# Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 03:09 PM EST

| | | |
|---|---|---|
| PDB ID | : | 6CNC |
| EMDB ID | : | EMD-7531 |
| Title | : | Yeast RNA polymerase III open complex |
| Authors | : | Han, Y.; He, Y. |
| Deposited on | : | 2018-03-08 |
| Resolution | : | 4.10 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:

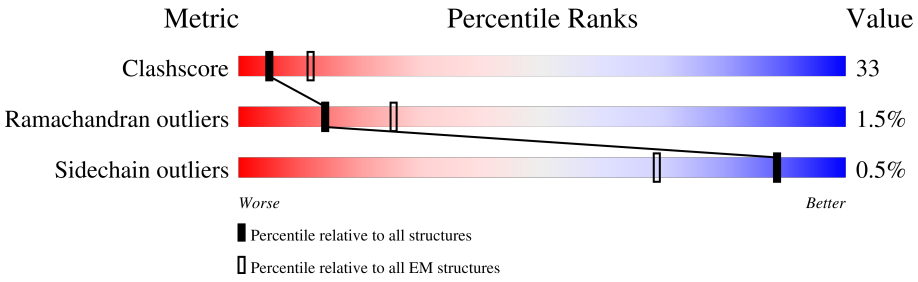
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1460 | 5% 47% 50% |
| 2 | B | 1149 | 47% 49% |
| 3 | C | 335 | 59% 40% |
| 4 | D | 161 | 12% 40% 34% 26% |
| 5 | E | 215 | 38% 60% |
| 6 | F | 155 | 34% 19% 46% |
| 7 | G | 212 | 9% 34% 50% 13% |
| 8 | H | 146 | 5% 49% 47% |

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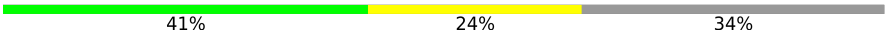
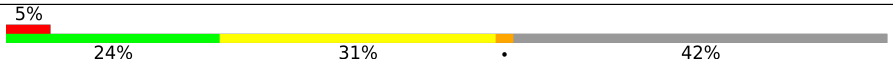
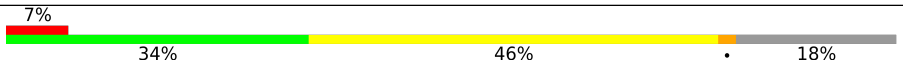
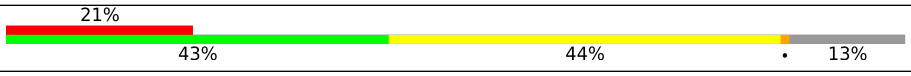
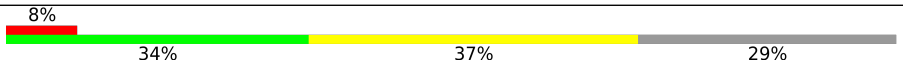
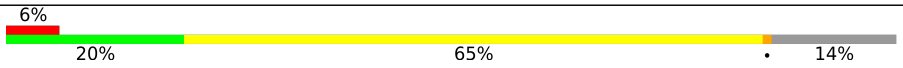
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | I | 110 |   |
| 10 | J | 70 |   |
| 11 | K | 142 |   |
| 12 | L | 70 |   |
| 13 | M | 282 |   |
| 14 | N | 422 |   |
| 15 | O | 654 |   |
| 16 | P | 317 |   |
| 17 | Q | 251 |   |
| 18 | R | 736 |   |
| 19 | S | 594 |   |
| 20 | X | 71 |   |
| 21 | Y | 71 |   |

## 2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 47836 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 DNA-directed RNA polymerase III subunit RPC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 1428 | 11159 | 7029 | 1972 | 2099 | 59 | 0 | 0 |

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 1114 | 8788 | 5558 | 1516 | 1654 | 60 | 0 | 0 |

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 335 | 2655 | 1681 | 454 | 511 | 9 | 0 | 0 |

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 119 | 977 | 628 | 156 | 187 | 6 | 0 | 0 |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 215 | 1759 | 1116 | 310 | 321 | 12 | 0 | 0 |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 83 | 671 | 429 | 114 | 125 | 3 | 0 | 0 |

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 184 | Total | C | N | O | S | 0 | 0 |
| | | | 1484 | 972 | 239 | 267 | 6 | | |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1120 | 703 | 188 | 224 | 5 | | |

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 321 | 204 | 47 | 64 | 6 | | |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 350 | 95 | 98 | 6 | | |

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 792 | 496 | 130 | 161 | 5 | | |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 363 | 224 | 72 | 63 | 4 | | |

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1338 | 857 | 227 | 253 | 1 | | |

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | N | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 845 | 536 | 152 | 154 | 3 | | |

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | O | 539 | Total | C | N | O | S | 0 | 0 |
| | | | 4329 | 2756 | 741 | 813 | 19 | | |

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | P | 277 | Total | C | N | O | S | 0 | 0 |
| | | | 2242 | 1438 | 368 | 425 | 11 | | |

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 17 | Q | 54 | Total | C | N | O | 0 | 0 |
| | | | 368 | 238 | 64 | 66 | | |

- Molecule 18 is a protein called Transcription factor IIIB 70 kDa subunit,TATA-box-bindin g protein,Transcription factor IIIB 70 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | R | 522 | Total | C | N | O | S | 0 | 0 |
| | | | 4131 | 2621 | 733 | 757 | 20 | | |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| R | 383 | ALA | - | linker | UNP P29056 |
| R | 384 | MET | - | linker | UNP P29056 |
| R | 385 | PRO | - | linker | UNP P29056 |
| R | 386 | TRP | - | linker | UNP P29056 |
| R | 567 | GLY | - | linker | UNP P13393 |
| R | 568 | SER | - | linker | UNP P13393 |
| R | 569 | GLY | - | linker | UNP P13393 |
| R | 570 | SER | - | linker | UNP P13393 |
| R | 571 | GLY | - | linker | UNP P13393 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| R | 572 | SER | - | linker | UNP P13393 |
| R | 573 | GLY | - | linker | UNP P13393 |
| R | 574 | SER | - | linker | UNP P13393 |
| R | 575 | GLY | - | linker | UNP P13393 |
| R | 576 | SER | - | linker | UNP P13393 |
| R | 577 | GLY | - | linker | UNP P13393 |
| R | 578 | SER | CYS | engineered mutation | UNP P29056 |

- Molecule 19 is a protein called Transcription factor TFIIIB component B",Transcription factor TFIIIB component B",Transcription factor TFIIIB component B",Transcription factor TFIIIB component B",Transcription factor TFIIIB component B".

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | S | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1649 | 1035 | 286 | 321 | 7 | | |

- Molecule 20 is a DNA chain called DNA (71-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | X | 51 | Total | C | N | O | P | 0 | 0 |
| | | | 1040 | 503 | 181 | 306 | 50 | | |

- Molecule 21 is a DNA chain called DNA (71-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | Y | 61 | Total | C | N | O | P | 0 | 0 |
| | | | 1249 | 602 | 223 | 364 | 60 | | |

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 22 | A | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 22 | B | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 22 | I | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 22 | J | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 22 | L | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

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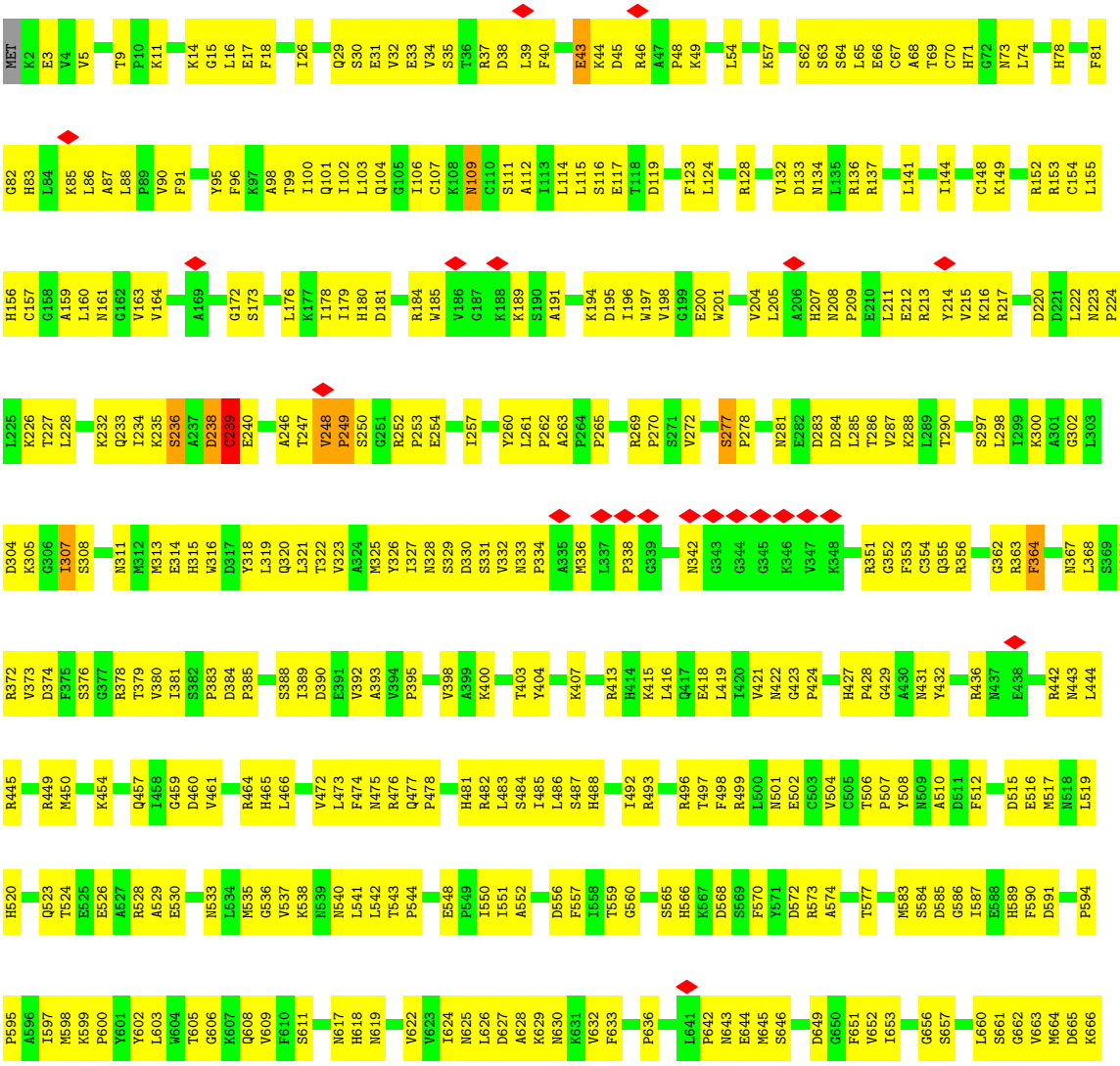
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 22 | R | 1 | 1 | 1 | 0 |

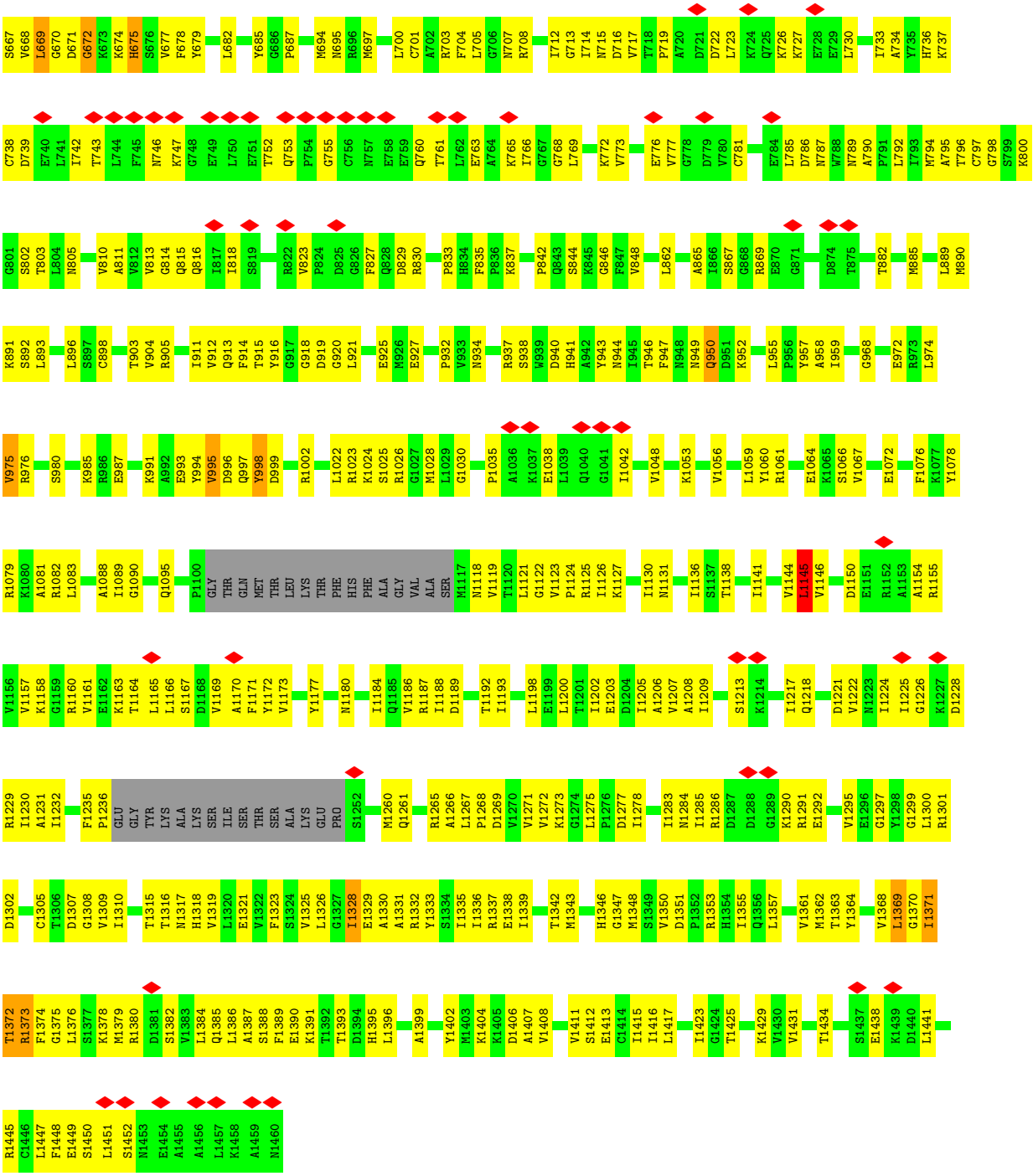
# 3 Residue-property plots (i)

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.

