:B:3668:ARG:O | 1:B:3671:ILE:HG13 | 2.18 | 0.43 |
| 5:A:1988:PHE:O | 5:A:1991:SER:N | 2.42 | 0.43 |
| 5:A:2168:LEU:O | 5:A:2172:PHE:N | 2.49 | 0.43 |
| 6:F:128:LEU:HD13 | 6:F:134:PHE:CD2 | 2.53 | 0.43 |
| 6:F:302:ALA:C | 6:F:304:TRP:H | 2.22 | 0.43 |
| 6:F:416:SER:HA | 6:F:448:ARG:NH1 | 2.34 | 0.43 |
| 6:F:462:LEU:HD23 | 6:F:462:LEU:HA | 1.84 | 0.43 |
| 1:B:2898:TRP:HE3 | 1:B:2898:TRP:O | 2.00 | 0.43 |
| 1:B:2947:ILE:CB | 1:B:2970:ILE:HD12 | 2.49 | 0.43 |
| 1:B:3394:ARG:CA | 1:B:3398:GLY:HA2 | 2.49 | 0.43 |
| 5:A:1417:LYS:O | 5:A:1421:ILE:N | 2.51 | 0.43 |
| 5:A:1986:TYR:HA | 5:A:1989:LEU:CB | 2.49 | 0.43 |
| 6:F:440:LEU:HD13 | 6:F:440:LEU:HA | 1.75 | 0.43 |
| 7:G:116:ARG:HG2 | 7:G:370:VAL:HG21 | 2.01 | 0.43 |
| 1:B:3062:PHE:CZ | 1:B:3658:GLU:HA | 2.50 | 0.42 |
| 5:A:21:LEU:O | 5:A:25:TYR:N | 2.44 | 0.42 |
| 6:F:40:LEU:HB3 | 6:F:89:GLN:HE21 | 1.84 | 0.42 |
| 6:F:116:ASN:OD1 | 6:F:120:ASN:HB2 | 2.19 | 0.42 |
| 7:G:103:VAL:O | 7:G:132:PHE:HD1 | 2.02 | 0.42 |
| 7:G:151:ILE:CG2 | 7:G:297:ILE:CG1 | 2.95 | 0.42 |
| 6:F:10:GLY:HA2 | 6:F:463:GLY:N | 2.34 | 0.42 |
| 6:F:272:SER:HB3 | 6:F:278:ILE:CG1 | 2.49 | 0.42 |
| 1:B:2966:GLN:OE1 | 1:B:2966:GLN:HA | 2.19 | 0.42 |
| 1:B:3493:LEU:CD1 | 1:B:3497:HIS:HB2 | 2.49 | 0.42 |
| 7:G:70:PRO:HG2 | 7:G:85:ILE:HD11 | 2.01 | 0.42 |
| 1:B:2844:HIS:HA | 1:B:2847:GLN:CB | 2.47 | 0.42 |
| 1:B:3168:HIS:ND1 | 1:B:3168:HIS:C | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3296:PHE:CD1 | 1:B:3296:PHE:C | 2.92 | 0.42 |
| 1:B:3667:ILE:HG21 | 1:B:3696:VAL:CB | 2.49 | 0.42 |
| 6:F:56:ILE:HD12 | 6:F:56:ILE:HA | 1.68 | 0.42 |
| 6:F:87:GLN:O | 6:F:132:MET:HE1 | 2.11 | 0.42 |
| 7:G:105:LEU:HD13 | 7:G:132:PHE:CE1 | 2.54 | 0.42 |
| 7:G:255:PHE:O | 7:G:259:GLU:HG2 | 2.19 | 0.42 |
| 1:B:2648:SER:O | 1:B:2649:ILE:CB | 2.68 | 0.42 |
| 5:A:369:TYR:O | 5:A:372:ASP:N | 2.52 | 0.42 |
| 5:A:1249:GLN:C | 5:A:1251:GLU:H | 2.14 | 0.42 |
| 5:A:1581:GLU:O | 5:A:1585:ARG:N | 2.53 | 0.42 |
| 6:F:2:SER:HB2 | 7:G:371:HIS:O | 2.19 | 0.42 |
| 6:F:238:PHE:HZ | 6:F:278:ILE:HG21 | 1.85 | 0.42 |
| 7:G:102:PRO:HA | 7:G:131:ALA:O | 2.20 | 0.42 |
| 1:B:2761:GLU:O | 1:B:2765:ARG:N | 2.52 | 0.42 |
| 1:B:3163:TYR:CB | 1:B:3167:LEU:CB | 2.98 | 0.42 |
| 1:B:3247:ARG:O | 1:B:3251:VAL:HG23 | 2.18 | 0.42 |
| 1:B:3418:ARG:HA | 1:B:3418:ARG:HD3 | 1.26 | 0.42 |
| 1:B:3462:VAL:O | 1:B:3464:PHE:CG | 2.72 | 0.42 |
| 2:C:691:ARG:O | 2:C:695:GLN:HG3 | 2.20 | 0.42 |
| 4:H:223:ASP:O | 4:H:227:GLU:N | 2.44 | 0.42 |
| 1:B:2635:GLN:N | 1:B:2635:GLN:CD | 2.72 | 0.42 |
| 1:B:2885:ARG:HD3 | 1:B:2886:ASP:N | 2.34 | 0.42 |
| 1:B:3512:GLU:O | 1:B:3515:ASN:HB3 | 2.19 | 0.42 |
| 1:B:3724:ILE:O | 1:B:3727:ALA:N | 2.50 | 0.42 |
| 2:C:649:ILE:O | 2:C:653:GLU:N | 2.49 | 0.42 |
| 3:D:424:UNK:O | 3:D:425:UNK:C | 2.67 | 0.42 |
| 5:A:1345:LEU:O | 5:A:1349:MET:CB | 2.67 | 0.42 |
| 6:F:175:THR:O | 6:F:489[B]:ARG:NH2 | 2.48 | 0.42 |
| 6:F:243:LYS:HG2 | 6:F:247:CYS:SG | 2.59 | 0.42 |
| 6:F:287:GLY:HA2 | 6:F:290:GLU:HB3 | 2.01 | 0.42 |
| 6:F:437:PHE:CD1 | 6:F:437:PHE:N | 2.86 | 0.42 |
| 7:G:174:ALA:O | 7:G:281:SER:OG | 2.34 | 0.42 |
| 7:G:230:ALA:HB2 | 7:G:252:ASN:HB3 | 2.02 | 0.42 |
| 4:H:186:LYS:O | 4:H:190:ASP:N | 2.51 | 0.42 |
| 6:F:62:ILE:HG12 | 6:F:71:LEU:CD2 | 2.49 | 0.42 |
| 6:F:484:LEU:O | 6:F:487:ARG:HG2 | 2.19 | 0.42 |
| 7:G:355:MET:HA | 7:G:373:LYS:NZ | 2.34 | 0.42 |
| 1:B:3101:LEU:C | 1:B:3101:LEU:CD1 | 2.86 | 0.42 |
| 1:B:3360:LEU:CB | 1:B:3424:ARG:HG2 | 2.50 | 0.42 |
| 6:F:19:ILE:HA | 6:F:28:ILE:HG12 | 2.02 | 0.42 |
| 6:F:213:LYS:CA | 6:F:213:LYS:CE | 2.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3106:TRP:CH2 | 1:B:3668:ARG:CZ | 3.00 | 0.42 |
| 1:B:3492:LYS:O | 1:B:3510:LYS:HE2 | 2.20 | 0.42 |
| 3:D:396:UNK:CA | 6:F:436:LYS:HE3 | 2.48 | 0.42 |
| 5:A:2180:ILE:O | 5:A:2184:LEU:N | 2.52 | 0.42 |
| 6:F:30:TYR:HB2 | 7:G:113:LYS:HE3 | 2.02 | 0.42 |
| 7:G:133:TYR:CZ | 7:G:374:CYS:HA | 2.54 | 0.42 |
| 1:B:2778:GLN:O | 1:B:2782:SER:N | 2.30 | 0.41 |
| 1:B:3719:PHE:HA | 1:B:3722:ASP:CB | 2.49 | 0.41 |
| 1:B:3720:ILE:O | 1:B:3723:CYS:N | 2.52 | 0.41 |
| 6:F:164:THR:HG22 | 6:F:184:PHE:CD1 | 2.54 | 0.41 |
| 7:G:109:PRO:CD | 7:G:161:HIS:CD2 | 3.03 | 0.41 |
| 7:G:163:VAL:HA | 7:G:164:PRO:HD3 | 1.65 | 0.41 |
| 1:B:3229:LEU:C | 1:B:3229:LEU:CD1 | 2.85 | 0.41 |
| 1:B:3354:ILE:CA | 1:B:3371:ILE:H | 2.22 | 0.41 |
| 1:B:3540:ASP:HA | 1:B:3543:LEU:HD13 | 2.02 | 0.41 |
| 5:A:1300:ASN:C | 5:A:1302:LYS:N | 2.56 | 0.41 |
| 6:F:151:GLY:N | 8:E:370:GLN:OE1 | 2.53 | 0.41 |
| 6:F:213:LYS:CG | 6:F:214:PRO:HD3 | 2.50 | 0.41 |
| 7:G:149:THR:HG21 | 7:G:292:GLU:OE1 | 2.19 | 0.41 |
| 7:G:151:ILE:HD12 | 7:G:152:VAL:N | 2.36 | 0.41 |
| 7:G:180:LEU:HD21 | 7:G:269:LEU:HD11 | 2.01 | 0.41 |
| 2:C:694:TRP:HA | 2:C:697:PHE:CD2 | 2.53 | 0.41 |
| 5:A:580:ILE:HA | 5:A:583:ALA:HB3 | 2.01 | 0.41 |
| 5:A:1673:PHE:O | 5:A:1674:ASN:C | 2.58 | 0.41 |
| 6:F:122:LYS:HA | 6:F:125:LEU:CD1 | 2.50 | 0.41 |