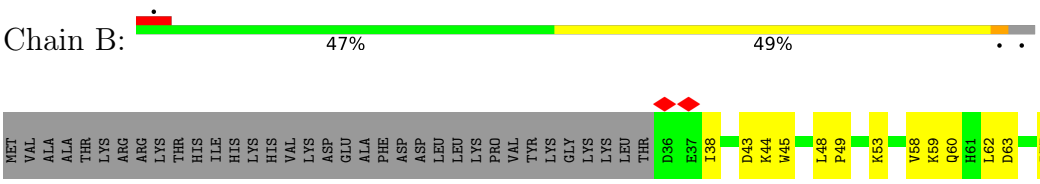
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

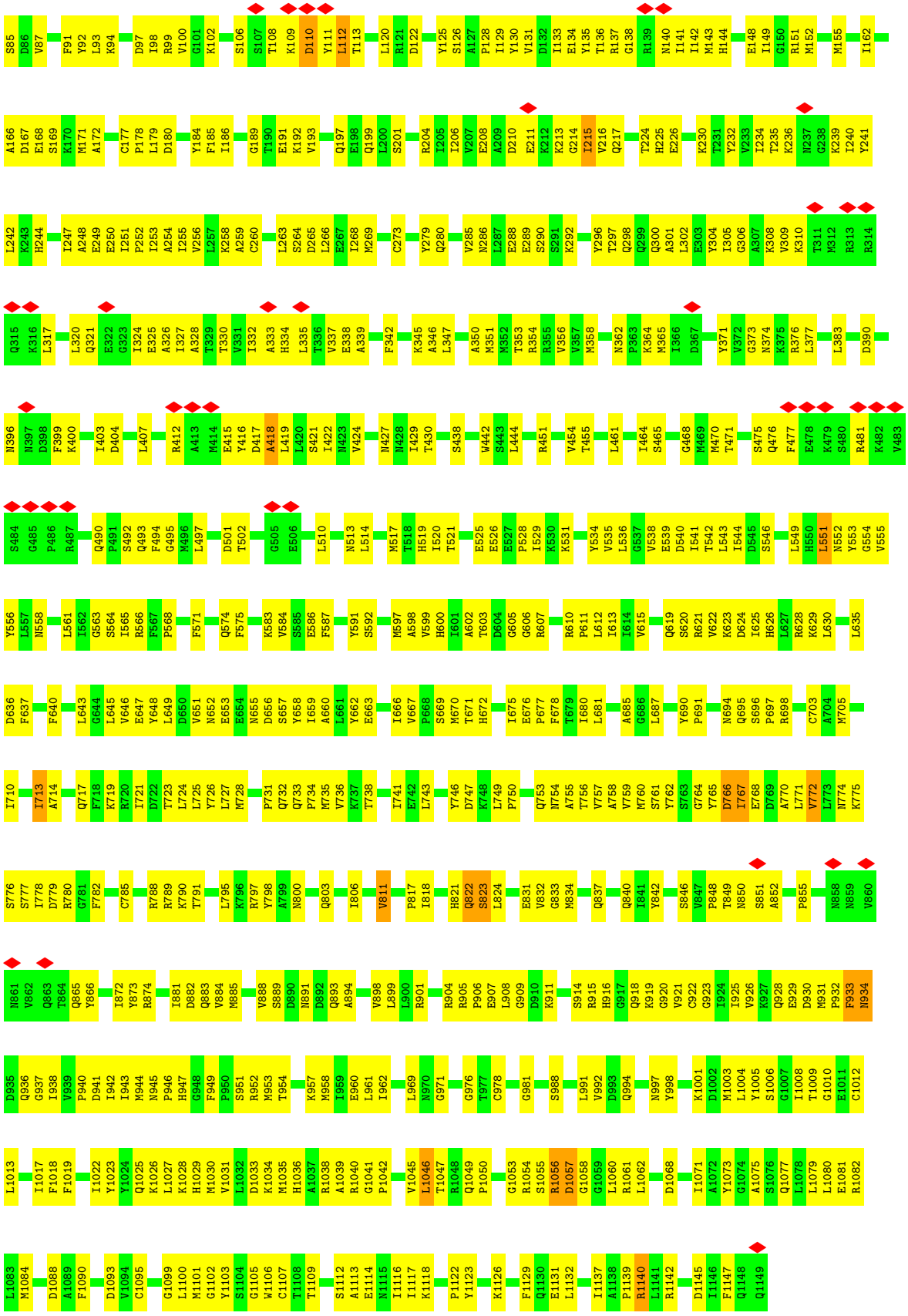
Chain A:



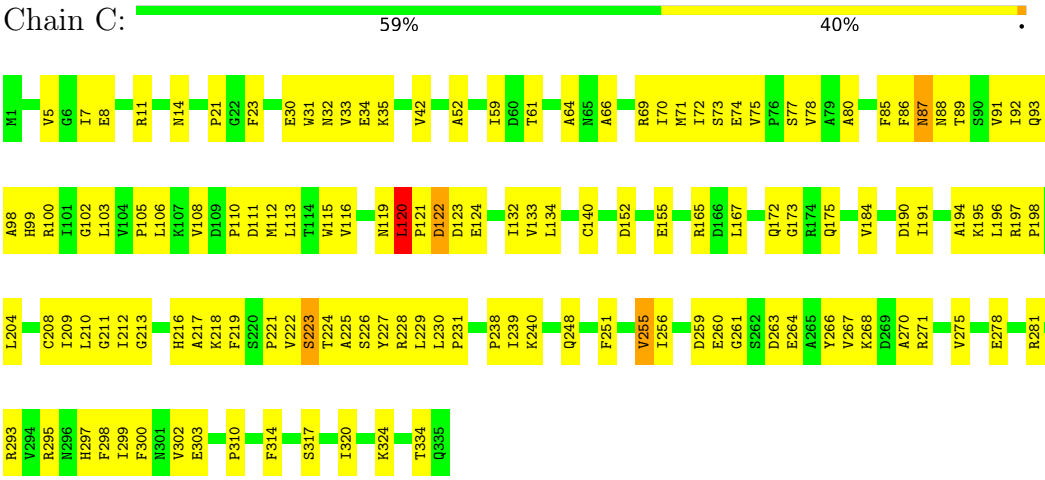
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2





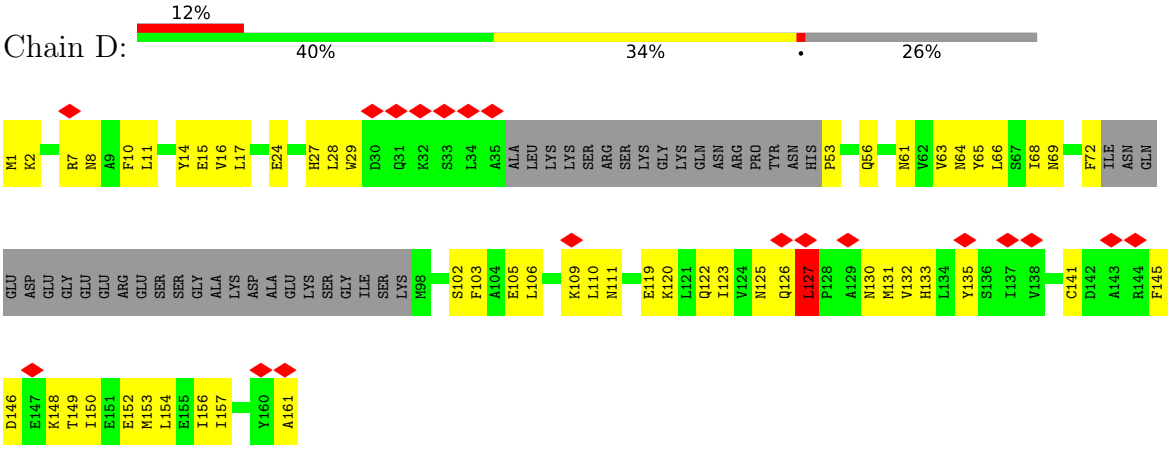
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:




• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D:

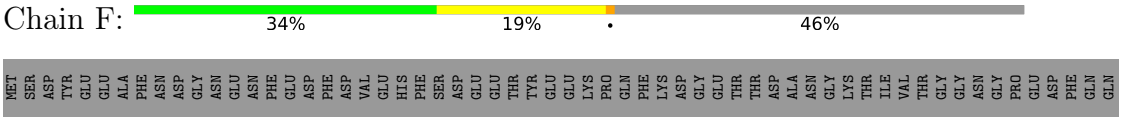


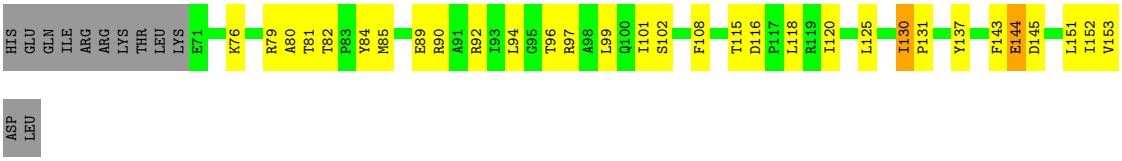

• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

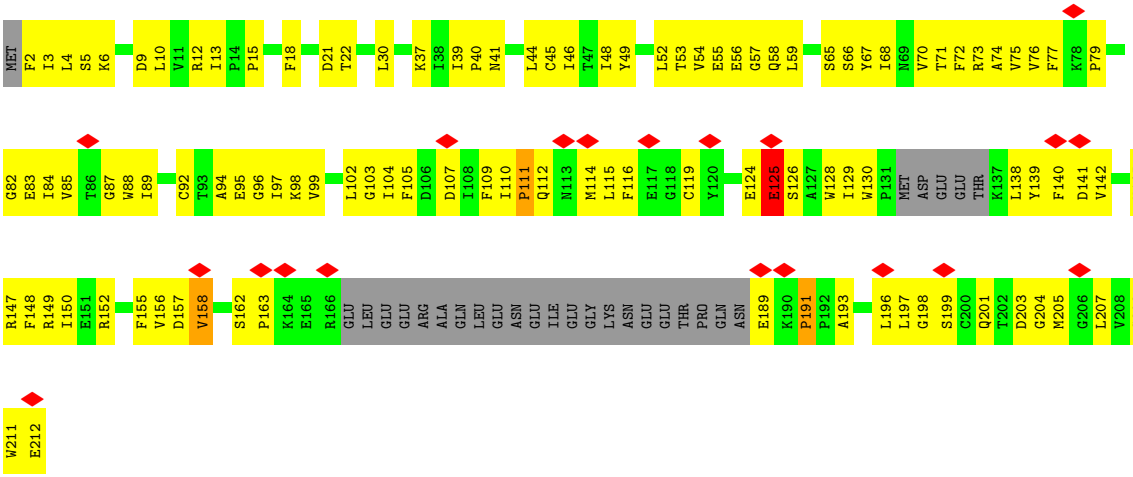






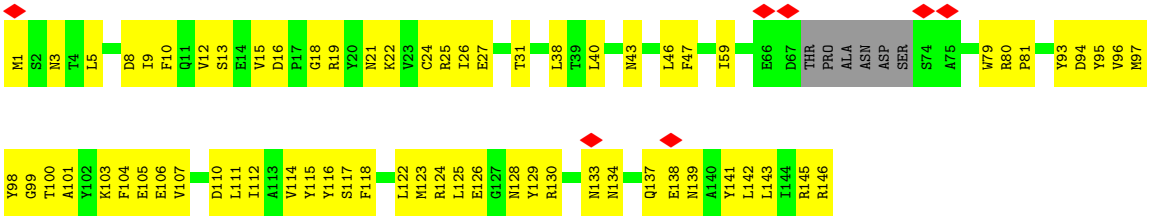
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:

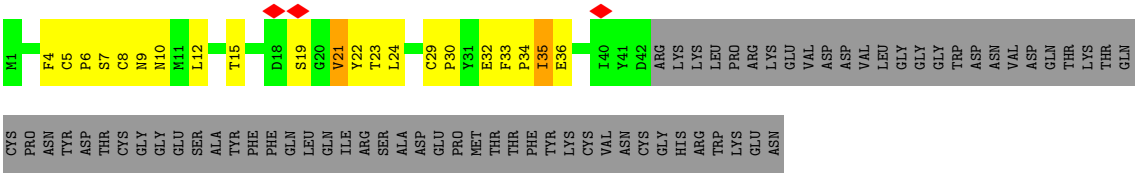
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I:

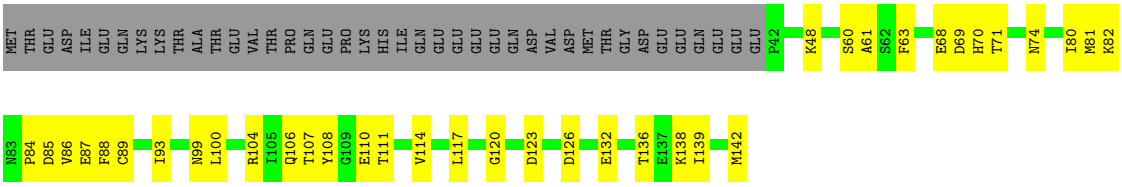



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

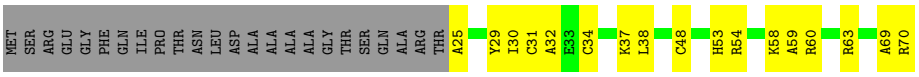

• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:

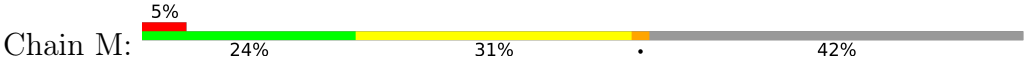

• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

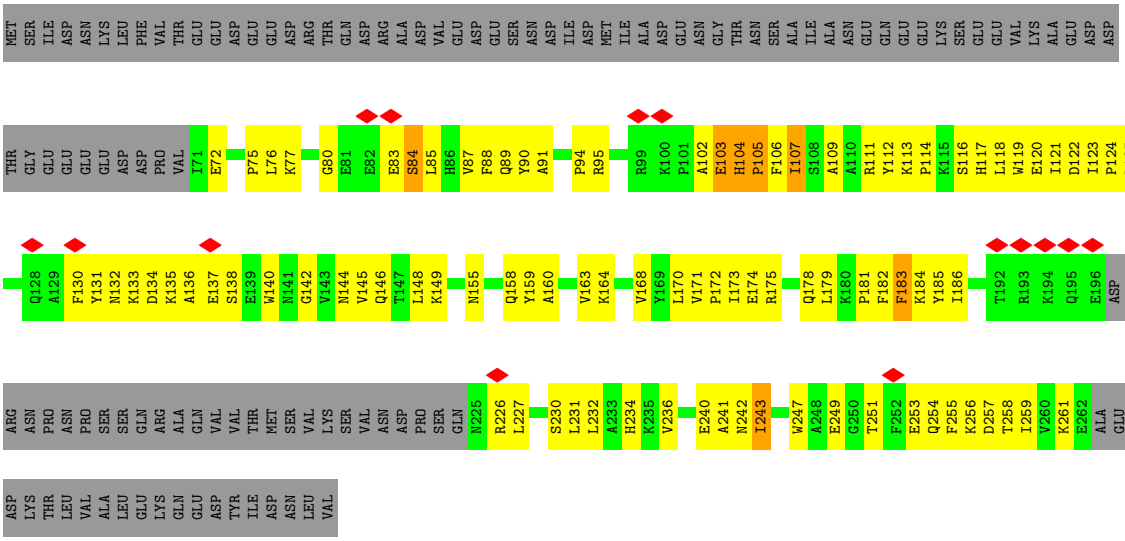
Chain L:


• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

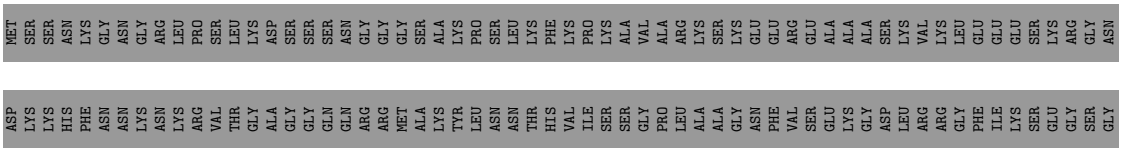
Chain M:

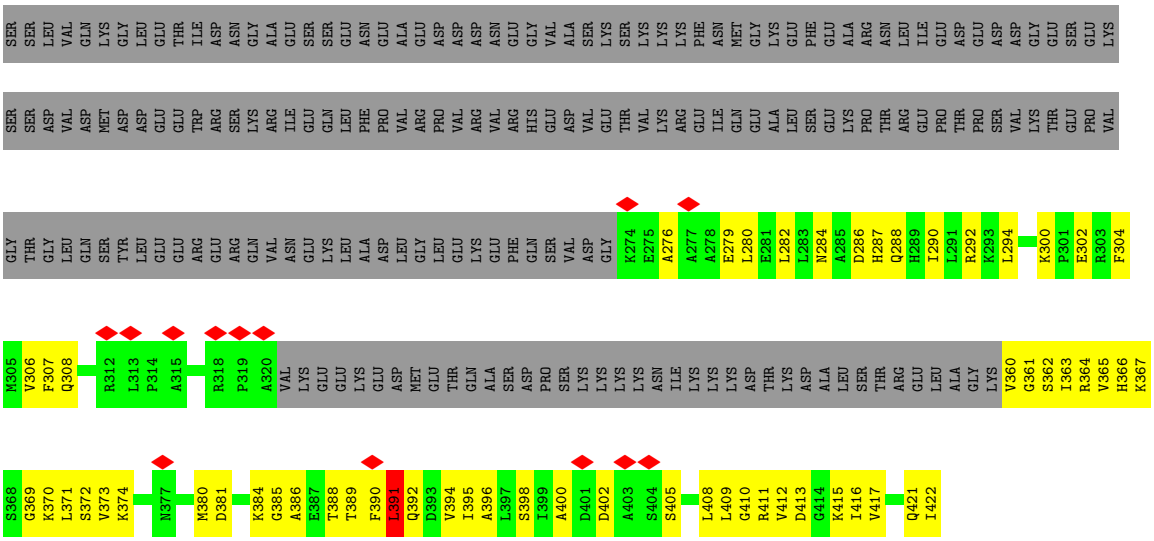



• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

Chain N:



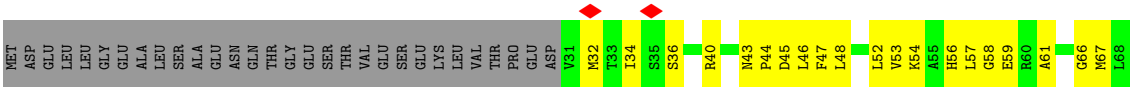


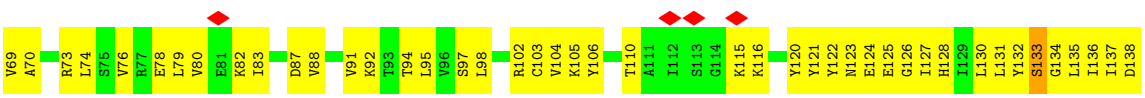


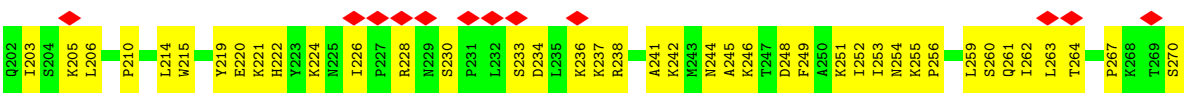


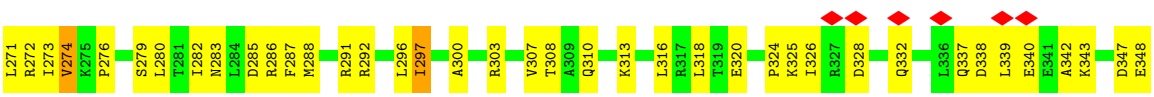


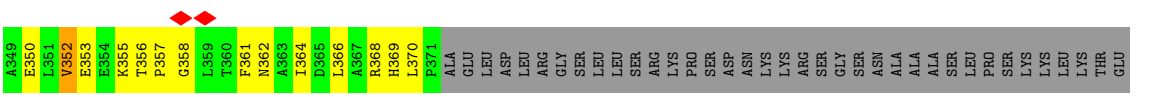
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

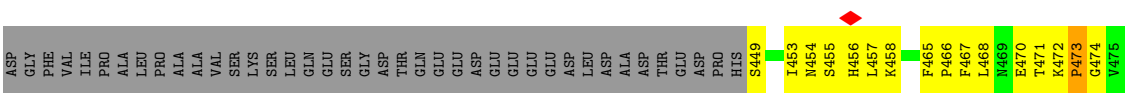



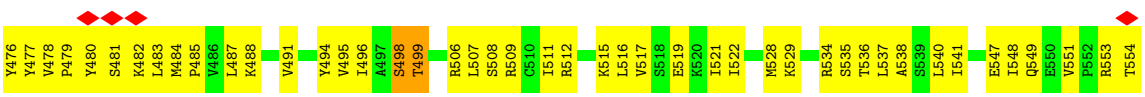


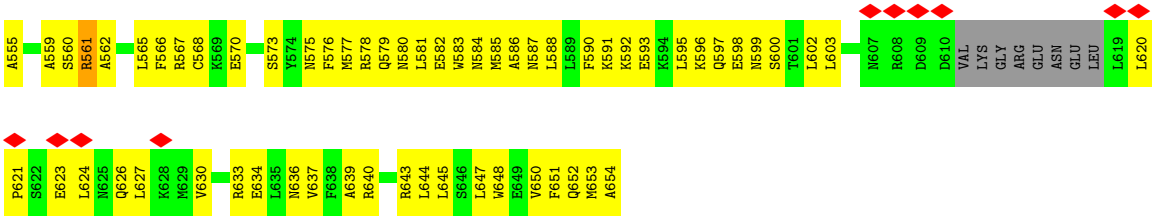








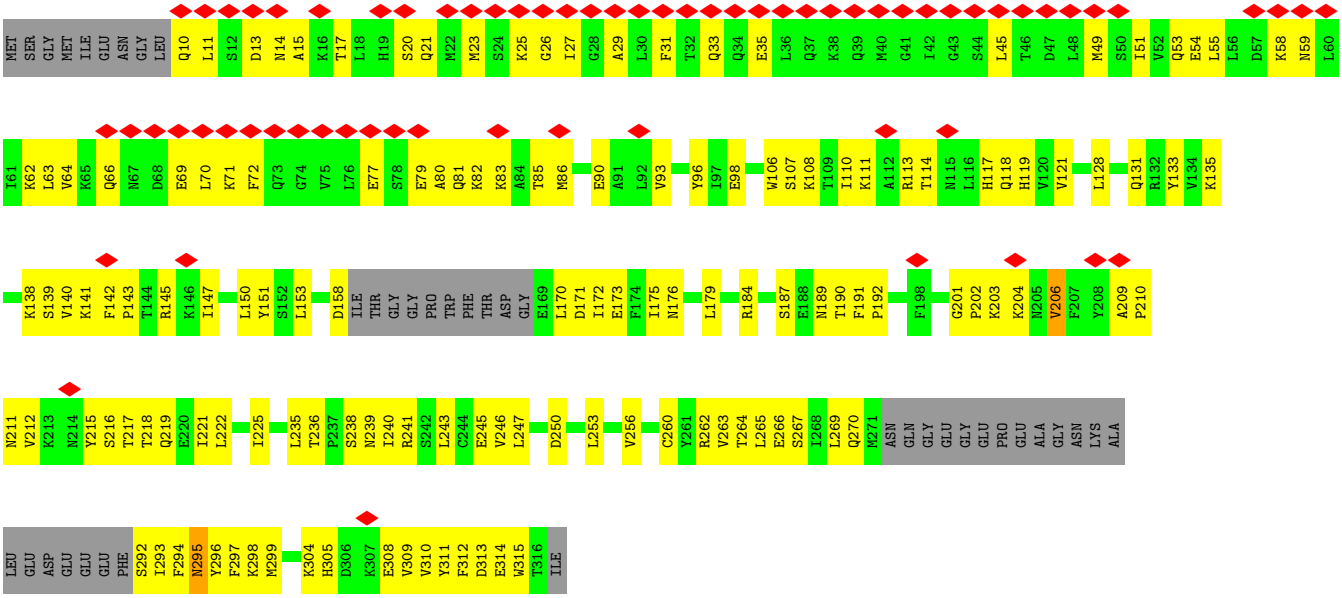






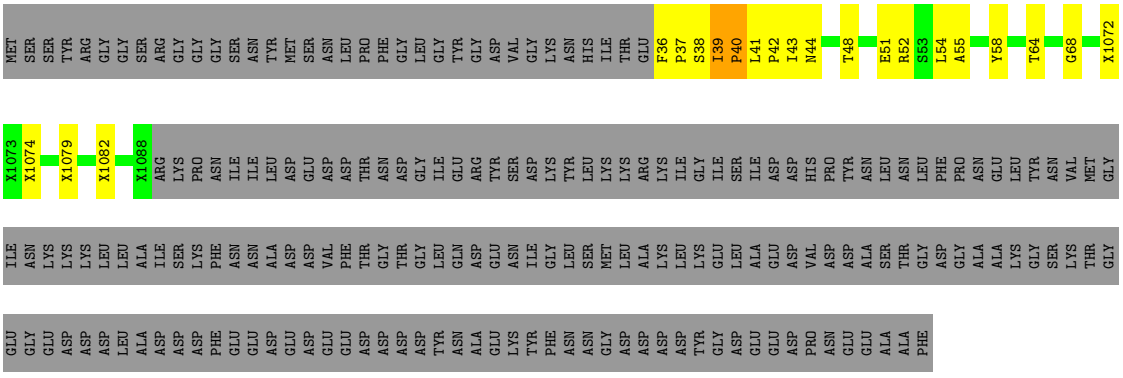
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P:

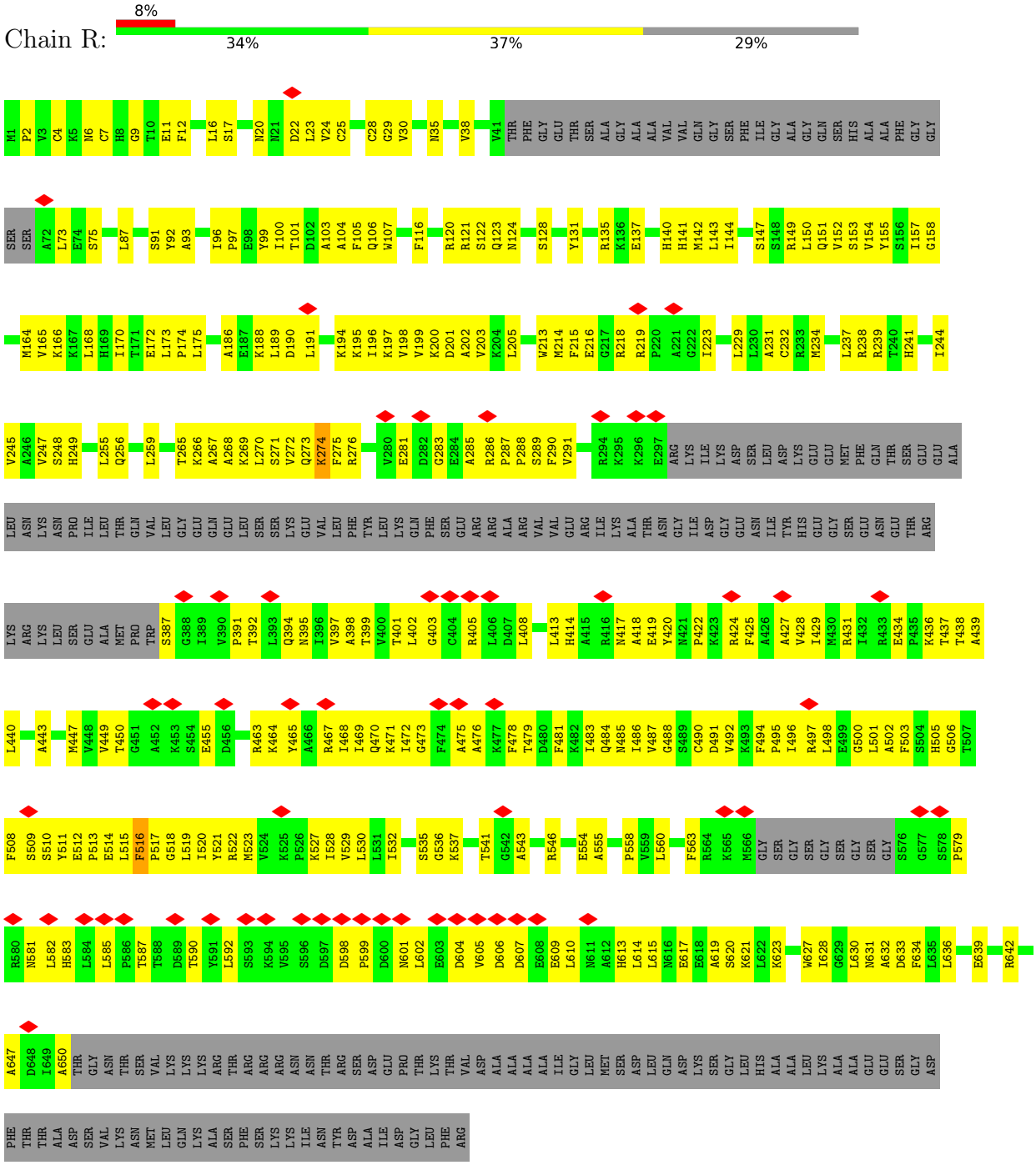



• Molecule 17: DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7

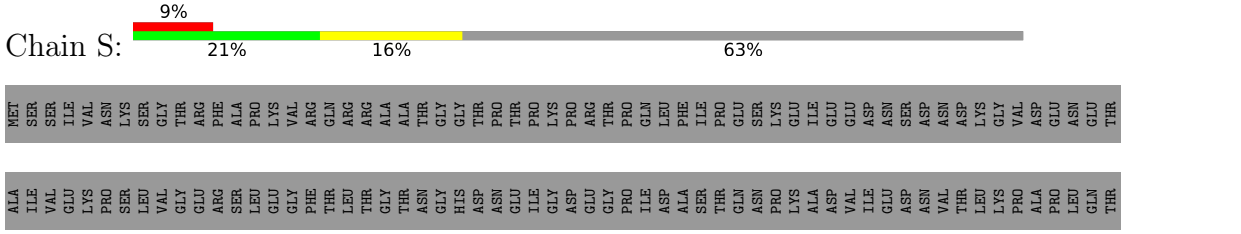
Chain Q:

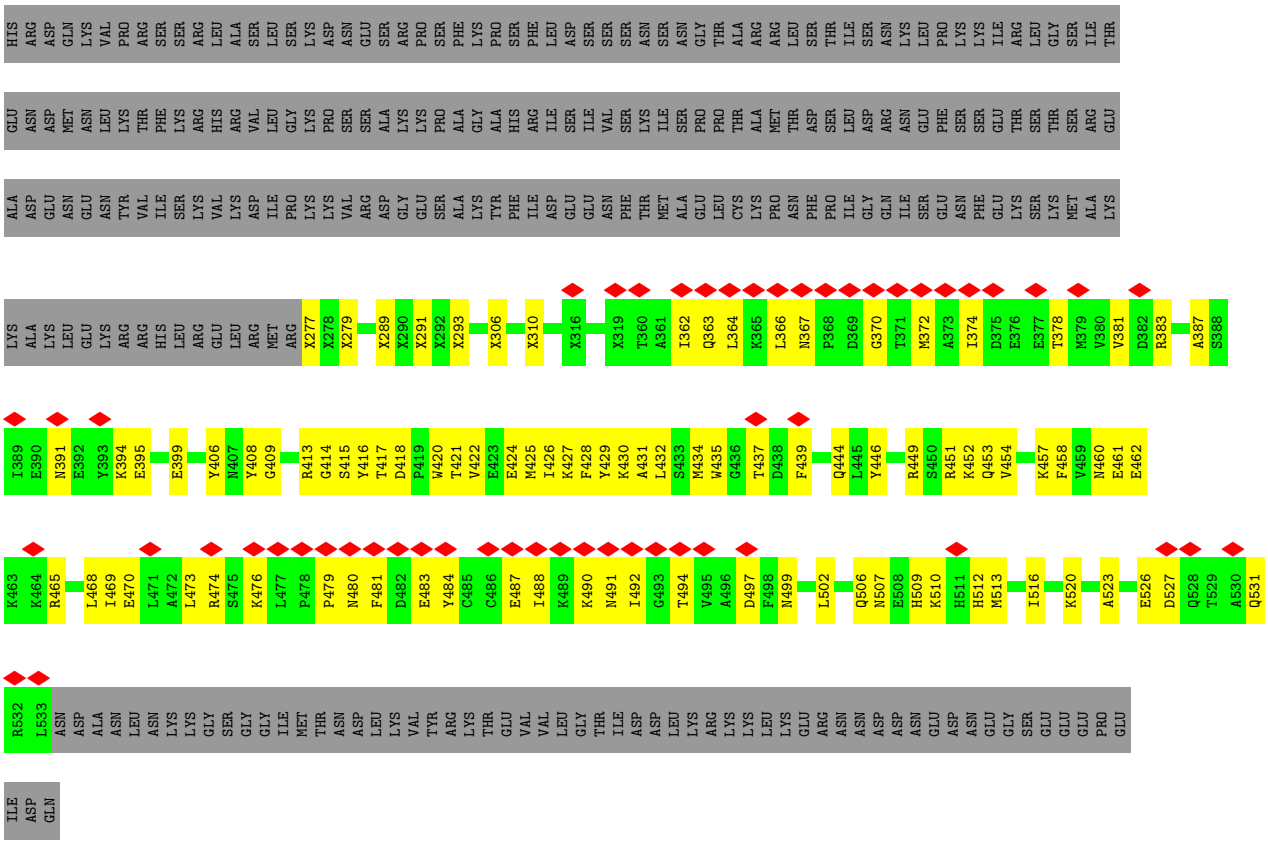



• Molecule 18: Transcription factor IIIB 70 kDa subunit,TATA-box-binding protein,Transcriptio n factor IIIB 70 kDa subunit



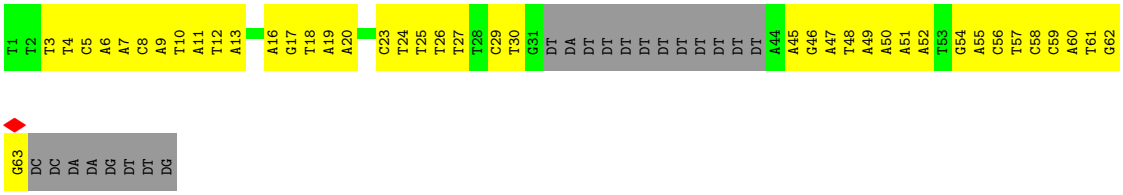

• Molecule 19: Transcription factor TFIIIB component B",Transcription factor TFIIIB component B",Transcription factor TFIIIB component B",Transcription factor TFIIIB component B",Transcription factor TFIIIB component B"





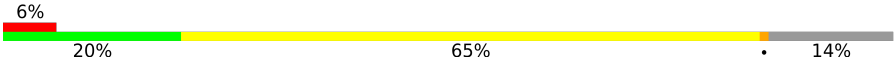
• Molecule 20: DNA (71-MER)

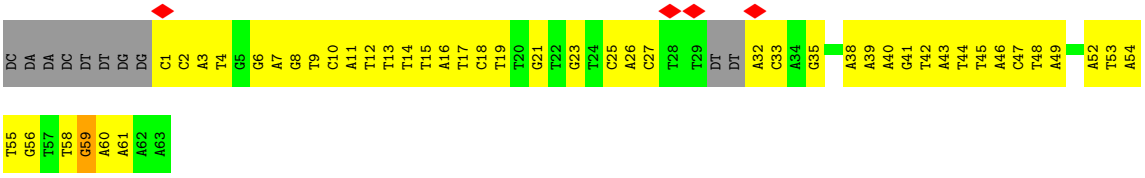
Chain X:

• Molecule 21: DNA (71-MER)

Chain Y:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 74281 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion. | Depositor |
| Microscope | JEOL 3200FS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 68.9 | 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 | 0.279 | Depositor |
| Minimum map value | -0.190 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.009 | Depositor |
| Recommended contour level | 0.04 | Depositor |
| Map size (Å) | 339.84, 339.84, 339.84 | wwPDB |
| Map dimensions | 288, 288, 288 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.18, 1.18, 1.18 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.43 | 0/11358 | 0.63 | 0/15345 |
| 2 | B | 0.43 | 0/8943 | 0.63 | 0/12068 |
| 3 | C | 0.45 | 0/2711 | 0.57 | 0/3676 |
| 4 | D | 0.27 | 0/991 | 0.51 | 0/1328 |
| 5 | E | 0.35 | 0/1795 | 0.55 | 0/2416 |
| 6 | F | 0.50 | 1/683 (0.1%) | 0.64 | 0/923 |
| 7 | G | 0.32 | 0/1523 | 0.56 | 0/2066 |
| 8 | H | 0.43 | 0/1138 | 0.61 | 0/1540 |
| 9 | I | 0.36 | 0/328 | 0.63 | 0/445 |
| 10 | J | 0.51 | 0/558 | 0.73 | 0/750 |
| 11 | K | 0.47 | 0/803 | 0.63 | 0/1083 |
| 12 | L | 0.40 | 0/365 | 0.60 | 0/485 |
| 13 | M | 0.30 | 0/1369 | 0.56 | 0/1851 |
| 14 | N | 0.28 | 0/855 | 0.60 | 0/1149 |
| 15 | O | 0.34 | 0/4394 | 0.63 | 0/5928 |
| 16 | P | 0.30 | 0/2282 | 0.52 | 0/3075 |
| 17 | Q | 0.30 | 0/281 | 0.45 | 0/381 |
| 18 | R | 0.30 | 0/4200 | 0.51 | 0/5659 |
| 19 | S | 0.29 | 0/1464 | 0.48 | 0/1971 |
| 20 | X | 0.65 | 0/1164 | 1.05 | 0/1792 |
| 21 | Y | 0.63 | 0/1400 | 1.03 | 1/2157 (0.0%) |
| All | All | 0.41 | 1/48605 (0.0%) | 0.63 | 1/66088 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | F | 130 | ILE | C-N | -6.92 | 1.21 | 1.34 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | Y | 59 | DG | O4'-C1'-N9 | 6.44 | 112.50 | 108.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 11159 | 0 | 11285 | 860 | 0 |
| 2 | B | 8788 | 0 | 8902 | 703 | 0 |
| 3 | C | 2655 | 0 | 2628 | 155 | 0 |
| 4 | D | 977 | 0 | 983 | 55 | 0 |
| 5 | E | 1759 | 0 | 1788 | 124 | 0 |
| 6 | F | 671 | 0 | 692 | 27 | 0 |
| 7 | G | 1484 | 0 | 1485 | 115 | 0 |
| 8 | H | 1120 | 0 | 1089 | 67 | 0 |
| 9 | I | 321 | 0 | 303 | 27 | 0 |
| 10 | J | 549 | 0 | 560 | 63 | 0 |
| 11 | K | 792 | 0 | 790 | 45 | 0 |
| 12 | L | 363 | 0 | 386 | 20 | 0 |
| 13 | M | 1338 | 0 | 1307 | 158 | 0 |
| 14 | N | 845 | 0 | 891 | 104 | 0 |
| 15 | O | 4329 | 0 | 4497 | 345 | 0 |
| 16 | P | 2242 | 0 | 2265 | 140 | 0 |
| 17 | Q | 368 | 0 | 308 | 21 | 0 |
| 18 | R | 4131 | 0 | 4230 | 255 | 0 |
| 19 | S | 1649 | 0 | 1457 | 88 | 0 |
| 20 | X | 1040 | 0 | 584 | 66 | 0 |
| 21 | Y | 1249 | 0 | 696 | 69 | 0 |
| 22 | A | 2 | 0 | 0 | 0 | 0 |
| 22 | B | 1 | 0 | 0 | 0 | 0 |
| 22 | I | 1 | 0 | 0 | 0 | 0 |
| 22 | J | 1 | 0 | 0 | 0 | 0 |
| 22 | L | 1 | 0 | 0 | 0 | 0 |
| 22 | R | 1 | 0 | 0 | 0 | 0 |
| All | All | 47836 | 0 | 47126 | 3059 | 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 33.

All (3059) 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) |
|---|---|---|---|
| 13:M:84:SER:O | 13:M:85:LEU:HD12 | 1.26 | 1.31 |
| 2:B:546:SER:HB2 | 14:N:391:LEU:CD2 | 1.63 | 1.29 |
| 1:A:249:PRO:CD | 1:A:250:SER:H | 1.43 | 1.29 |
| 16:P:264:THR:O | 16:P:265:LEU:HG | 1.23 | 1.29 |
| 1:A:1145:LEU:HD11 | 1:A:1157:VAL:CG2 | 1.61 | 1.28 |
| 15:O:516:LEU:HD12 | 15:O:516:LEU:O | 1.17 | 1.24 |
| 1:A:1369:LEU:CD2 | 1:A:1374:PHE:HE2 | 1.49 | 1.23 |
| 13:M:183:PHE:CE1 | 13:M:185:TYR:CD2 | 2.27 | 1.23 |
| 1:A:327:ILE:HA | 1:A:353:PHE:CD2 | 1.74 | 1.20 |
| 10:J:42:LYS:HE3 | 10:J:43:ARG:NH1 | 1.55 | 1.20 |
| 8:H:104:PHE:O | 8:H:105:GLU:HG3 | 1.42 | 1.18 |
| 13:M:104:HIS:CG | 13:M:105:PRO:HD2 | 1.77 | 1.18 |
| 18:R:7:CYS:SG | 18:R:28:CYS:HB3 | 1.82 | 1.18 |
| 2:B:933:PHE:CE2 | 3:C:226:SER:HB2 | 1.79 | 1.17 |
| 1:A:1145:LEU:CD1 | 1:A:1157:VAL:HG21 | 1.74 | 1.17 |
| 1:A:1169:VAL:HG23 | 1:A:1170:ALA:H | 1.10 | 1.15 |
| 13:M:183:PHE:CD1 | 13:M:185:TYR:CD2 | 2.34 | 1.14 |
| 15:O:303:ARG:HA | 16:P:265:LEU:HD21 | 1.22 | 1.14 |
| 2:B:934:ASN:HB3 | 2:B:1004:LEU:HD23 | 1.26 | 1.12 |
| 1:A:1369:LEU:CD2 | 1:A:1374:PHE:CE2 | 2.33 | 1.11 |
| 1:A:372:ARG:HD2 | 2:B:1050:PRO:O | 1.49 | 1.11 |
| 15:O:353:GLU:HA | 15:O:357:PRO:HD2 | 1.29 | 1.10 |
| 15:O:515:LYS:O | 15:O:516:LEU:HG | 1.48 | 1.10 |
| 16:P:311:TYR:HA | 17:Q:40:PRO:HA | 1.30 | 1.09 |
| 1:A:371:LYS:NZ | 2:B:1122:PRO:HB3 | 1.67 | 1.08 |
| 2:B:780:ARG:HH12 | 10:J:6:ARG:CD | 1.65 | 1.08 |
| 7:G:87:GLY:O | 7:G:146:ILE:HB | 1.54 | 1.08 |
| 12:L:31:CYS:HB2 | 12:L:34:CYS:SG | 1.94 | 1.08 |
| 2:B:546:SER:CB | 14:N:391:LEU:CD2 | 2.30 | 1.08 |
| 1:A:1369:LEU:HD21 | 1:A:1374:PHE:HE2 | 1.19 | 1.08 |
| 15:O:352:VAL:HG13 | 15:O:353:GLU:OE1 | 1.53 | 1.08 |
| 1:A:249:PRO:HD2 | 1:A:250:SER:N | 1.54 | 1.07 |
| 13:M:183:PHE:CE1 | 13:M:185:TYR:HD2 | 1.66 | 1.06 |
| 2:B:546:SER:CB | 14:N:391:LEU:HD23 | 1.84 | 1.06 |
| 1:A:18:PHE:HE1 | 2:B:1139:PRO:HB3 | 1.22 | 1.05 |
| 1:A:235:LYS:HB3 | 1:A:252:ARG:HE | 1.16 | 1.05 |
| 2:B:671:THR:HG22 | 2:B:672:HIS:CE1 | 1.92 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:183:PHE:CD1 | 13:M:185:TYR:HD2 | 1.73 | 1.05 |
| 1:A:974:LEU:HD21 | 1:A:998:TYR:HB3 | 1.40 | 1.04 |
| 2:B:780:ARG:HH12 | 10:J:6:ARG:HD3 | 1.21 | 1.04 |
| 15:O:498:SER:HB2 | 16:P:296:TYR:HB2 | 1.39 | 1.04 |
| 2:B:780:ARG:NH2 | 3:C:217:ALA:HB1 | 1.72 | 1.04 |
| 2:B:1045:VAL:HG23 | 2:B:1046:LEU:HD12 | 1.40 | 1.04 |
| 2:B:780:ARG:NH1 | 10:J:6:ARG:CD | 2.20 | 1.03 |
| 15:O:516:LEU:O | 15:O:516:LEU:CD1 | 2.06 | 1.03 |
| 10:J:42:LYS:HE3 | 10:J:43:ARG:HH12 | 0.86 | 1.02 |
| 13:M:183:PHE:CE1 | 13:M:185:TYR:CE2 | 2.47 | 1.01 |
| 19:S:483:GLU:O | 19:S:487:GLU:HB2 | 1.61 | 1.01 |
| 15:O:110:THR:HG22 | 15:O:116:LYS:HA | 1.41 | 1.00 |
| 1:A:371:LYS:HZ3 | 2:B:1122:PRO:HB3 | 1.21 | 0.99 |
| 2:B:546:SER:HB2 | 14:N:391:LEU:HD23 | 1.38 | 0.99 |
| 11:K:88:PHE:HB3 | 11:K:106:GLN:HG2 | 1.41 | 0.99 |
| 1:A:239:CYS:SG | 1:A:246:ALA:HB2 | 2.03 | 0.99 |
| 7:G:83:GLU:O | 7:G:149:ARG:HA | 1.63 | 0.99 |
| 2:B:551:LEU:HD11 | 14:N:388:THR:H | 1.25 | 0.98 |
| 2:B:671:THR:CG2 | 2:B:672:HIS:CE1 | 2.47 | 0.98 |
| 15:O:498:SER:CB | 16:P:296:TYR:HB2 | 1.94 | 0.98 |
| 13:M:104:HIS:CG | 13:M:105:PRO:CD | 2.47 | 0.98 |
| 2:B:671:THR:HG22 | 2:B:672:HIS:ND1 | 1.78 | 0.98 |
| 1:A:975:VAL:HG22 | 1:A:976:ARG:H | 1.30 | 0.97 |
| 2:B:933:PHE:CE2 | 3:C:226:SER:CB | 2.47 | 0.97 |
| 15:O:498:SER:HB2 | 16:P:296:TYR:CB | 1.94 | 0.97 |
| 2:B:415:GLU:HG2 | 2:B:416:TYR:H | 1.30 | 0.96 |
| 1:A:285:LEU:HD21 | 1:A:353:PHE:HD1 | 1.28 | 0.96 |
| 2:B:933:PHE:HE2 | 3:C:226:SER:CB | 1.76 | 0.95 |
| 2:B:780:ARG:NH1 | 10:J:6:ARG:HD3 | 1.79 | 0.95 |
| 3:C:222:VAL:HG11 | 3:C:225:ALA:HB2 | 1.48 | 0.95 |
| 2:B:780:ARG:NH1 | 10:J:6:ARG:HD2 | 1.81 | 0.95 |
| 1:A:617:ASN:OD1 | 1:A:618:HIS:N | 2.00 | 0.94 |
| 1:A:18:PHE:CE1 | 2:B:1139:PRO:HB3 | 2.02 | 0.94 |
| 13:M:94:PRO:HA | 14:N:391:LEU:O | 1.67 | 0.94 |
| 1:A:18:PHE:HD1 | 2:B:1139:PRO:HA | 1.30 | 0.94 |
| 4:D:126:GLN:O | 4:D:127:LEU:HG | 1.68 | 0.93 |
| 1:A:373:VAL:O | 2:B:1050:PRO:HG2 | 1.67 | 0.93 |
| 2:B:772:VAL:HG13 | 2:B:943:ILE:HG23 | 1.49 | 0.93 |
| 3:C:33:VAL:O | 3:C:34:GLU:HB2 | 1.68 | 0.93 |
| 13:M:104:HIS:HE1 | 14:N:395:ILE:HD13 | 1.31 | 0.93 |
| 1:A:1266:ALA:O | 1:A:1269:ASP:HB3 | 1.67 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:110:LEU:HB3 | 4:D:120:LYS:HE3 | 1.50 | 0.92 |
| 13:M:84:SER:C | 13:M:85:LEU:HD12 | 1.89 | 0.92 |
| 18:R:22:ASP:OD1 | 18:R:23:LEU:N | 2.02 | 0.92 |
| 1:A:664:MET:HB3 | 1:A:669:LEU:CD2 | 2.00 | 0.92 |
| 1:A:15:GLY:H | 1:A:1408:VAL:HG12 | 1.31 | 0.92 |
| 3:C:119:ASN:C | 3:C:120:LEU:HG | 1.90 | 0.91 |
| 1:A:285:LEU:HD21 | 1:A:353:PHE:CD1 | 2.05 | 0.91 |
| 1:A:196:ILE:O | 1:A:200:GLU:HG3 | 1.67 | 0.91 |
| 16:P:33:GLN:NE2 | 16:P:49:MET:SD | 2.44 | 0.91 |
| 11:K:88:PHE:HB3 | 11:K:106:GLN:CG | 2.02 | 0.90 |
| 15:O:303:ARG:HA | 16:P:265:LEU:CD2 | 2.01 | 0.90 |
| 15:O:105:LYS:HB2 | 15:O:121:TYR:HB2 | 1.53 | 0.90 |
| 19:S:458:PHE:O | 19:S:462:GLU:HB2 | 1.71 | 0.90 |
| 2:B:1139:PRO:O | 2:B:1140:ARG:O | 1.87 | 0.90 |
| 18:R:213:TRP:HH2 | 18:R:497:ARG:HA | 1.36 | 0.90 |
| 1:A:444:LEU:HD11 | 1:A:445:ARG:HH11 | 1.37 | 0.89 |
| 1:A:393:ALA:HB3 | 1:A:499:ARG:HB2 | 1.52 | 0.89 |
| 1:A:1369:LEU:HD22 | 1:A:1374:PHE:HE2 | 1.38 | 0.89 |
| 1:A:314:GLU:HB2 | 15:O:559:ALA:HB1 | 1.54 | 0.89 |
| 2:B:734:PRO:HB2 | 2:B:915:ARG:HH12 | 1.37 | 0.89 |
| 5:E:181:ALA:O | 5:E:182:ASP:O | 1.91 | 0.89 |
| 3:C:172:GLN:H | 3:C:175:GLN:HB3 | 1.38 | 0.89 |
| 1:A:154:CYS:CB | 1:A:157:CYS:SG | 2.60 | 0.88 |
| 2:B:933:PHE:HE1 | 2:B:1005:TYR:HD2 | 1.17 | 0.88 |
| 15:O:554:THR:HG23 | 15:O:561:ARG:HE | 1.36 | 0.88 |
| 13:M:183:PHE:HE1 | 13:M:185:TYR:CE2 | 1.90 | 0.88 |
| 18:R:397:VAL:HA | 18:R:449:VAL:O | 1.74 | 0.88 |
| 1:A:235:LYS:HB3 | 1:A:252:ARG:NE | 1.88 | 0.88 |
| 1:A:109:ASN:HD22 | 1:A:159:ALA:CB | 1.85 | 0.88 |
| 1:A:1369:LEU:HD21 | 1:A:1374:PHE:CE2 | 2.03 | 0.88 |
| 1:A:1145:LEU:CD2 | 1:A:1308:GLY:O | 2.21 | 0.88 |
| 18:R:232:CYS:HB3 | 18:R:237:LEU:HD11 | 1.54 | 0.88 |
| 20:X:6:DA:H4' | 20:X:7:DA:OP1 | 1.73 | 0.88 |
| 1:A:100:ILE:O | 1:A:104:GLN:HB2 | 1.73 | 0.88 |
| 1:A:1169:VAL:HG23 | 1:A:1170:ALA:N | 1.88 | 0.87 |
| 1:A:154:CYS:HB3 | 1:A:157:CYS:SG | 2.14 | 0.87 |
| 1:A:1369:LEU:HD22 | 1:A:1374:PHE:CE2 | 2.09 | 0.87 |
| 16:P:11:LEU:O | 16:P:15:ALA:HB2 | 1.73 | 0.87 |
| 16:P:264:THR:O | 16:P:265:LEU:CG | 2.18 | 0.87 |
| 1:A:249:PRO:HD2 | 1:A:250:SER:H | 0.71 | 0.87 |
| 15:O:193:GLN:O | 15:O:195:CYS:N | 2.08 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:735:MET:HB2 | 2:B:754:ASN:HD21 | 1.39 | 0.87 |
| 7:G:53:THR:HG21 | 7:G:71:THR:HG22 | 1.57 | 0.86 |
| 1:A:327:ILE:HG22 | 1:A:353:PHE:CE2 | 2.11 | 0.86 |
| 5:E:181:ALA:O | 5:E:182:ASP:C | 2.12 | 0.86 |
| 7:G:125:GLU:HG2 | 7:G:126:SER:N | 1.88 | 0.86 |
| 13:M:94:PRO:CA | 14:N:391:LEU:O | 2.22 | 0.86 |
| 1:A:172:GLY:HA3 | 1:A:331:SER:HB3 | 1.58 | 0.86 |
| 1:A:238:ASP:OD1 | 1:A:239:CYS:N | 2.09 | 0.86 |
| 1:A:664:MET:CB | 1:A:669:LEU:HD21 | 2.06 | 0.86 |
| 3:C:119:ASN:O | 3:C:120:LEU:HG | 1.76 | 0.86 |
| 16:P:138:LYS:HD2 | 16:P:143:PRO:HB3 | 1.57 | 0.86 |
| 13:M:90:TYR:O | 14:N:392:GLN:HG3 | 1.76 | 0.86 |
| 15:O:156:VAL:HG12 | 15:O:189:SER:HB3 | 1.56 | 0.85 |
| 12:L:31:CYS:SG | 12:L:48:CYS:HB3 | 2.16 | 0.85 |
| 1:A:946:THR:HG21 | 1:A:1066:SER:HA | 1.58 | 0.85 |
| 4:D:145:PHE:HB2 | 4:D:149:THR:HG21 | 1.56 | 0.85 |
| 1:A:49:LYS:HD2 | 1:A:54:LEU:HB3 | 1.59 | 0.85 |
| 13:M:158:GLN:HE21 | 14:N:308:GLN:HE21 | 1.25 | 0.85 |
| 10:J:42:LYS:CE | 10:J:43:ARG:HH12 | 1.82 | 0.85 |
| 15:O:143:GLN:HE21 | 15:O:196:GLU:HG2 | 1.41 | 0.85 |
| 15:O:263:LEU:HB3 | 15:O:272:ARG:HH21 | 1.41 | 0.85 |
| 1:A:327:ILE:HA | 1:A:353:PHE:CE2 | 2.12 | 0.85 |
| 15:O:190:LEU:HD13 | 15:O:194:LEU:HD23 | 1.57 | 0.85 |
| 1:A:1166:LEU:HA | 1:A:1169:VAL:HG22 | 1.56 | 0.84 |
| 12:L:31:CYS:SG | 12:L:48:CYS:CB | 2.64 | 0.84 |
| 1:A:356:ARG:HG3 | 2:B:1131:GLU:OE2 | 1.76 | 0.84 |
| 13:M:90:TYR:O | 14:N:392:GLN:CG | 2.26 | 0.84 |
| 15:O:190:LEU:HA | 15:O:193:GLN:HB3 | 1.60 | 0.84 |
| 15:O:547:GLU:HG2 | 15:O:548:ILE:H | 1.43 | 0.84 |
| 15:O:640:ARG:HH12 | 16:P:309:VAL:HA | 1.43 | 0.84 |
| 2:B:780:ARG:CZ | 3:C:217:ALA:HB1 | 2.07 | 0.84 |
| 13:M:89:GLN:HE21 | 13:M:178:GLN:HE22 | 1.20 | 0.84 |
| 1:A:235:LYS:HD2 | 1:A:252:ARG:HB2 | 1.58 | 0.84 |
| 2:B:933:PHE:CD2 | 2:B:937:GLY:HA2 | 2.11 | 0.84 |
| 14:N:302:GLU:HB3 | 14:N:410:GLY:HA2 | 1.59 | 0.83 |
| 15:O:597:GLN:HA | 15:O:600:SER:HB2 | 1.61 | 0.83 |
| 7:G:84:ILE:HA | 7:G:148:PHE:O | 1.78 | 0.83 |
| 1:A:235:LYS:CB | 1:A:252:ARG:HE | 1.91 | 0.83 |