| 8:E:361:ILE:HA | 8:E:364:GLU:CD | 2.41 | 0.41 |
| 1:B:2690:ILE:C | 1:B:3715:VAL:CB | 2.89 | 0.41 |
| 1:B:3068:LEU:HB3 | 1:B:3078:ALA:CB | 2.44 | 0.41 |
| 4:H:59:LEU:O | 4:H:63:ARG:N | 2.54 | 0.41 |
| 6:F:110:LEU:HD13 | 6:F:124:SER:HB3 | 2.01 | 0.41 |
| 7:G:190:MET:SD | 7:G:206:ARG:NE | 2.93 | 0.41 |
| 1:B:2663:LEU:HD21 | 1:B:2678:LEU:CB | 2.50 | 0.41 |
| 1:B:3553:SER:O | 1:B:3555:PHE:N | 2.54 | 0.41 |
| 5:A:635:LYS:O | 5:A:636:ASP:C | 2.58 | 0.41 |
| 5:A:1222:ASN:O | 5:A:1223:VAL:C | 2.58 | 0.41 |
| 5:A:1581:GLU:C | 5:A:1583:LYS:N | 2.74 | 0.41 |
| 5:A:2036:LEU:O | 5:A:2037:TYR:C | 2.59 | 0.41 |
| 6:F:6:LEU:HA | 6:F:6:LEU:HD23 | 1.84 | 0.41 |
| 6:F:71:LEU:CD1 | 6:F:229:LEU:HA | 2.50 | 0.41 |
| 6:F:213:LYS:HG3 | 6:F:214:PRO:HD3 | 2.02 | 0.41 |
| 6:F:434:SER:O | 6:F:435:LEU:HD12 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:487:ARG:HA | 6:F:487:ARG:NE | 2.36 | 0.41 |
| 1:B:2634:TYR:HD1 | 1:B:2634:TYR:H | 1.66 | 0.41 |
| 1:B:3316:TYR:CD1 | 1:B:3316:TYR:C | 2.90 | 0.41 |
| 1:B:3418:ARG:HB2 | 1:B:3418:ARG:NH1 | 2.24 | 0.41 |
| 1:B:3663:LEU:O | 1:B:3667:ILE:HG23 | 2.20 | 0.41 |
| 2:C:701:VAL:HG13 | 2:C:711:ASP:CB | 2.51 | 0.41 |
| 6:F:61:SER:OG | 7:G:270:GLU:O | 2.25 | 0.41 |
| 7:G:8:LEU:HD13 | 7:G:10:ILE:HD11 | 2.03 | 0.41 |
| 7:G:18:LYS:HA | 7:G:30:VAL:HA | 2.02 | 0.41 |
| 7:G:351:THR:HG22 | 7:G:354:GLN:NE2 | 2.36 | 0.41 |
| 8:E:390:ALA:HB1 | 8:E:394:TYR:CE2 | 2.55 | 0.41 |
| 1:B:3249:ILE:O | 1:B:3253:LEU:HG | 2.21 | 0.41 |
| 1:B:3492:LYS:O | 1:B:3510:LYS:CE | 2.68 | 0.41 |
| 5:A:1286:GLU:O | 5:A:1290:THR:N | 2.34 | 0.41 |
| 6:F:105:GLY:O | 6:F:106:ILE:HD13 | 2.21 | 0.41 |
| 7:G:18:LYS:HB3 | 7:G:30:VAL:HG22 | 2.02 | 0.41 |
| 1:B:2654:ILE:HD12 | 1:B:2654:ILE:HA | 1.81 | 0.41 |
| 1:B:3220:PRO:C | 1:B:3222:LEU:H | 2.24 | 0.41 |
| 5:A:566:TYR:C | 5:A:568:PRO:N | 2.73 | 0.41 |
| 6:F:304:TRP:O | 6:F:306:ARG:HG3 | 2.21 | 0.41 |
| 7:G:163:VAL:HG22 | 7:G:175:ILE:HG13 | 1.67 | 0.41 |
| 1:B:3068:LEU:HD22 | 1:B:3078:ALA:O | 2.20 | 0.41 |
| 1:B:3464:PHE:CD2 | 1:B:3575:ASP:CB | 3.04 | 0.41 |
| 1:B:3666:PHE:O | 1:B:3669:ASP:N | 2.54 | 0.41 |
| 3:D:442:UNK:O | 3:D:443:UNK:C | 2.69 | 0.41 |
| 5:A:137:LEU:O | 5:A:140:PHE:N | 2.51 | 0.41 |
| 5:A:1044:LYS:O | 5:A:1045:THR:C | 2.58 | 0.41 |
| 5:A:1262:LYS:O | 5:A:1265:ILE:N | 2.54 | 0.41 |
| 6:F:397:ASP:O | 6:F:401:ARG:HG3 | 2.21 | 0.41 |
| 7:G:124:PHE:CD1 | 7:G:359:LYS:HG2 | 2.56 | 0.41 |
| 7:G:149:THR:HG22 | 7:G:150:GLY:N | 2.36 | 0.41 |
| 8:E:361:ILE:HA | 8:E:364:GLU:OE1 | 2.21 | 0.41 |
| 8:E:384:CYS:O | 8:E:387:MET:HB2 | 2.20 | 0.41 |
| 1:B:2849:TYR:HA | 1:B:2852:PHE:CB | 2.50 | 0.41 |
| 1:B:3078:ALA:O | 1:B:3081:ALA:HB3 | 2.21 | 0.41 |
| 1:B:3360:LEU:CB | 1:B:3424:ARG:CG | 2.99 | 0.41 |
| 1:B:3551:GLN:HA | 1:B:3554:SER:HG | 1.86 | 0.41 |
| 3:D:418:UNK:C | 3:D:420:UNK:N | 2.83 | 0.41 |
| 7:G:9:VAL:HG12 | 7:G:340:TRP:CD1 | 2.55 | 0.41 |
| 1:B:3038:GLU:N | 1:B:3038:GLU:CD | 2.73 | 0.40 |
| 1:B:3236:ARG:CD | 1:B:3338:CYS:CB | 2.95 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:996:GLY:C | 5:A:998:GLN:N | 2.73 | 0.40 |
| 1:B:3435:GLU:N | 1:B:3435:GLU:CD | 2.73 | 0.40 |
| 5:A:890:TYR:O | 5:A:892:ASP:N | 2.54 | 0.40 |
| 6:F:23:SER:HB3 | 6:F:163:ASP:H | 1.85 | 0.40 |
| 6:F:94:LEU:HA | 6:F:98:LEU:HB2 | 2.02 | 0.40 |
| 6:F:463:GLY:O | 6:F:466:HIS:HD2 | 2.04 | 0.40 |
| 7:G:27:PRO:HA | 7:G:340:TRP:CZ2 | 2.56 | 0.40 |
| 1:B:3136:PHE:O | 1:B:3141:LEU:N | 2.54 | 0.40 |
| 1:B:3733:LEU:HD23 | 1:B:3733:LEU:O | 2.21 | 0.40 |
| 5:A:1295:GLU:O | 5:A:1356:ALA:CB | 2.68 | 0.40 |
| 1:B:2941:HIS:C | 1:B:2943:ILE:N | 2.74 | 0.40 |
| 1:B:3391:LEU:C | 1:B:3402:SER:CB | 2.87 | 0.40 |
| 1:B:3559:SER:HG | 1:B:3560:TYR:H | 1.67 | 0.40 |
| 5:A:2517:LEU:O | 5:A:2519:LEU:N | 2.54 | 0.40 |
| 6:F:466:HIS:CG | 6:F:467:GLN:N | 2.90 | 0.40 |
| 7:G:310:ALA:O | 7:G:314:GLN:N | 2.36 | 0.40 |
| 1:B:2819:GLU:C | 1:B:2821:ILE:N | 2.75 | 0.40 |
| 1:B:3071:GLU:O | 1:B:3071:GLU:HG2 | 2.21 | 0.40 |
| 1:B:3486:GLN:NE2 | 1:B:3486:GLN:C | 2.73 | 0.40 |
| 1:B:3544:PHE:CE1 | 1:B:3579:GLY:HA2 | 2.52 | 0.40 |
| 1:B:3661:THR:HA | 1:B:3664:ALA:HB2 | 2.04 | 0.40 |
| 1:B:3668:ARG:O | 1:B:3671:ILE:N | 2.52 | 0.40 |
| 4:H:183:LYS:O | 4:H:185:LEU:N | 2.54 | 0.40 |
| 5:A:1103:LEU:C | 5:A:1105:ASN:N | 2.74 | 0.40 |
| 7:G:103:VAL:O | 7:G:356:TRP:HZ3 | 2.05 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | B | 935/1115 (84%) | 658 (70%) | 205 (22%) | 72 (8%) | 1 15 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | C | 136/336 (40%) | 99 (73%) | 24 (18%) | 13 (10%) | 0 11 |
| 4 | H | 136/279 (49%) | 120 (88%) | 14 (10%) | 2 (2%) | 10 46 |
| 5 | A | 1857/2627 (71%) | 1494 (80%) | 251 (14%) | 112 (6%) | 1 19 |
| 6 | F | 417/490 (85%) | 350 (84%) | 62 (15%) | 5 (1%) | 13 50 |
| 7 | G | 345/375 (92%) | 311 (90%) | 32 (9%) | 2 (1%) | 25 65 |
| 8 | E | 39/41 (95%) | 29 (74%) | 10 (26%) | 0 | 100 100 |
| All | All | 3865/5263 (73%) | 3061 (79%) | 598 (16%) | 206 (5%) | 3 21 |