| 2:B:931:MET:CG | 2:B:932:PRO:HD2 | 2.09 | 0.83 |
| 1:A:556:ASP:HB3 | 2:B:767:ILE:CD1 | 2.09 | 0.83 |
| 1:A:1305:CYS:SG | 5:E:11:ARG:NH1 | 2.49 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:321:GLN:H | 2:B:324:ILE:HB | 1.41 | 0.83 |
| 9:I:8:CYS:HB3 | 9:I:29:CYS:SG | 2.17 | 0.83 |
| 15:O:288:MET:SD | 15:O:291:ARG:NH2 | 2.51 | 0.83 |
| 1:A:664:MET:HB3 | 1:A:669:LEU:HD21 | 1.60 | 0.83 |
| 15:O:292:ARG:HH12 | 15:O:650:VAL:HA | 1.44 | 0.82 |
| 1:A:235:LYS:CE | 1:A:254:GLU:HG3 | 2.09 | 0.82 |
| 1:A:239:CYS:SG | 1:A:240:GLU:N | 2.51 | 0.82 |
| 2:B:109:LYS:HG3 | 2:B:111:TYR:H | 1.42 | 0.82 |
| 2:B:373:GLY:HA2 | 2:B:651:VAL:HG21 | 1.61 | 0.82 |
| 13:M:104:HIS:CD2 | 13:M:105:PRO:HD2 | 2.14 | 0.82 |
| 8:H:104:PHE:O | 8:H:105:GLU:CG | 2.27 | 0.82 |
| 17:Q:38:SER:O | 17:Q:39:ILE:O | 1.98 | 0.82 |
| 2:B:936:GLN:HB3 | 10:J:43:ARG:HD3 | 1.62 | 0.82 |
| 1:A:642:PRO:HB2 | 1:A:644:GLU:HG2 | 1.62 | 0.81 |
| 2:B:538:VAL:HG12 | 2:B:565:ILE:HB | 1.62 | 0.81 |
| 5:E:109:ILE:HG22 | 5:E:133:GLU:HB3 | 1.59 | 0.81 |
| 1:A:644:GLU:OE2 | 1:A:651:PHE:HD2 | 1.63 | 0.81 |
| 2:B:933:PHE:CE2 | 2:B:937:GLY:HA2 | 2.15 | 0.81 |
| 13:M:112:TYR:HD1 | 13:M:119:TRP:HE1 | 1.28 | 0.81 |
| 1:A:373:VAL:O | 2:B:1050:PRO:CG | 2.28 | 0.81 |
| 2:B:934:ASN:HB3 | 2:B:1004:LEU:CD2 | 2.07 | 0.81 |
| 1:A:1330:ALA:HB2 | 5:E:150:VAL:HG22 | 1.63 | 0.81 |
| 2:B:933:PHE:CG | 2:B:934:ASN:N | 2.48 | 0.81 |
| 5:E:179:GLN:O | 5:E:180:ARG:O | 1.98 | 0.80 |
| 15:O:124:GLU:HG3 | 15:O:126:GLY:H | 1.44 | 0.80 |
| 1:A:1038:GLU:HB3 | 1:A:1042:ILE:HD11 | 1.62 | 0.80 |
| 2:B:933:PHE:CZ | 3:C:226:SER:HB2 | 2.15 | 0.80 |
| 2:B:1047:THR:HG22 | 2:B:1049:GLN:H | 1.45 | 0.80 |
| 13:M:94:PRO:HB3 | 14:N:391:LEU:O | 1.81 | 0.80 |
| 15:O:183:MET:O | 15:O:187:ILE:HG12 | 1.81 | 0.80 |
| 15:O:105:LYS:HG2 | 15:O:123:ASN:HA | 1.62 | 0.80 |
| 13:M:112:TYR:H | 13:M:243:ILE:HG21 | 1.45 | 0.80 |
| 1:A:18:PHE:CD1 | 2:B:1139:PRO:HA | 2.16 | 0.80 |
| 18:R:213:TRP:HD1 | 18:R:287:PRO:HD3 | 1.46 | 0.80 |
| 15:O:48:LEU:HD22 | 15:O:581:LEU:HD11 | 1.63 | 0.80 |
| 15:O:324:PRO:HB2 | 15:O:328:ASP:HB3 | 1.64 | 0.80 |
| 2:B:364:LYS:HG3 | 2:B:365:MET:H | 1.46 | 0.79 |
| 2:B:1026:LYS:NZ | 2:B:1030:MET:SD | 2.54 | 0.79 |
| 16:P:176:ASN:HA | 16:P:179:LEU:HB2 | 1.64 | 0.79 |
| 4:D:126:GLN:C | 4:D:127:LEU:HG | 2.01 | 0.79 |
| 5:E:88:VAL:HG23 | 5:E:117:THR:HG22 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:117:THR:HG23 | 5:E:120:ALA:H | 1.45 | 0.79 |
| 1:A:400:LYS:HA | 1:A:465:HIS:HD2 | 1.45 | 0.79 |
| 2:B:915:ARG:HD3 | 2:B:960:GLU:OE2 | 1.82 | 0.79 |
| 15:O:200:LEU:HB3 | 15:O:280:LEU:HB3 | 1.64 | 0.79 |
| 2:B:546:SER:CB | 14:N:391:LEU:HD21 | 2.12 | 0.79 |
| 13:M:104:HIS:ND1 | 13:M:105:PRO:HD3 | 1.98 | 0.79 |
| 1:A:371:LYS:NZ | 2:B:1122:PRO:CB | 2.45 | 0.79 |
| 2:B:932:PRO:O | 2:B:940:PRO:HD2 | 1.82 | 0.79 |
| 9:I:29:CYS:HA | 13:M:183:PHE:HE2 | 1.47 | 0.79 |
| 1:A:235:LYS:NZ | 1:A:254:GLU:HG3 | 1.96 | 0.79 |
| 1:A:353:PHE:O | 1:A:356:ARG:HG2 | 1.82 | 0.79 |
| 2:B:1112:SER:HB2 | 2:B:1114:GLU:HG2 | 1.63 | 0.79 |
| 1:A:675:HIS:HA | 1:A:937:ARG:HH22 | 1.46 | 0.79 |
| 13:M:94:PRO:HA | 14:N:392:GLN:HA | 1.63 | 0.79 |
| 15:O:110:THR:HG21 | 15:O:115:LYS:O | 1.83 | 0.79 |
| 1:A:197:TRP:CZ3 | 15:O:567:ARG:NH1 | 2.51 | 0.78 |
| 15:O:80:VAL:HG11 | 15:O:87:ASP:HB2 | 1.64 | 0.78 |
| 12:L:31:CYS:CB | 12:L:34:CYS:SG | 2.63 | 0.78 |
| 1:A:124:LEU:HB3 | 1:A:128:ARG:HH12 | 1.48 | 0.78 |
| 16:P:235:LEU:HD21 | 16:P:239:ASN:HB3 | 1.65 | 0.78 |
| 19:S:494:THR:HB | 19:S:497:ASP:HB2 | 1.65 | 0.78 |
| 3:C:134:LEU:HD23 | 3:C:167:LEU:HD23 | 1.65 | 0.78 |
| 2:B:741:ILE:HG23 | 2:B:746:TYR:HB3 | 1.66 | 0.78 |
| 2:B:915:ARG:HD2 | 2:B:1023:TYR:HB3 | 1.66 | 0.78 |
| 3:C:103:LEU:HD22 | 10:J:5:VAL:HG23 | 1.66 | 0.78 |
| 2:B:931:MET:HG2 | 2:B:932:PRO:HD2 | 1.66 | 0.78 |
| 2:B:108:THR:HG22 | 2:B:109:LYS:H | 1.49 | 0.77 |
| 2:B:757:VAL:O | 2:B:1019:PHE:HB2 | 1.83 | 0.77 |
| 13:M:183:PHE:HE1 | 13:M:185:TYR:HE2 | 1.30 | 0.77 |
| 7:G:5:SER:O | 7:G:73:ARG:HA | 1.83 | 0.77 |
| 1:A:269:ARG:NH2 | 1:A:286:THR:H | 1.83 | 0.77 |
| 1:A:1145:LEU:HD23 | 1:A:1308:GLY:O | 1.84 | 0.77 |
| 1:A:1163:LYS:HG3 | 1:A:1164:THR:H | 1.47 | 0.77 |
| 15:O:156:VAL:HG12 | 15:O:189:SER:CB | 2.15 | 0.77 |
| 19:S:458:PHE:O | 19:S:462:GLU:CB | 2.33 | 0.77 |
| 19:S:470:GLU:O | 19:S:474:ARG:HB3 | 1.84 | 0.77 |
| 1:A:1048:VAL:HG11 | 1:A:1053:LYS:HG3 | 1.65 | 0.77 |
| 16:P:69:GLU:HG3 | 16:P:70:LEU:H | 1.50 | 0.77 |
| 1:A:235:LYS:CD | 1:A:252:ARG:HB2 | 2.14 | 0.77 |
| 3:C:224:THR:HB | 10:J:10:CYS:SG | 2.25 | 0.77 |
| 2:B:266:LEU:HD21 | 9:I:4:PHE:HA | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:705:LEU:CD2 | 2:B:761:SER:HB2 | 2.15 | 0.77 |
| 3:C:152:ASP:HB2 | 3:C:155:GLU:HG2 | 1.67 | 0.77 |
| 15:O:172:GLU:HG3 | 15:O:276:PRO:HB2 | 1.66 | 0.77 |
| 5:E:29:PHE:HB2 | 5:E:65:THR:HB | 1.65 | 0.77 |
| 18:R:632:ALA:O | 18:R:636:LEU:HB2 | 1.85 | 0.77 |
| 1:A:200:GLU:HB3 | 15:O:516:LEU:CD2 | 2.15 | 0.76 |
| 2:B:971:GLY:HA2 | 10:J:51:LEU:HD11 | 1.66 | 0.76 |
| 3:C:231:PRO:HB3 | 3:C:275:VAL:HG22 | 1.67 | 0.76 |
| 11:K:60:SER:HA | 11:K:106:GLN:HA | 1.65 | 0.76 |
| 15:O:515:LYS:O | 15:O:516:LEU:CG | 2.33 | 0.76 |
| 13:M:105:PRO:O | 13:M:106:PHE:HB2 | 1.85 | 0.76 |
| 2:B:671:THR:CG2 | 2:B:672:HIS:ND1 | 2.47 | 0.76 |
| 15:O:98:LEU:HB3 | 15:O:103:CYS:HB2 | 1.65 | 0.76 |
| 3:C:275:VAL:HG21 | 3:C:293:ARG:HD3 | 1.66 | 0.76 |
| 3:C:70:ILE:HG13 | 3:C:74:GLU:HB2 | 1.68 | 0.76 |
| 15:O:91:VAL:O | 15:O:95:LEU:HB2 | 1.85 | 0.76 |
| 15:O:196:GLU:HG3 | 15:O:197:MET:H | 1.49 | 0.76 |
| 1:A:645:MET:HE1 | 8:H:124:ARG:HB2 | 1.66 | 0.76 |
| 1:A:1396:LEU:HD13 | 2:B:1132:LEU:HD21 | 1.68 | 0.76 |
| 2:B:551:LEU:CD1 | 14:N:388:THR:H | 1.99 | 0.75 |
| 1:A:329:SER:O | 1:A:351:ARG:NH2 | 2.20 | 0.75 |
| 1:A:1184:ILE:HB | 1:A:1232:ILE:HB | 1.66 | 0.75 |
| 1:A:373:VAL:HG12 | 1:A:374:ASP:H | 1.51 | 0.75 |
| 15:O:353:GLU:CA | 15:O:357:PRO:HD2 | 2.12 | 0.75 |
| 18:R:200:LYS:HG2 | 18:R:276:ARG:HH22 | 1.50 | 0.75 |
| 1:A:197:TRP:HZ3 | 15:O:567:ARG:NH1 | 1.85 | 0.75 |
| 2:B:901:ARG:NH2 | 3:C:94:ASP:OD1 | 2.20 | 0.75 |
| 1:A:332:VAL:HG13 | 1:A:333:ASN:H | 1.51 | 0.75 |
| 1:A:541:LEU:HG | 1:A:551:ILE:HD11 | 1.69 | 0.75 |
| 15:O:292:ARG:HD2 | 15:O:488:LYS:HZ2 | 1.51 | 0.75 |
| 2:B:930:ASP:OD1 | 3:C:69:ARG:NH1 | 2.20 | 0.75 |
| 18:R:419:GLU:HB3 | 18:R:429:ILE:HD13 | 1.68 | 0.75 |
| 15:O:353:GLU:HB2 | 15:O:481:SER:OG | 1.85 | 0.75 |
| 1:A:114:LEU:HD11 | 1:A:148:CYS:HA | 1.68 | 0.75 |
| 3:C:119:ASN:O | 3:C:120:LEU:O | 2.05 | 0.75 |
| 1:A:1170:ALA:HA | 1:A:1188:ILE:HG12 | 1.67 | 0.74 |
| 2:B:671:THR:HG21 | 2:B:672:HIS:CE1 | 2.22 | 0.74 |
| 8:H:96:VAL:HG12 | 8:H:143:LEU:HD13 | 1.69 | 0.74 |
| 15:O:124:GLU:HG3 | 15:O:126:GLY:N | 2.02 | 0.74 |
| 1:A:1166:LEU:O | 1:A:1166:LEU:HD23 | 1.86 | 0.74 |
| 16:P:172:ILE:HG22 | 16:P:173:GLU:H | 1.52 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:321:LEU:O | 1:A:325:MET:HB2 | 1.88 | 0.74 |
| 1:A:1169:VAL:CG2 | 1:A:1170:ALA:H | 1.94 | 0.74 |
| 2:B:546:SER:OG | 14:N:391:LEU:HD23 | 1.87 | 0.74 |
| 18:R:467:ARG:HB2 | 18:R:602:LEU:HD11 | 1.68 | 0.74 |
| 2:B:551:LEU:HD11 | 14:N:388:THR:N | 2.02 | 0.74 |
| 15:O:54:LYS:HA | 15:O:58:GLY:HA2 | 1.68 | 0.74 |
| 7:G:96:GLY:N | 7:G:112:GLN:HG2 | 2.02 | 0.74 |
| 7:G:104:ILE:HG23 | 7:G:105:PHE:H | 1.52 | 0.74 |
| 1:A:1095:GLN:NE2 | 2:B:1068:ASP:OD2 | 2.20 | 0.74 |
| 18:R:266:LYS:HG2 | 18:R:283:GLY:HA3 | 1.69 | 0.74 |
| 1:A:181:ASP:HB2 | 1:A:220:ASP:OD1 | 1.88 | 0.74 |
| 1:A:200:GLU:HB3 | 15:O:516:LEU:HD23 | 1.68 | 0.74 |
| 5:E:87:SER:HA | 5:E:115:ASN:HB3 | 1.70 | 0.74 |
| 20:X:56:DC:O2 | 21:Y:8:DG:N2 | 2.20 | 0.74 |
| 15:O:110:THR:CG2 | 15:O:115:LYS:O | 2.35 | 0.74 |
| 2:B:933:PHE:O | 2:B:1004:LEU:HD22 | 1.88 | 0.74 |
| 3:C:121:PRO:O | 3:C:122:ASP:OD1 | 2.06 | 0.74 |
| 10:J:43:ARG:HH11 | 10:J:43:ARG:HG2 | 1.53 | 0.74 |
| 1:A:163:VAL:C | 1:A:180:HIS:HD2 | 1.91 | 0.73 |
| 1:A:395:PRO:HB3 | 1:A:496:ARG:HA | 1.69 | 0.73 |
| 3:C:256:ILE:HA | 3:C:268:LYS:H | 1.53 | 0.73 |
| 5:E:180:ARG:O | 5:E:182:ASP:N | 2.21 | 0.73 |
| 21:Y:55:DT:H2" | 21:Y:56:DG:C8 | 2.22 | 0.73 |
| 7:G:39:ILE:HD12 | 7:G:40:PRO:HD2 | 1.69 | 0.73 |
| 14:N:389:THR:HG23 | 14:N:390:PHE:H | 1.50 | 0.73 |
| 13:M:104:HIS:ND1 | 13:M:105:PRO:CD | 2.52 | 0.73 |
| 15:O:467:PHE:HD1 | 15:O:468:LEU:HD13 | 1.54 | 0.73 |
| 2:B:767:ILE:O | 2:B:945:ASN:ND2 | 2.21 | 0.73 |
| 3:C:116:VAL:HB | 3:C:209:ILE:HD11 | 1.71 | 0.73 |
| 5:E:21:GLU:HB3 | 5:E:35:VAL:HG21 | 1.71 | 0.73 |
| 15:O:292:ARG:NH2 | 15:O:653:MET:O | 2.22 | 0.73 |
| 13:M:90:TYR:HB3 | 13:M:179:LEU:HB3 | 1.69 | 0.73 |
| 13:M:158:GLN:HG2 | 14:N:308:GLN:HG2 | 1.69 | 0.73 |