All (206) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 2649 | ILE |
| 1 | B | 2652 | THR |
| 1 | B | 2787 | PRO |
| 1 | B | 2788 | THR |
| 1 | B | 3056 | ALA |
| 1 | B | 3117 | LEU |
| 1 | B | 3164 | PRO |
| 1 | B | 3223 | ALA |
| 1 | B | 3242 | ASP |
| 1 | B | 3293 | ARG |
| 1 | B | 3367 | HIS |
| 1 | B | 3401 | HIS |
| 1 | B | 3407 | TYR |
| 1 | B | 3453 | PRO |
| 1 | B | 3463 | SER |
| 1 | B | 3480 | PHE |
| 1 | B | 3481 | ASP |
| 1 | B | 3552 | TYR |
| 1 | B | 3592 | PRO |
| 1 | B | 3598 | PRO |
| 1 | B | 3657 | ASN |
| 1 | B | 3704 | ALA |
| 1 | B | 3742 | PRO |
| 2 | C | 674 | ALA |
| 2 | C | 678 | HIS |
| 2 | C | 714 | GLY |
| 2 | C | 715 | PRO |
| 2 | C | 716 | ARG |
| 2 | C | 739 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 740 | PRO |
| 5 | A | 138 | ASP |
| 5 | A | 218 | MET |
| 5 | A | 231 | MET |
| 5 | A | 240 | GLN |
| 5 | A | 245 | SER |
| 5 | A | 303 | SER |
| 5 | A | 411 | ILE |
| 5 | A | 425 | GLU |
| 5 | A | 431 | VAL |
| 5 | A | 517 | PHE |
| 5 | A | 567 | ALA |
| 5 | A | 777 | PRO |
| 5 | A | 866 | PRO |
| 5 | A | 924 | VAL |
| 5 | A | 958 | GLN |
| 5 | A | 962 | PRO |
| 5 | A | 963 | PRO |
| 5 | A | 968 | GLU |
| 5 | A | 970 | THR |
| 5 | A | 973 | ASP |
| 5 | A | 977 | ILE |
| 5 | A | 994 | THR |
| 5 | A | 997 | ILE |
| 5 | A | 1035 | PHE |
| 5 | A | 1069 | LYS |
| 5 | A | 1094 | GLU |
| 5 | A | 1098 | ASP |
| 5 | A | 1153 | LEU |
| 5 | A | 1158 | PRO |
| 5 | A | 1223 | VAL |
| 5 | A | 1250 | SER |
| 5 | A | 1293 | VAL |
| 5 | A | 1301 | PRO |
| 5 | A | 1346 | PRO |
| 5 | A | 1362 | SER |
| 5 | A | 1364 | PRO |
| 5 | A | 1373 | GLU |
| 5 | A | 1507 | LEU |
| 5 | A | 1591 | PRO |
| 5 | A | 1605 | ASN |
| 5 | A | 1630 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 1651 | TYR |
| 5 | A | 1860 | PHE |
| 5 | A | 2369 | VAL |
| 5 | A | 2419 | PRO |
| 5 | A | 2497 | PRO |
| 5 | A | 2506 | GLU |
| 5 | A | 2568 | TYR |
| 5 | A | 2572 | PRO |
| 6 | F | 49 | ALA |
| 6 | F | 213 | LYS |
| 6 | F | 445 | THR |
| 7 | G | 16 | MET |
| 1 | B | 2997 | ASN |
| 1 | B | 3368 | PHE |
| 1 | B | 3388 | TYR |
| 1 | B | 3394 | ARG |
| 1 | B | 3403 | PHE |
| 1 | B | 3455 | VAL |
| 1 | B | 3568 | THR |
| 1 | B | 3595 | ARG |
| 5 | A | 572 | LEU |
| 5 | A | 959 | PHE |
| 5 | A | 976 | ALA |
| 5 | A | 980 | PHE |
| 5 | A | 1011 | ILE |
| 5 | A | 1033 | ALA |
| 5 | A | 1037 | THR |
| 5 | A | 1091 | SER |
| 5 | A | 1295 | GLU |
| 5 | A | 1653 | SER |
| 5 | A | 2384 | ILE |
| 5 | A | 2401 | LEU |
| 5 | A | 2491 | ILE |
| 1 | B | 2823 | LEU |
| 1 | B | 3115 | GLY |
| 1 | B | 3149 | ALA |
| 1 | B | 3150 | ASN |
| 1 | B | 3366 | VAL |
| 1 | B | 3482 | PRO |
| 1 | B | 3590 | ARG |
| 1 | B | 3599 | LEU |
| 1 | B | 3619 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 3707 | GLY |
| 1 | B | 3709 | LEU |
| 1 | B | 3717 | THR |
| 1 | B | 3737 | ASP |
| 1 | B | 3743 | TRP |
| 2 | C | 680 | LEU |
| 2 | C | 718 | HIS |
| 2 | C | 719 | SER |
| 4 | H | 131 | MET |
| 5 | A | 389 | PRO |
| 5 | A | 426 | SER |
| 5 | A | 889 | GLN |
| 5 | A | 967 | THR |
| 5 | A | 995 | PRO |
| 5 | A | 1070 | ARG |
| 5 | A | 1104 | ASN |
| 5 | A | 1204 | GLU |
| 5 | A | 1225 | SER |
| 5 | A | 1229 | PHE |
| 5 | A | 1302 | LYS |
| 5 | A | 1335 | SER |
| 5 | A | 1606 | PRO |
| 5 | A | 1615 | MET |
| 5 | A | 1895 | LYS |
| 5 | A | 2226 | ILE |
| 5 | A | 2518 | GLU |
| 6 | F | 405 | ALA |
| 1 | B | 2647 | THR |
| 1 | B | 2958 | ASN |
| 1 | B | 2962 | VAL |
| 1 | B | 3291 | TYR |
| 1 | B | 3356 | GLY |
| 1 | B | 3409 | ALA |
| 1 | B | 3410 | VAL |
| 1 | B | 3462 | VAL |
| 1 | B | 3706 | LEU |
| 1 | B | 3741 | MET |
| 2 | C | 679 | ARG |
| 2 | C | 690 | ARG |
| 4 | H | 129 | ILE |
| 5 | A | 833 | PRO |
| 5 | A | 978 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 983 | ASN |
| 5 | A | 986 | PRO |
| 5 | A | 1006 | SER |
| 5 | A | 1095 | LEU |
| 5 | A | 1105 | ASN |
| 5 | A | 1207 | TYR |
| 5 | A | 1898 | ASP |
| 5 | A | 2612 | LYS |
| 6 | F | 70 | GLU |
| 1 | B | 2671 | GLU |
| 1 | B | 2942 | GLU |
| 1 | B | 2961 | ASP |
| 1 | B | 3054 | ALA |
| 1 | B | 3165 | GLN |
| 1 | B | 3219 | TYR |
| 1 | B | 3618 | GLU |
| 5 | A | 637 | LEU |
| 5 | A | 1067 | VAL |
| 5 | A | 1203 | ASP |
| 5 | A | 1321 | PRO |
| 5 | A | 1650 | PHE |
| 5 | A | 1894 | ILE |
| 5 | A | 2390 | LEU |
| 5 | A | 2557 | HIS |
| 5 | A | 2570 | SER |
| 1 | B | 2789 | PRO |
| 1 | B | 3344 | PHE |
| 1 | B | 3602 | ASN |
| 1 | B | 3625 | THR |
| 1 | B | 3627 | ASN |
| 2 | C | 675 | HIS |
| 5 | A | 246 | LEU |
| 5 | A | 314 | ALA |
| 5 | A | 890 | TYR |
| 5 | A | 991 | LEU |
| 5 | A | 1051 | LYS |
| 5 | A | 1583 | LYS |
| 5 | A | 1596 | LEU |
| 5 | A | 1647 | PHE |
| 5 | A | 1897 | GLU |
| 1 | B | 2902 | VAL |
| 1 | B | 3400 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 776 | PHE |
| 5 | A | 993 | VAL |
| 5 | A | 1036 | PRO |
| 1 | B | 3393 | ILE |
| 1 | B | 3612 | PRO |
| 1 | B | 3381 | VAL |
| 5 | A | 1256 | ILE |
| 7 | G | 287 | VAL |
| 5 | A | 982 | ILE |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | B | 300/1012 (30%) | 198 (66%) | 102 (34%) | 0 1 |
| 2 | C | 26/309 (8%) | 10 (38%) | 16 (62%) | 0 0 |
| 5 | A | 7/2438 (0%) | 5 (71%) | 2 (29%) | 0 3 |
| 6 | F | 372/435 (86%) | 360 (97%) | 12 (3%) | 39 62 |
| 7 | G | 297/320 (93%) | 284 (96%) | 13 (4%) | 28 54 |
| 8 | E | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 64 |
| All | All | 1036/4548 (23%) | 890 (86%) | 146 (14%) | 6 18 |