| 1:A:572:ASP:OD1 | 1:A:573:ARG:N | 2.22 | 0.73 |
| 13:M:94:PRO:CB | 14:N:391:LEU:O | 2.35 | 0.73 |
| 2:B:167:ASP:O | 2:B:169:SER:N | 2.21 | 0.72 |
| 2:B:475:SER:HB3 | 2:B:510:LEU:O | 1.89 | 0.72 |
| 2:B:929:GLU:HG2 | 3:C:72:ILE:HG23 | 1.69 | 0.72 |
| 1:A:665:ASP:OD1 | 1:A:798:GLY:N | 2.23 | 0.72 |
| 14:N:290:ILE:O | 14:N:294:LEU:HB2 | 1.89 | 0.72 |
| 18:R:467:ARG:HA | 18:R:602:LEU:HD21 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:476:ARG:NH2 | 1:A:515:ASP:OD2 | 2.23 | 0.72 |
| 1:A:249:PRO:CD | 1:A:250:SER:N | 2.13 | 0.72 |
| 2:B:476:GLN:HG2 | 2:B:477:PHE:H | 1.53 | 0.72 |
| 2:B:933:PHE:O | 2:B:1004:LEU:CD2 | 2.37 | 0.72 |
| 2:B:1106:TRP:HE1 | 7:G:162:SER:HA | 1.55 | 0.72 |
| 3:C:197:ARG:HB3 | 3:C:198:PRO:HD2 | 1.72 | 0.72 |
| 15:O:584:ASN:O | 15:O:588:LEU:N | 2.22 | 0.72 |
| 19:S:483:GLU:O | 19:S:487:GLU:CB | 2.37 | 0.72 |
| 2:B:1019:PHE:HE1 | 10:J:44:TYR:HH | 1.38 | 0.72 |
| 6:F:76:LYS:HD2 | 6:F:79:ARG:HE | 1.53 | 0.72 |
| 2:B:1139:PRO:O | 2:B:1140:ARG:C | 2.27 | 0.72 |
| 1:A:388:SER:OG | 1:A:695:ASN:ND2 | 2.23 | 0.72 |
| 15:O:46:LEU:HD13 | 15:O:69:VAL:HB | 1.71 | 0.72 |
| 1:A:327:ILE:HG22 | 1:A:353:PHE:CZ | 2.24 | 0.72 |
| 5:E:86:PRO:HA | 5:E:113:GLN:HB3 | 1.72 | 0.72 |
| 7:G:57:GLY:HA3 | 7:G:68:ILE:HG12 | 1.70 | 0.72 |
| 7:G:204:GLY:HA2 | 7:G:210:TRP:HB2 | 1.70 | 0.72 |
| 16:P:264:THR:C | 16:P:265:LEU:HG | 2.09 | 0.72 |
| 7:G:150:ILE:HG21 | 7:G:196:LEU:HD23 | 1.71 | 0.71 |
| 1:A:154:CYS:SG | 1:A:155:LEU:N | 2.62 | 0.71 |
| 1:A:869:ARG:HH22 | 2:B:502:THR:HB | 1.53 | 0.71 |
| 16:P:135:LYS:NZ | 16:P:150:LEU:O | 2.23 | 0.71 |
| 1:A:164:VAL:HB | 1:A:180:HIS:HB2 | 1.71 | 0.71 |
| 1:A:671:ASP:OD1 | 1:A:671:ASP:O | 2.08 | 0.71 |
| 1:A:330:ASP:OD1 | 1:A:331:SER:N | 2.23 | 0.71 |
| 1:A:597:ILE:HD11 | 1:A:603:LEU:HD12 | 1.73 | 0.71 |
| 2:B:197:GLN:NE2 | 2:B:476:GLN:OE1 | 2.21 | 0.71 |
| 15:O:156:VAL:CG1 | 15:O:189:SER:HB3 | 2.20 | 0.71 |
| 19:S:506:GLN:O | 19:S:510:LYS:HB2 | 1.91 | 0.71 |
| 1:A:1121:LEU:O | 1:A:1346:HIS:NE2 | 2.24 | 0.71 |
| 2:B:248:ALA:HB3 | 2:B:308:LYS:HG2 | 1.71 | 0.71 |
| 14:N:371:LEU:HD22 | 14:N:384:LYS:HD3 | 1.73 | 0.71 |
| 8:H:130:ARG:O | 8:H:134:ASN:ND2 | 2.24 | 0.71 |
| 1:A:249:PRO:CG | 1:A:250:SER:N | 2.54 | 0.71 |
| 2:B:795:LEU:HB2 | 2:B:894:ALA:HB3 | 1.73 | 0.71 |
| 2:B:1057:ASP:CG | 2:B:1058:GLY:H | 1.93 | 0.71 |
| 1:A:556:ASP:HB3 | 2:B:767:ILE:HD12 | 1.72 | 0.71 |
| 1:A:666:LYS:HA | 1:A:670:GLY:HA3 | 1.72 | 0.71 |
| 15:O:499:THR:HG23 | 16:P:312:PHE:CB | 2.21 | 0.70 |
| 2:B:481:ARG:HH21 | 21:Y:21:DG:H2' | 1.54 | 0.70 |
| 16:P:54:GLU:O | 16:P:58:LYS:N | 2.22 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1266:ALA:O | 1:A:1269:ASP:CB | 2.37 | 0.70 |
| 8:H:21:ASN:OD1 | 8:H:22:LYS:N | 2.25 | 0.70 |
| 18:R:152:VAL:HG22 | 18:R:153:SER:H | 1.57 | 0.70 |
| 1:A:400:LYS:HA | 1:A:465:HIS:CD2 | 2.26 | 0.70 |
| 1:A:827:PHE:HE2 | 1:A:833:PRO:HG3 | 1.55 | 0.70 |
| 7:G:45:CYS:HA | 7:G:76:VAL:HA | 1.74 | 0.70 |
| 2:B:658:TYR:CE2 | 2:B:670:MET:HG2 | 2.27 | 0.70 |
| 2:B:944:MET:HG2 | 2:B:945:ASN:H | 1.57 | 0.70 |
| 3:C:229:LEU:HB2 | 3:C:293:ARG:HH11 | 1.57 | 0.70 |
| 13:M:104:HIS:HE1 | 14:N:395:ILE:CD1 | 2.05 | 0.70 |
| 1:A:552:ALA:CB | 1:A:671:ASP:HB3 | 2.20 | 0.70 |
| 2:B:1055:SER:O | 2:B:1056:ARG:C | 2.27 | 0.70 |
| 1:A:664:MET:HB3 | 1:A:669:LEU:HD23 | 1.71 | 0.70 |
| 1:A:1145:LEU:HD11 | 1:A:1157:VAL:HG21 | 0.79 | 0.70 |
| 19:S:444:GLN:HE22 | 19:S:490:LYS:NZ | 1.90 | 0.70 |
| 1:A:373:VAL:C | 2:B:1050:PRO:HG2 | 2.12 | 0.70 |
| 4:D:7:ARG:HE | 4:D:10:PHE:HZ | 1.37 | 0.70 |
| 15:O:620:LEU:HD12 | 15:O:621:PRO:HD2 | 1.73 | 0.70 |
| 1:A:356:ARG:CG | 2:B:1131:GLU:OE2 | 2.40 | 0.69 |
| 1:A:705:LEU:HD21 | 2:B:761:SER:HB2 | 1.74 | 0.69 |
| 1:A:1429:LYS:HD3 | 6:F:137:TYR:HE2 | 1.57 | 0.69 |
| 2:B:774:ASN:ND2 | 2:B:777:SER:OG | 2.25 | 0.69 |
| 10:J:36:LEU:HD23 | 10:J:47:ARG:HG3 | 1.72 | 0.69 |
| 1:A:82:GLY:O | 1:A:263:ALA:N | 2.20 | 0.69 |
| 1:A:109:ASN:HD22 | 1:A:159:ALA:HB2 | 1.55 | 0.69 |
| 1:A:141:LEU:HA | 1:A:144:ILE:HG22 | 1.73 | 0.69 |
| 2:B:811:VAL:HA | 2:B:817:PRO:HA | 1.74 | 0.69 |
| 3:C:92:ILE:HD13 | 3:C:194:ALA:HB1 | 1.74 | 0.69 |
| 15:O:515:LYS:C | 15:O:516:LEU:HG | 2.13 | 0.69 |
| 2:B:186:ILE:HA | 2:B:191:GLU:HA | 1.74 | 0.69 |
| 1:A:1202:ILE:HD13 | 1:A:1224:ILE:HD12 | 1.75 | 0.69 |
| 2:B:612:LEU:HD13 | 2:B:672:HIS:HB3 | 1.75 | 0.69 |
| 1:A:325:MET:SD | 1:A:351:ARG:NH2 | 2.66 | 0.69 |
| 18:R:144:ILE:HD12 | 18:R:154:VAL:HG21 | 1.75 | 0.69 |
| 4:D:24:GLU:HG3 | 4:D:29:TRP:HA | 1.73 | 0.69 |
| 11:K:136:THR:HA | 11:K:139:ILE:HG22 | 1.74 | 0.69 |
| 1:A:205:LEU:HG | 1:A:212:GLU:HA | 1.74 | 0.69 |
| 2:B:705:MET:SD | 2:B:919:LYS:NZ | 2.65 | 0.69 |
| 14:N:363:ILE:HG12 | 14:N:373:VAL:HG22 | 1.75 | 0.69 |
| 1:A:164:VAL:CB | 1:A:180:HIS:HB2 | 2.23 | 0.69 |
| 2:B:77:ILE:HD13 | 2:B:98:ILE:HG12 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:325:GLU:HG3 | 2:B:328:ALA:HB3 | 1.75 | 0.69 |
| 3:C:42:VAL:O | 11:K:138:LYS:NZ | 2.26 | 0.69 |
| 16:P:131:GLN:HB3 | 16:P:133:TYR:CD2 | 2.28 | 0.69 |
| 18:R:213:TRP:CH2 | 18:R:497:ARG:HA | 2.25 | 0.69 |
| 1:A:107:CYS:HA | 1:A:161:ASN:HD22 | 1.57 | 0.69 |
| 1:A:643:ASN:HB2 | 1:A:651:PHE:CZ | 2.27 | 0.69 |
| 2:B:933:PHE:CE1 | 2:B:1005:TYR:HD2 | 2.05 | 0.69 |
| 7:G:96:GLY:H | 7:G:112:GLN:HG2 | 1.58 | 0.69 |
| 1:A:238:ASP:CG | 1:A:239:CYS:H | 1.94 | 0.69 |
| 1:A:1164:THR:HB | 1:A:1271:VAL:HA | 1.74 | 0.69 |
| 2:B:914:SER:OG | 2:B:957:LYS:NZ | 2.23 | 0.69 |
| 5:E:172:GLU:HG2 | 5:E:173:SER:H | 1.58 | 0.68 |
| 1:A:600:PRO:HG2 | 8:H:95:TYR:HD1 | 1.56 | 0.68 |
| 2:B:613:ILE:HA | 2:B:646:VAL:HG12 | 1.75 | 0.68 |
| 1:A:444:LEU:HD11 | 1:A:445:ARG:NH1 | 2.08 | 0.68 |
| 15:O:554:THR:HG23 | 15:O:561:ARG:NE | 2.07 | 0.68 |
| 2:B:138:GLY:H | 2:B:141:ILE:HG21 | 1.57 | 0.68 |
| 2:B:1101:MET:SD | 2:B:1126:LYS:HG3 | 2.34 | 0.68 |
| 1:A:552:ALA:HB2 | 1:A:671:ASP:HB3 | 1.74 | 0.68 |
| 1:A:664:MET:CB | 1:A:669:LEU:CD2 | 2.70 | 0.68 |
| 1:A:1166:LEU:HA | 1:A:1169:VAL:CG2 | 2.22 | 0.68 |
| 21:Y:41:DG:H2' | 21:Y:42:DT:H71 | 1.74 | 0.68 |
| 1:A:736:HIS:HA | 1:A:739:ASP:HB3 | 1.74 | 0.68 |
| 11:K:89:CYS:HA | 11:K:104:ARG:O | 1.94 | 0.68 |
| 15:O:339:LEU:O | 15:O:343:LYS:NZ | 2.26 | 0.68 |
| 18:R:636:LEU:HD13 | 19:S:502:LEU:HD21 | 1.75 | 0.68 |
| 5:E:79:TRP:O | 5:E:108:GLY:HA2 | 1.94 | 0.68 |
| 7:G:126:SER:HB3 | 7:G:139:TYR:CB | 2.23 | 0.68 |
| 18:R:135:ARG:NH2 | 18:R:174:PRO:O | 2.27 | 0.68 |
| 20:X:25:DT:H2' | 20:X:26:DT:C6 | 2.29 | 0.68 |
| 13:M:171:VAL:HG13 | 13:M:172:PRO:HD2 | 1.76 | 0.68 |
| 18:R:402:LEU:HD22 | 18:R:476:ALA:HB1 | 1.76 | 0.68 |
| 18:R:467:ARG:HG3 | 18:R:610:LEU:HD22 | 1.75 | 0.68 |
| 1:A:327:ILE:CA | 1:A:353:PHE:CD2 | 2.66 | 0.68 |
| 2:B:122:ASP:HA | 2:B:189:GLY:HA3 | 1.74 | 0.68 |
| 2:B:938:ILE:HD13 | 10:J:44:TYR:CE2 | 2.30 | 0.68 |
| 13:M:104:HIS:CE1 | 14:N:395:ILE:HD13 | 2.21 | 0.68 |
| 20:X:6:DA:C6 | 20:X:7:DA:N6 | 2.62 | 0.68 |
| 3:C:209:ILE:HG13 | 3:C:210:LEU:H | 1.59 | 0.67 |
| 15:O:46:LEU:HD22 | 15:O:70:ALA:HB2 | 1.74 | 0.67 |
| 2:B:129:ILE:HD11 | 2:B:152:MET:HB2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:24:LYS:HB2 | 5:E:30:ILE:HD11 | 1.76 | 0.67 |
| 5:E:56:LYS:HE2 | 5:E:84:ASP:HB2 | 1.75 | 0.67 |
| 10:J:52:THR:HG22 | 10:J:53:HIS:H | 1.57 | 0.67 |
| 2:B:102:LYS:NZ | 2:B:106:SER:O | 2.26 | 0.67 |
| 4:D:17:LEU:HD22 | 4:D:66:LEU:HB3 | 1.75 | 0.67 |
| 5:E:12:LEU:HD22 | 5:E:42:PHE:HZ | 1.60 | 0.67 |
| 11:K:80:ILE:HG22 | 11:K:86:VAL:HG11 | 1.77 | 0.67 |
| 2:B:622:VAL:HG12 | 2:B:624:ASP:H | 1.59 | 0.67 |
| 14:N:290:ILE:O | 14:N:294:LEU:CB | 2.42 | 0.67 |
| 15:O:43:ASN:HB3 | 15:O:47:PHE:HB2 | 1.75 | 0.67 |
| 1:A:1371:ILE:O | 1:A:1372:THR:OG1 | 2.11 | 0.67 |
| 7:G:129:ILE:HG12 | 7:G:139:TYR:HB3 | 1.75 | 0.67 |
| 15:O:499:THR:HG23 | 16:P:312:PHE:HB2 | 1.76 | 0.67 |
| 1:A:248:VAL:N | 1:A:249:PRO:HD3 | 2.09 | 0.67 |
| 1:A:976:ARG:HG3 | 1:A:1002:ARG:NH2 | 2.10 | 0.67 |
| 2:B:1103:TYR:HE2 | 7:G:163:PRO:HG2 | 1.59 | 0.67 |
| 3:C:190:ASP:O | 10:J:16:ASP:HB3 | 1.95 | 0.67 |
| 15:O:303:ARG:CA | 16:P:265:LEU:HD21 | 2.13 | 0.67 |
| 18:R:215:PHE:HD1 | 18:R:223:ILE:HD13 | 1.59 | 0.67 |
| 20:X:6:DA:C4 | 20:X:7:DA:N7 | 2.62 | 0.67 |
| 1:A:431:ASN:OD1 | 1:A:432:TYR:N | 2.24 | 0.67 |
| 7:G:92:CYS:SG | 7:G:98:LYS:N | 2.61 | 0.67 |
| 15:O:292:ARG:NH1 | 15:O:650:VAL:HA | 2.08 | 0.67 |
| 1:A:338:PRO:HG2 | 1:A:342:ASN:HD22 | 1.60 | 0.67 |
| 1:A:1145:LEU:HG | 1:A:1308:GLY:O | 1.94 | 0.67 |
| 2:B:717:GLN:HE21 | 2:B:727:LEU:HD22 | 1.60 | 0.67 |
| 2:B:1006:SER:HB2 | 2:B:1013:LEU:HD21 | 1.74 | 0.67 |
| 10:J:42:LYS:CE | 10:J:43:ARG:NH1 | 2.47 | 0.67 |
| 13:M:122:ASP:HB3 | 13:M:145:VAL:HG21 | 1.77 | 0.67 |