All (146) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 2636 | SER |
| 1 | B | 2637 | ILE |
| 1 | B | 2639 | ILE |
| 1 | B | 2651 | ASN |
| 1 | B | 2652 | THR |
| 1 | B | 2654 | ILE |
| 1 | B | 2655 | ILE |
| 1 | B | 2663 | LEU |
| 1 | B | 2665 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 2674 | MET |
| 1 | B | 2826 | ILE |
| 1 | B | 2847 | GLN |
| 1 | B | 2856 | THR |
| 1 | B | 2882 | GLN |
| 1 | B | 2885 | ARG |
| 1 | B | 2894 | ASP |
| 1 | B | 2896 | ASN |
| 1 | B | 2897 | MET |
| 1 | B | 2898 | TRP |
| 1 | B | 2899 | ASN |
| 1 | B | 2900 | ASP |
| 1 | B | 2902 | VAL |
| 1 | B | 2906 | GLN |
| 1 | B | 2912 | ILE |
| 1 | B | 2941 | HIS |
| 1 | B | 2946 | VAL |
| 1 | B | 2952 | HIS |
| 1 | B | 2965 | SER |
| 1 | B | 2966 | GLN |
| 1 | B | 2967 | LEU |
| 1 | B | 2970 | ILE |
| 1 | B | 2971 | TYR |
| 1 | B | 3007 | SER |
| 1 | B | 3019 | LYS |
| 1 | B | 3023 | PHE |
| 1 | B | 3038 | GLU |
| 1 | B | 3041 | GLN |
| 1 | B | 3059 | GLN |
| 1 | B | 3062 | PHE |
| 1 | B | 3066 | ARG |
| 1 | B | 3067 | ARG |
| 1 | B | 3069 | SER |
| 1 | B | 3095 | SER |
| 1 | B | 3097 | ILE |
| 1 | B | 3099 | GLU |
| 1 | B | 3100 | LEU |
| 1 | B | 3104 | ILE |
| 1 | B | 3105 | LEU |
| 1 | B | 3107 | LEU |
| 1 | B | 3108 | ILE |
| 1 | B | 3111 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 3143 | SER |
| 1 | B | 3145 | SER |
| 1 | B | 3162 | SER |
| 1 | B | 3167 | LEU |
| 1 | B | 3168 | HIS |
| 1 | B | 3169 | PHE |
| 1 | B | 3171 | LEU |
| 1 | B | 3172 | ARG |
| 1 | B | 3219 | TYR |
| 1 | B | 3229 | LEU |
| 1 | B | 3236 | ARG |
| 1 | B | 3247 | ARG |
| 1 | B | 3317 | TRP |
| 1 | B | 3318 | ARG |
| 1 | B | 3367 | HIS |
| 1 | B | 3411 | ARG |
| 1 | B | 3417 | GLU |
| 1 | B | 3418 | ARG |
| 1 | B | 3421 | GLN |
| 1 | B | 3422 | LEU |
| 1 | B | 3424 | ARG |
| 1 | B | 3427 | ASN |
| 1 | B | 3432 | LYS |
| 1 | B | 3435 | GLU |
| 1 | B | 3440 | SER |
| 1 | B | 3443 | PHE |
| 1 | B | 3444 | ASN |
| 1 | B | 3449 | ILE |
| 1 | B | 3462 | VAL |
| 1 | B | 3467 | LEU |
| 1 | B | 3468 | HIS |
| 1 | B | 3472 | ASN |
| 1 | B | 3474 | PHE |
| 1 | B | 3484 | ASP |
| 1 | B | 3485 | ILE |
| 1 | B | 3486 | GLN |
| 1 | B | 3487 | ASP |
| 1 | B | 3488 | PHE |
| 1 | B | 3489 | MET |
| 1 | B | 3492 | LYS |
| 1 | B | 3494 | ASN |
| 1 | B | 3499 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 3552 | TYR |
| 1 | B | 3568 | THR |
| 1 | B | 3570 | HIS |
| 1 | B | 3571 | LYS |
| 1 | B | 3611 | SER |
| 1 | B | 3647 | THR |
| 1 | B | 3652 | LEU |
| 1 | B | 3668 | ARG |
| 1 | B | 3674 | TRP |
| 2 | C | 680 | LEU |
| 2 | C | 681 | THR |
| 2 | C | 684 | TYR |
| 2 | C | 685 | LEU |
| 2 | C | 687 | ASN |
| 2 | C | 688 | ILE |
| 2 | C | 689 | GLU |
| 2 | C | 694 | TRP |
| 2 | C | 695 | GLN |
| 2 | C | 696 | CYS |
| 2 | C | 697 | PHE |
| 2 | C | 699 | ARG |
| 2 | C | 702 | GLN |
| 2 | C | 703 | LEU |
| 2 | C | 706 | ARG |
| 2 | C | 707 | PHE |
| 5 | A | 948 | ILE |
| 5 | A | 1896 | LEU |
| 6 | F | 47 | TYR |
| 6 | F | 56 | ILE |
| 6 | F | 66 | ARG |
| 6 | F | 67 | LYS |
| 6 | F | 70 | GLU |
| 6 | F | 72 | LYS |
| 6 | F | 125 | LEU |
| 6 | F | 128 | LEU |
| 6 | F | 137 | CYS |
| 6 | F | 213 | LYS |
| 6 | F | 440 | LEU |
| 6 | F | 442 | THR |
| 7 | G | 16 | MET |
| 7 | G | 71 | ILE |
| 7 | G | 73 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | G | 135 | SER |
| 7 | G | 136 | ILE |
| 7 | G | 137 | GLN |
| 7 | G | 139 | VAL |
| 7 | G | 151 | ILE |
| 7 | G | 152 | VAL |
| 7 | G | 153 | LEU |
| 7 | G | 159 | VAL |
| 7 | G | 163 | VAL |
| 7 | G | 288 | ASP |
| 8 | E | 394 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 2752 | HIS |
| 1 | B | 2941 | HIS |
| 1 | B | 3041 | GLN |
| 1 | B | 3367 | HIS |
| 1 | B | 3427 | ASN |
| 1 | B | 3444 | ASN |
| 1 | B | 3486 | GLN |
| 1 | B | 3494 | ASN |
| 1 | B | 3497 | HIS |
| 1 | B | 3515 | ASN |
| 1 | B | 3570 | HIS |
| 1 | B | 3732 | ASN |
| 2 | C | 687 | ASN |
| 6 | F | 89 | GLN |
| 6 | F | 91 | GLN |
| 6 | F | 96 | ASN |
| 6 | F | 120 | ASN |
| 6 | F | 162 | HIS |
| 6 | F | 234 | ASN |
| 6 | F | 248 | HIS |
| 6 | F | 406 | HIS |
| 6 | F | 444 | HIS |
| 6 | F | 449 | GLN |
| 7 | G | 115 | ASN |
| 7 | G | 280 | ASN |
| 8 | E | 377 | HIS |

#### 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.

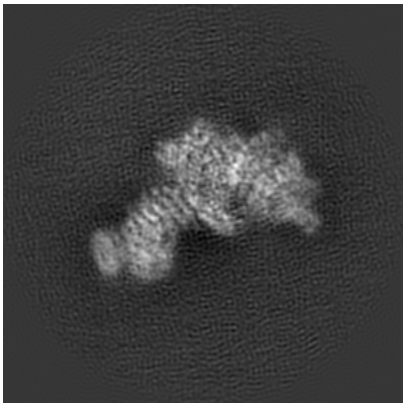
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6816. These allow visual inspection of the internal detail of the map and identification of artifacts.

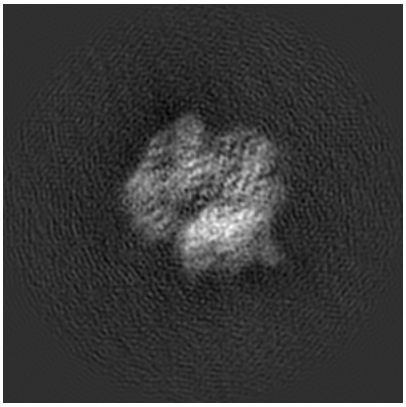
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

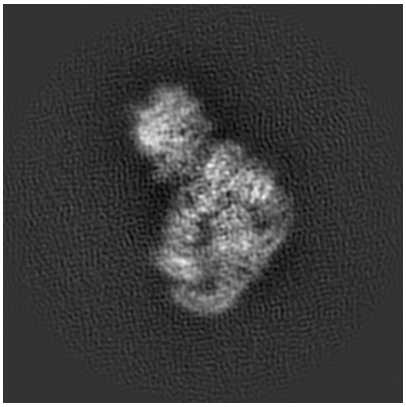
### 6.1.1 Primary map



X



Y

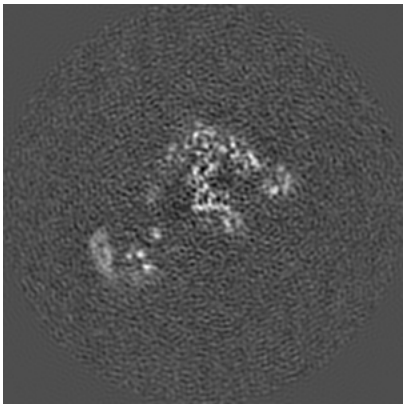


Z

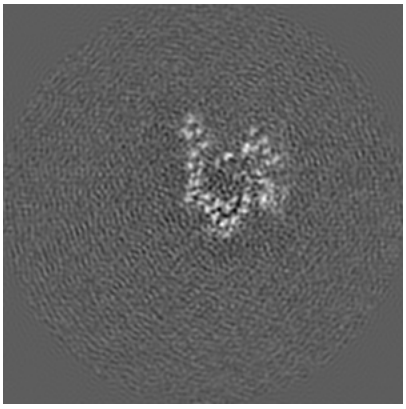
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

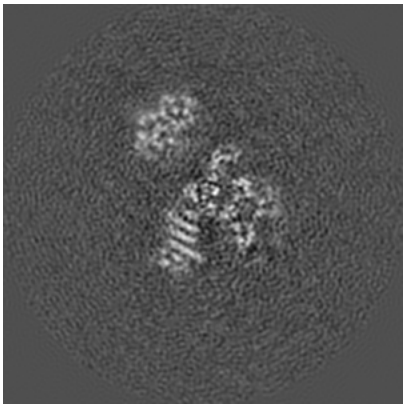
### 6.2.1 Primary map



X Index: 144



Y Index: 144

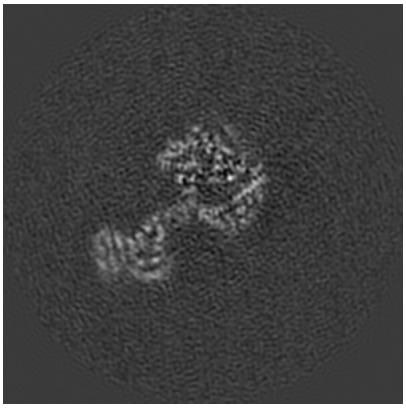


Z Index: 144

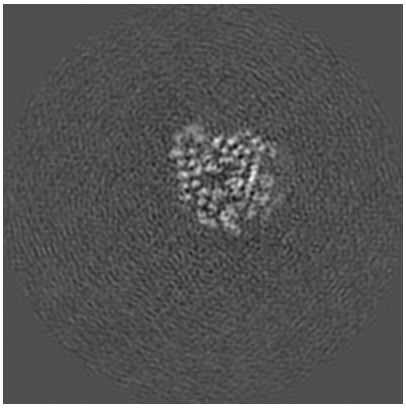
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

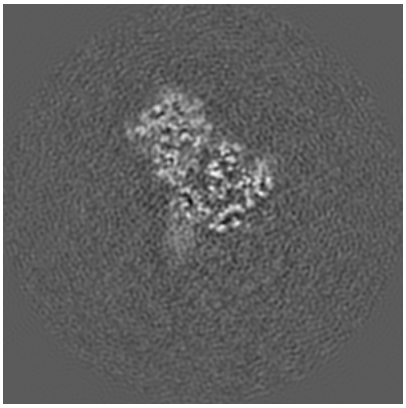
### 6.3.1 Primary map



X Index: 158



Y Index: 153



Z Index: 160

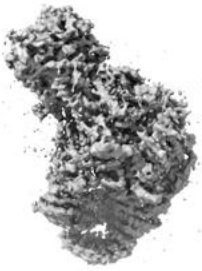
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0225. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

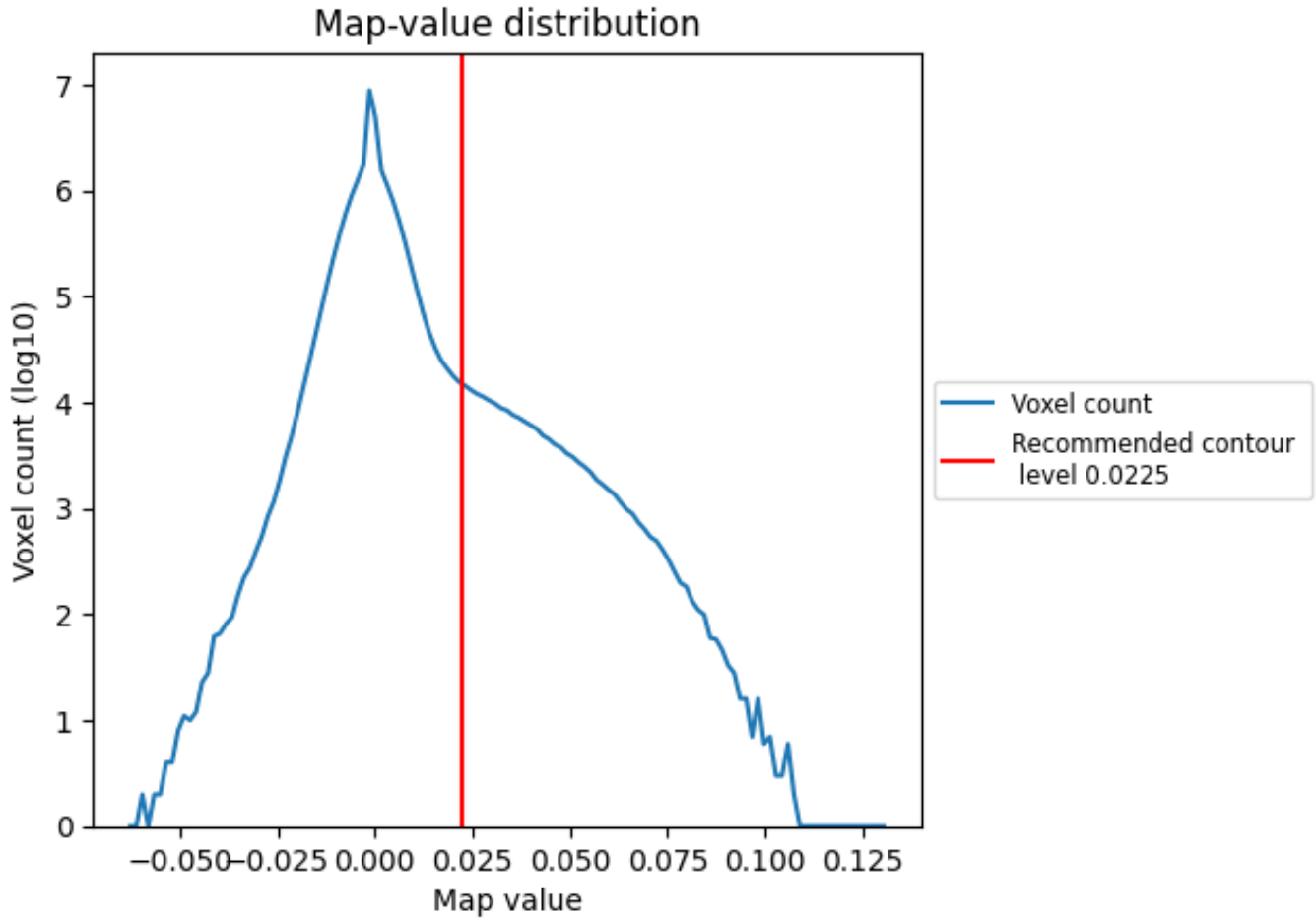
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

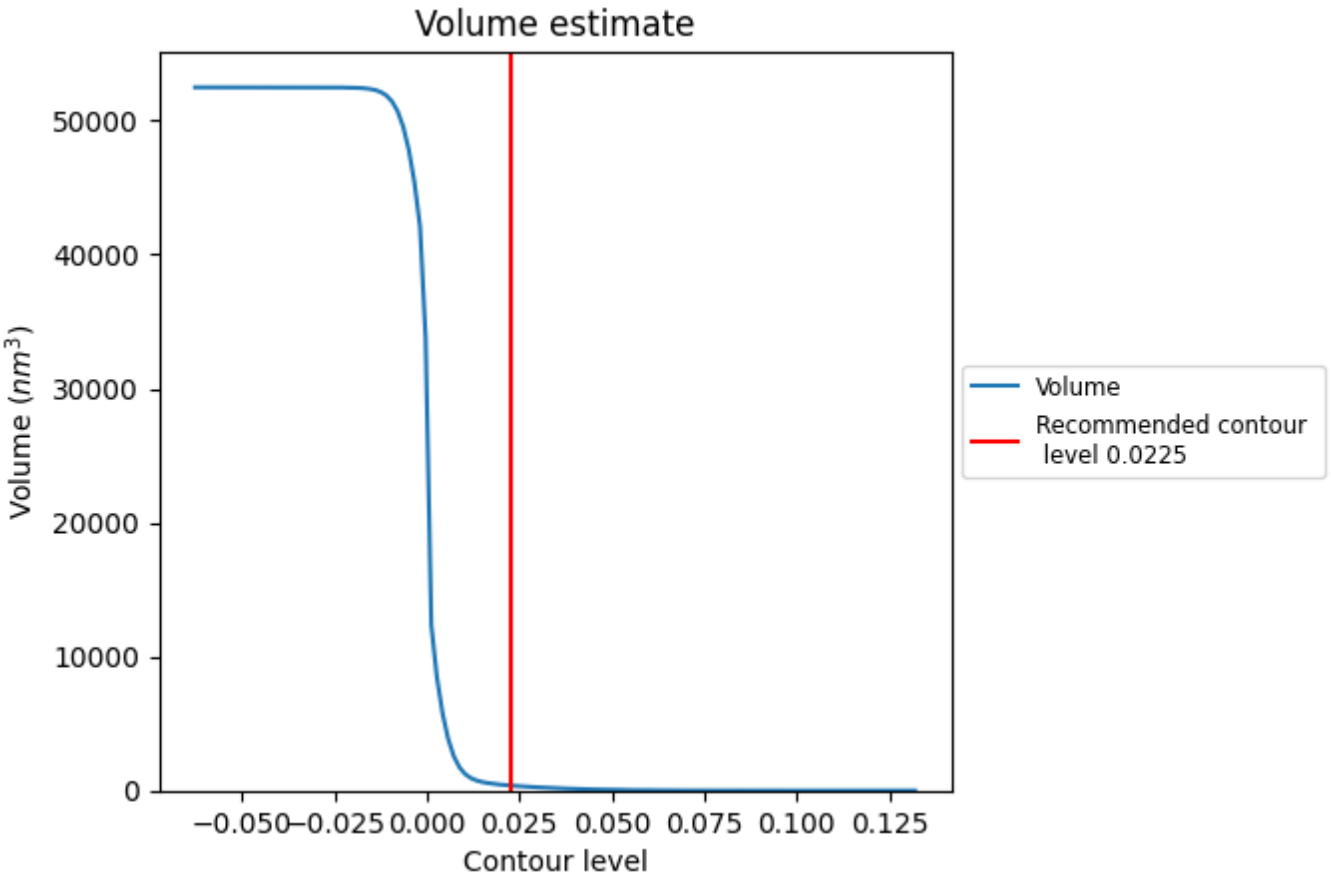
This section contains the results of statistical analysis of the map.

## 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.

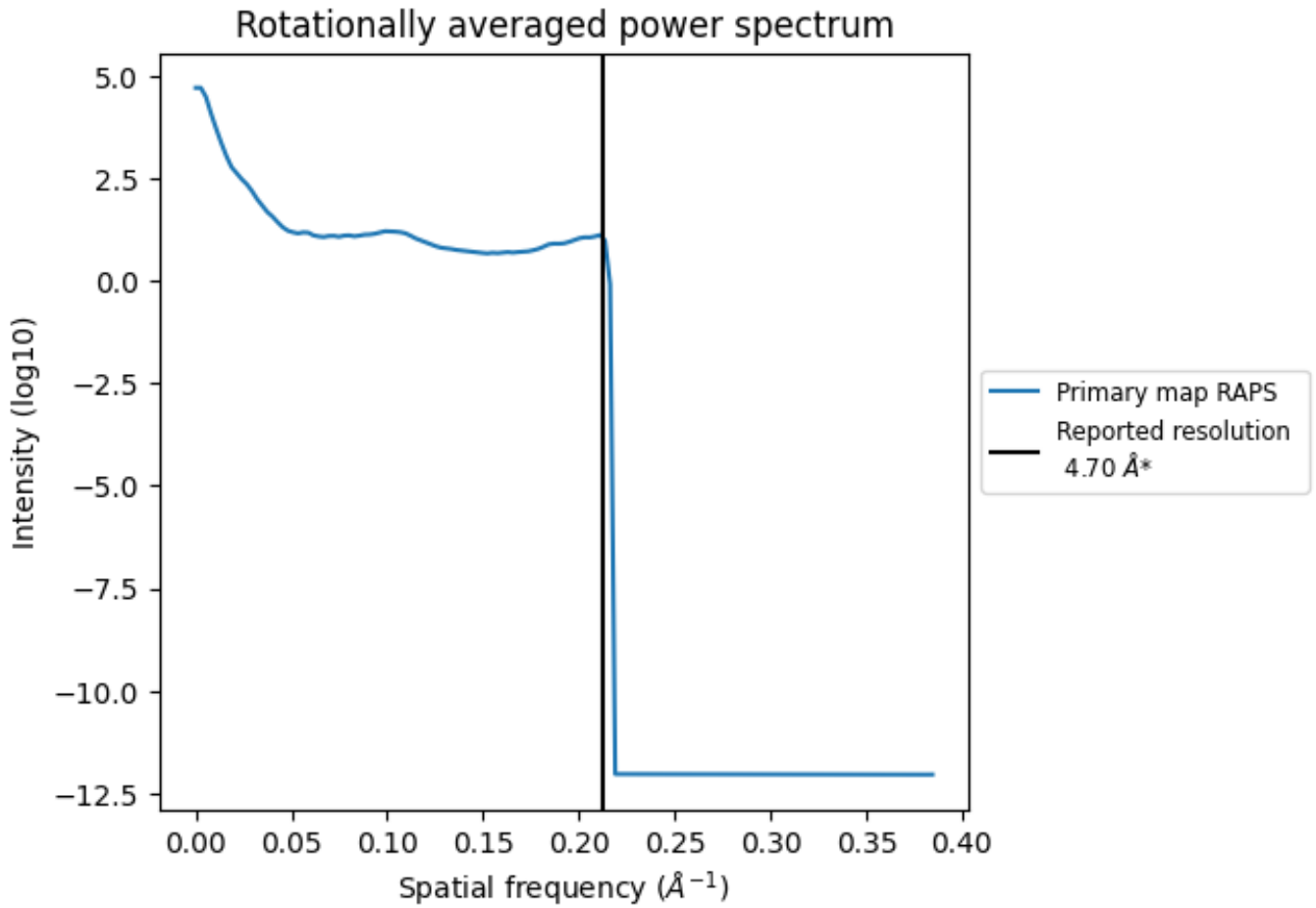
## 7.2 Volume estimate




The volume at the recommended contour level is 378 $nm^3$; this corresponds to an approximate mass of 341 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 (i)




*Reported resolution corresponds to spatial frequency of 0.213 $Å^{-1}$

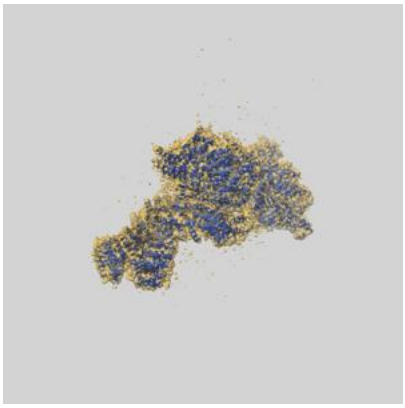
# 8 Fourier-Shell correlation

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

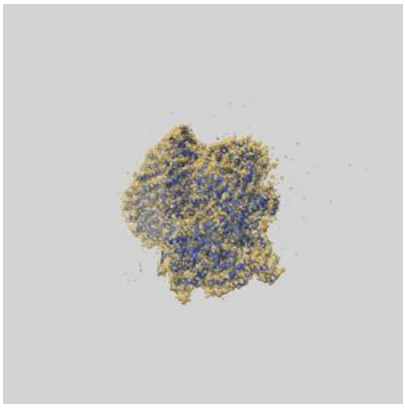
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6816 and PDB model 5Y81. Per-residue inclusion information can be found in section 3 on page 5.

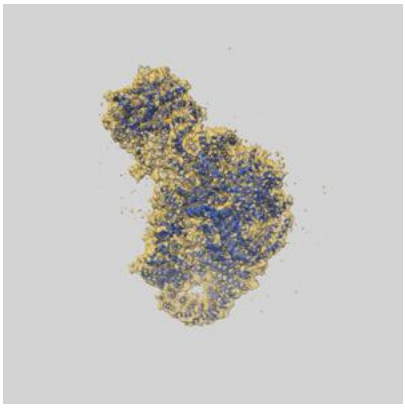
## 9.1 Map-model overlay



X



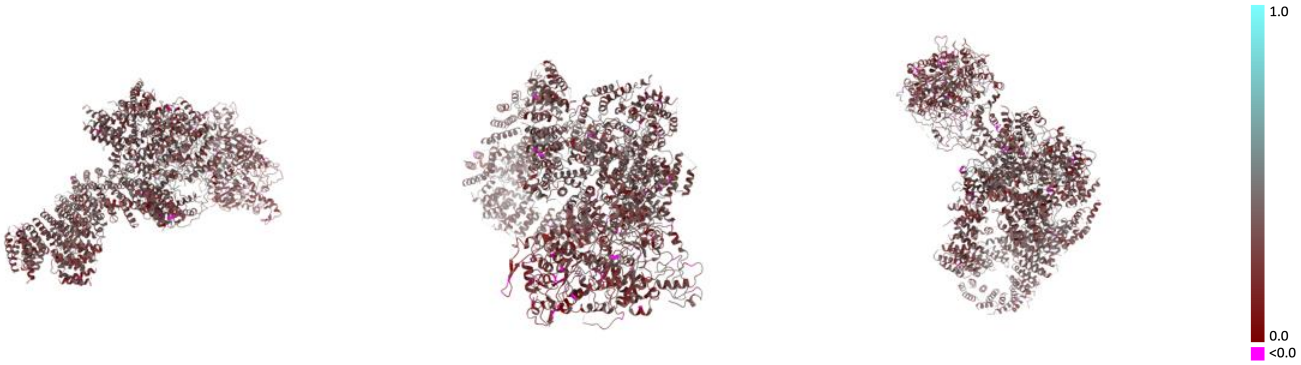
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0225 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.

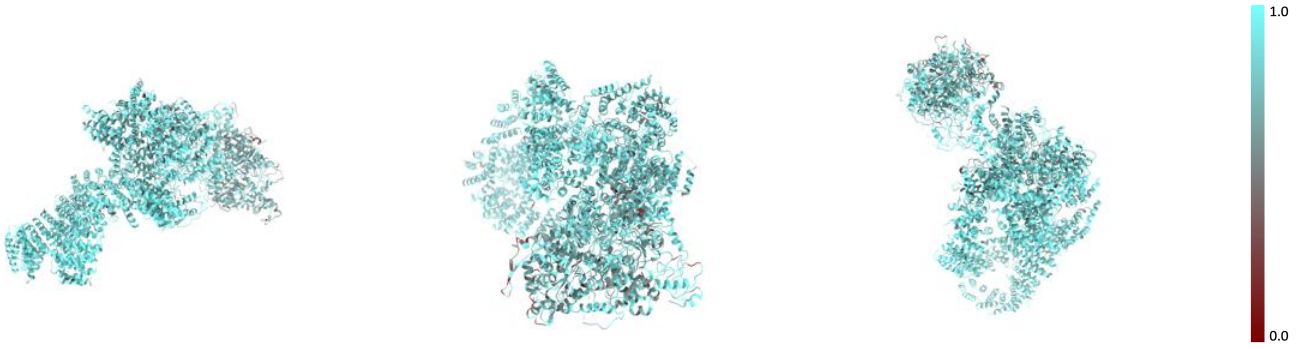
## 9.2 Q-score mapped to coordinate model (i)




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.

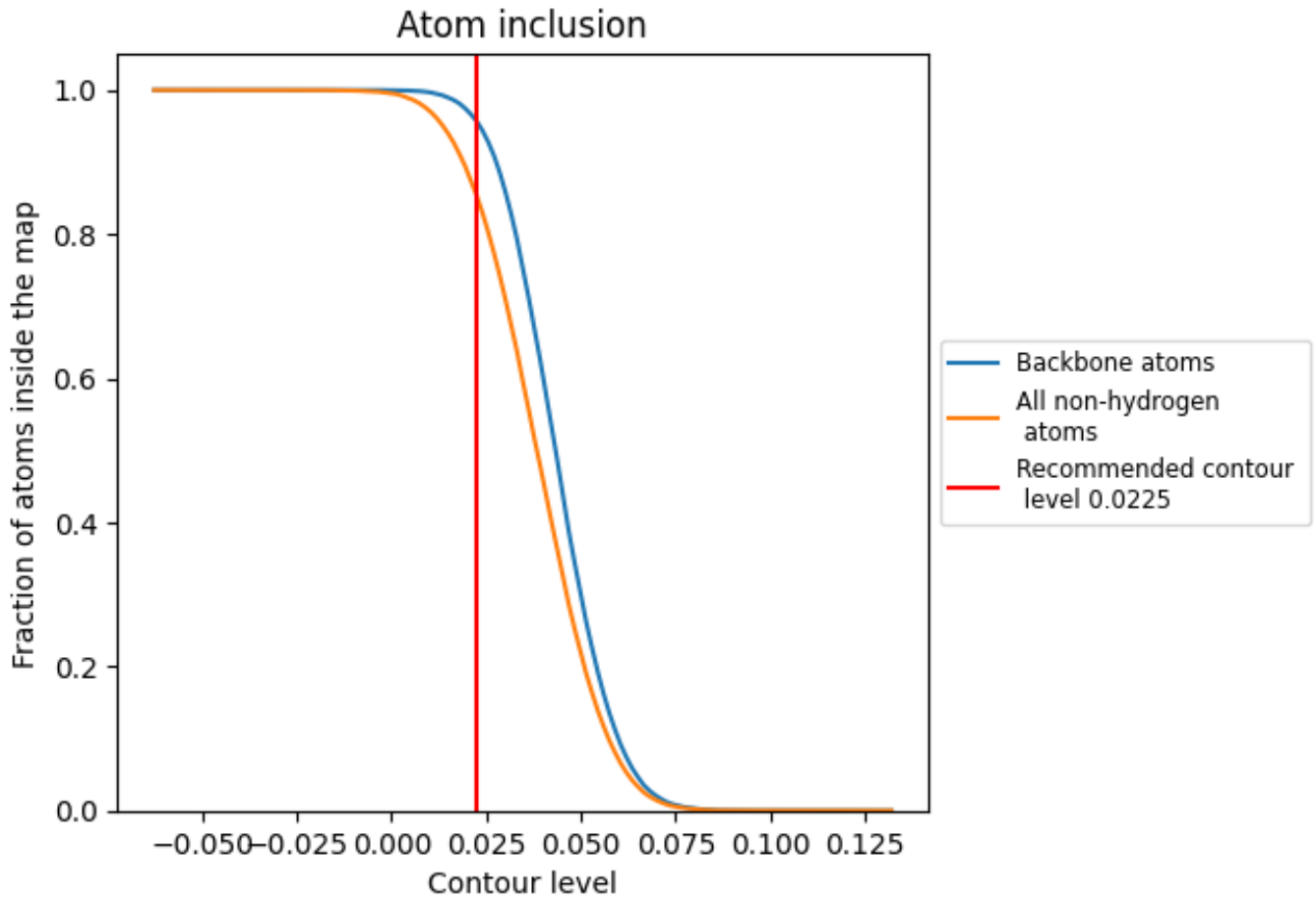
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.0225).

## 9.4 Atom inclusion (i)




At the recommended contour level, 96% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0225) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8530 | 0.3080 |
| A | 0.9246 | 0.3230 |
| B | 0.8590 | 0.3370 |
| C | 0.8949 | 0.3300 |
| D | 0.8833 | 0.3430 |
| E | 0.7092 | 0.2490 |
| F | 0.7102 | 0.2630 |
| G | 0.7175 | 0.2240 |
| H | 0.9018 | 0.3050 |