| 14:N:395:ILE:HA | 14:N:411:ARG:HA | 1.76 | 0.67 |
| 18:R:455:GLU:OE1 | 18:R:546:ARG:NH2 | 2.27 | 0.67 |
| 2:B:141:ILE:HG23 | 2:B:142:ILE:H | 1.60 | 0.67 |
| 1:A:390:ASP:OD2 | 1:A:538:LYS:NZ | 2.24 | 0.66 |
| 1:A:1186:VAL:H | 1:A:1230:ILE:HG12 | 1.60 | 0.66 |
| 6:F:96:THR:HG21 | 7:G:59:LEU:HD21 | 1.77 | 0.66 |
| 13:M:253:GLU:HB2 | 13:M:257:ASP:HB2 | 1.78 | 0.66 |
| 16:P:66:GLN:OE1 | 16:P:71:LYS:NZ | 2.25 | 0.66 |
| 16:P:131:GLN:HB3 | 16:P:133:TYR:HD2 | 1.59 | 0.66 |
| 19:S:428:PHE:HE1 | 19:S:454:VAL:HG13 | 1.58 | 0.66 |
| 19:S:460:ASN:ND2 | 20:X:9:DA:OP2 | 2.28 | 0.66 |
| 1:A:372:ARG:O | 2:B:1050:PRO:HD2 | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1145:LEU:O | 1:A:1310:ILE:HG22 | 1.94 | 0.66 |
| 2:B:882:ASP:OD1 | 2:B:883:GLN:N | 2.29 | 0.66 |
| 7:G:6:LYS:HA | 7:G:72:PHE:O | 1.94 | 0.66 |
| 15:O:599:ASN:O | 15:O:603:LEU:N | 2.25 | 0.66 |
| 18:R:517:PRO:HG3 | 21:Y:52:DA:H1' | 1.78 | 0.66 |
| 1:A:239:CYS:SG | 1:A:246:ALA:CB | 2.81 | 0.66 |
| 1:A:952:LYS:O | 1:A:1061:ARG:HD2 | 1.96 | 0.66 |
| 2:B:698:ARG:HH21 | 2:B:952:ARG:HG2 | 1.58 | 0.66 |
| 16:P:191:PHE:HB2 | 16:P:192:PRO:HD2 | 1.76 | 0.66 |
| 18:R:628:ILE:HG21 | 19:S:499:ASN:HD21 | 1.61 | 0.66 |
| 2:B:734:PRO:HB2 | 2:B:915:ARG:NH1 | 2.08 | 0.66 |
| 5:E:31:THR:HG22 | 5:E:34:GLU:HG2 | 1.77 | 0.66 |
| 18:R:123:GLN:HG2 | 18:R:150:LEU:HD21 | 1.77 | 0.66 |
| 15:O:353:GLU:O | 15:O:358:GLY:N | 2.29 | 0.66 |
| 1:A:363:ARG:HA | 1:A:367:ASN:HB2 | 1.78 | 0.66 |
| 1:A:664:MET:HB2 | 1:A:669:LEU:HD21 | 1.76 | 0.66 |
| 2:B:337:VAL:HG23 | 2:B:345:LYS:HZ3 | 1.61 | 0.66 |
| 7:G:87:GLY:HA3 | 7:G:148:PHE:HE2 | 1.59 | 0.66 |
| 15:O:102:ARG:NH2 | 15:O:282:ILE:O | 2.28 | 0.66 |
| 16:P:313:ASP:O | 16:P:314:GLU:HG2 | 1.96 | 0.66 |
| 2:B:734:PRO:CB | 2:B:915:ARG:HH12 | 2.09 | 0.66 |
| 7:G:12:ARG:NH2 | 7:G:65:SER:OG | 2.27 | 0.66 |
| 12:L:29:TYR:HB3 | 12:L:58:LYS:HA | 1.78 | 0.66 |
| 15:O:495:VAL:HG21 | 15:O:577:MET:HG3 | 1.76 | 0.66 |
| 1:A:865:ALA:HA | 2:B:696:SER:HB3 | 1.78 | 0.66 |
| 2:B:760:MET:HB3 | 2:B:943:ILE:HD11 | 1.77 | 0.66 |
| 16:P:11:LEU:O | 16:P:15:ALA:CB | 2.42 | 0.66 |
| 16:P:62:LYS:HD3 | 16:P:83:LYS:HE2 | 1.76 | 0.66 |
| 18:R:650:ALA:O | 19:S:520:LYS:NZ | 2.29 | 0.66 |
| 2:B:933:PHE:CD1 | 2:B:934:ASN:N | 2.64 | 0.66 |
| 19:S:426:ILE:HA | 19:S:429:TYR:HD2 | 1.61 | 0.66 |
| 1:A:766:ILE:HA | 1:A:769:LEU:HB2 | 1.76 | 0.66 |
| 5:E:101:GLN:O | 5:E:104:ASN:ND2 | 2.29 | 0.66 |
| 2:B:269:MET:O | 2:B:273:CYS:HB3 | 1.95 | 0.65 |
| 2:B:613:ILE:HG13 | 2:B:675:ILE:HG22 | 1.77 | 0.65 |
| 2:B:1147:PHE:HD2 | 7:G:10:LEU:HD11 | 1.61 | 0.65 |
| 15:O:201:ILE:HD12 | 15:O:283:ASN:HD22 | 1.59 | 0.65 |
| 15:O:297:ILE:O | 15:O:300:ALA:N | 2.29 | 0.65 |
| 1:A:1225:ILE:H | 1:A:1229:ARG:HE | 1.44 | 0.65 |
| 5:E:179:GLN:C | 5:E:180:ARG:O | 2.34 | 0.65 |
| 1:A:269:ARG:CZ | 1:A:285:LEU:HB2 | 2.26 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:305:ILE:HG22 | 2:B:325:GLU:HG2 | 1.79 | 0.65 |
| 2:B:396:ASN:O | 2:B:399:PHE:N | 2.28 | 0.65 |
| 13:M:182:PHE:CD1 | 13:M:183:PHE:N | 2.64 | 0.65 |
| 15:O:110:THR:CG2 | 15:O:116:LYS:HA | 2.24 | 0.65 |
| 1:A:632:VAL:HG21 | 1:A:796:THR:HG23 | 1.76 | 0.65 |
| 1:A:1171:PHE:CD2 | 1:A:1172:TYR:HD2 | 2.14 | 0.65 |
| 1:A:1378:LYS:HG3 | 1:A:1379:MET:H | 1.61 | 0.65 |
| 11:K:69:ASP:OD1 | 11:K:70:HIS:N | 2.26 | 0.65 |
| 1:A:955:LEU:HD12 | 1:A:959:ILE:HG13 | 1.78 | 0.65 |
| 2:B:192:LYS:NZ | 2:B:438:SER:O | 2.22 | 0.65 |
| 10:J:17:LYS:HB3 | 10:J:39:LEU:HD21 | 1.77 | 0.65 |
| 1:A:368:LEU:HD21 | 1:A:1416:ILE:HG23 | 1.79 | 0.65 |
| 3:C:121:PRO:O | 3:C:122:ASP:CG | 2.35 | 0.65 |
| 5:E:32:GLN:HA | 5:E:35:VAL:HG12 | 1.78 | 0.65 |
| 14:N:364:ARG:HH11 | 14:N:365:VAL:H | 1.44 | 0.65 |
| 1:A:18:PHE:HE1 | 2:B:1139:PRO:CB | 2.06 | 0.65 |
| 1:A:429:GLY:O | 1:A:465:HIS:ND1 | 2.24 | 0.65 |
| 1:A:1059:LEU:HD11 | 8:H:106:GLU:HB3 | 1.76 | 0.65 |
| 18:R:239:ARG:NH1 | 19:S:291:UNK:O | 2.30 | 0.65 |
| 1:A:674:LYS:HD2 | 1:A:927:GLU:O | 1.97 | 0.65 |
| 1:A:716:ASP:OD2 | 1:A:790:ALA:N | 2.27 | 0.65 |
| 1:A:898:CYS:HA | 1:A:904:VAL:HA | 1.77 | 0.65 |
| 1:A:1370:GLY:O | 1:A:1371:ILE:C | 2.34 | 0.65 |
| 8:H:38:LEU:HD21 | 8:H:40:LEU:HB2 | 1.77 | 0.65 |
| 16:P:189:ASN:ND2 | 16:P:217:THR:OG1 | 2.26 | 0.65 |
| 1:A:204:VAL:O | 1:A:208:ASN:N | 2.27 | 0.65 |
| 1:A:308:SER:HA | 15:O:534:ARG:HD2 | 1.79 | 0.65 |
| 1:A:644:GLU:OE2 | 1:A:651:PHE:CD2 | 2.49 | 0.65 |
| 1:A:1170:ALA:CA | 1:A:1188:ILE:HG12 | 2.27 | 0.65 |
| 2:B:914:SER:O | 2:B:915:ARG:HG2 | 1.97 | 0.65 |
| 7:G:2:PHE:N | 7:G:76:VAL:O | 2.30 | 0.65 |
| 15:O:370:LEU:HD22 | 15:O:453:ILE:HD11 | 1.77 | 0.65 |
| 17:Q:40:PRO:HB2 | 17:Q:44:ASN:ND2 | 2.11 | 0.65 |
| 18:R:581:ASN:ND2 | 18:R:583:HIS:O | 2.30 | 0.65 |
| 19:S:480:ASN:OD1 | 19:S:481:PHE:N | 2.26 | 0.65 |
| 2:B:137:ARG:HG3 | 2:B:138:GLY:H | 1.62 | 0.65 |
| 2:B:553:TYR:HB3 | 2:B:598:ALA:N | 2.11 | 0.65 |
| 3:C:231:PRO:HA | 3:C:293:ARG:HG2 | 1.79 | 0.65 |
| 1:A:429:GLY:C | 1:A:465:HIS:HD1 | 1.99 | 0.64 |
| 1:A:911:ILE:HG23 | 5:E:176:PRO:HD3 | 1.79 | 0.64 |
| 1:A:1222:VAL:HG23 | 1:A:1231:ALA:H | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:619:ALA:O | 18:R:623:LYS:CB | 2.44 | 0.64 |
| 15:O:163:VAL:HG22 | 15:O:169:LEU:HD22 | 1.78 | 0.64 |
| 16:P:107:SER:O | 16:P:110:ILE:HG22 | 1.97 | 0.64 |
| 2:B:797:ARG:HG2 | 2:B:803:GLN:HG2 | 1.78 | 0.64 |
| 6:F:115:THR:HG22 | 6:F:116:ASP:H | 1.63 | 0.64 |
| 16:P:77:GLU:HA | 16:P:80:ALA:HB3 | 1.79 | 0.64 |
| 1:A:649:ASP:OD2 | 1:A:663:VAL:N | 2.30 | 0.64 |
| 2:B:764:GLY:O | 2:B:767:ILE:HG12 | 1.97 | 0.64 |
| 3:C:88:ASN:HB3 | 12:L:60:ARG:NH1 | 2.11 | 0.64 |
| 5:E:18:THR:HG23 | 5:E:143:ASN:HB3 | 1.78 | 0.64 |
| 18:R:93:ALA:O | 18:R:149:ARG:NH2 | 2.31 | 0.64 |
| 1:A:99:THR:HA | 1:A:102:ILE:HG22 | 1.79 | 0.64 |
| 18:R:469:ILE:O | 18:R:473:GLY:N | 2.31 | 0.64 |
| 1:A:577:THR:HG23 | 11:K:88:PHE:CD1 | 2.32 | 0.64 |
| 1:A:1145:LEU:CG | 1:A:1308:GLY:O | 2.46 | 0.64 |
| 1:A:1284:ASN:OD1 | 1:A:1285:ILE:N | 2.30 | 0.64 |
| 2:B:214:GLY:HA3 | 2:B:234:ILE:HG21 | 1.79 | 0.64 |
| 15:O:47:PHE:HE2 | 15:O:586:ALA:HA | 1.62 | 0.64 |
| 15:O:102:ARG:O | 15:O:123:ASN:ND2 | 2.28 | 0.64 |
| 18:R:237:LEU:HD13 | 18:R:239:ARG:HG2 | 1.79 | 0.64 |
| 19:S:490:LYS:HG3 | 19:S:490:LYS:O | 1.98 | 0.64 |
| 1:A:1384:LEU:O | 1:A:1388:SER:N | 2.30 | 0.64 |
| 2:B:213:LYS:HD3 | 2:B:216:VAL:HG23 | 1.80 | 0.64 |
| 13:M:72:GLU:HB2 | 14:N:364:ARG:HE | 1.62 | 0.64 |
| 18:R:131:TYR:OH | 18:R:135:ARG:NH1 | 2.31 | 0.64 |
| 18:R:391:PRO:HA | 18:R:490:CYS:HB3 | 1.80 | 0.64 |
| 1:A:997:GLN:O | 1:A:999:ASP:N | 2.31 | 0.64 |
| 1:A:328:ASN:OD1 | 1:A:329:SER:N | 2.24 | 0.63 |
| 1:A:1333:TYR:CE2 | 1:A:1337:ARG:HD2 | 2.33 | 0.63 |
| 2:B:404:ASP:O | 2:B:407:LEU:N | 2.30 | 0.63 |
| 2:B:1040:ARG:HD3 | 18:R:35:ASN:HD21 | 1.63 | 0.63 |
| 15:O:233:SER:O | 15:O:236:LYS:HG2 | 1.97 | 0.63 |
| 19:S:469:ILE:O | 19:S:473:LEU:HB3 | 1.98 | 0.63 |
| 15:O:599:ASN:OD1 | 15:O:626:GLN:NE2 | 2.30 | 0.63 |
| 18:R:463:ARG:NH1 | 18:R:601:ASN:O | 2.30 | 0.63 |
| 19:S:306:UNK:O | 19:S:310:UNK:CB | 2.46 | 0.63 |
| 1:A:109:ASN:ND2 | 1:A:159:ALA:HB2 | 2.12 | 0.63 |
| 1:A:1333:TYR:CZ | 1:A:1337:ARG:HD2 | 2.34 | 0.63 |
| 4:D:125:ASN:OD1 | 4:D:126:GLN:N | 2.27 | 0.63 |
| 1:A:493:ARG:HB2 | 1:A:499:ARG:HH21 | 1.63 | 0.63 |
| 1:A:1272:VAL:HG13 | 1:A:1273:LYS:H | 1.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:190:ASP:O | 3:C:191:ILE:HG13 | 1.98 | 0.63 |
| 1:A:869:ARG:HH12 | 2:B:502:THR:HB | 1.64 | 0.63 |
| 2:B:1028:LYS:HG2 | 2:B:1029:HIS:H | 1.64 | 0.63 |
| 13:M:91:ALA:HA | 14:N:392:GLN:CD | 2.19 | 0.63 |
| 15:O:47:PHE:HZ | 15:O:590:PHE:CE2 | 2.15 | 0.63 |
| 16:P:10:GLN:HB3 | 16:P:13:ASP:HB3 | 1.80 | 0.63 |
| 18:R:245:VAL:HA | 18:R:248:SER:HB3 | 1.79 | 0.63 |
| 19:S:418:ASP:O | 19:S:449:ARG:NH1 | 2.31 | 0.63 |
| 6:F:80:ALA:O | 6:F:81:THR:OG1 | 2.14 | 0.63 |
| 1:A:533:ASN:HD21 | 6:F:90:ARG:HG2 | 1.62 | 0.63 |
| 3:C:133:VAL:HG11 | 3:C:172:GLN:HE22 | 1.64 | 0.63 |
| 13:M:117:HIS:HB2 | 13:M:119:TRP:NE1 | 2.14 | 0.63 |
| 1:A:148:CYS:SG | 1:A:149:LYS:N | 2.72 | 0.63 |
| 2:B:258:LYS:HE2 | 2:B:265:ASP:HB2 | 1.81 | 0.63 |
| 2:B:587:PHE:CZ | 2:B:607:ARG:HD3 | 2.34 | 0.63 |
| 3:C:31:TRP:CZ2 | 11:K:123:ASP:HB3 | 2.34 | 0.63 |
| 17:Q:40:PRO:HB2 | 17:Q:44:ASN:HD21 | 1.64 | 0.63 |
| 18:R:392:THR:O | 18:R:488:GLY:HA2 | 1.98 | 0.63 |
| 20:X:30:DT:O4 | 21:Y:33:DC:N4 | 2.32 | 0.63 |
| 20:X:63:DG:N2 | 21:Y:2:DC:O2 | 2.31 | 0.63 |
| 15:O:151:GLU:O | 15:O:155:LEU:N | 2.25 | 0.62 |
| 15:O:183:MET:HB2 | 15:O:186:THR:HB | 1.80 | 0.62 |
| 15:O:233:SER:HA | 20:X:59:DC:OP2 | 1.98 | 0.62 |
| 18:R:485:ASN:OD1 | 18:R:486:ILE:N | 2.32 | 0.62 |
| 18:R:619:ALA:O | 18:R:623:LYS:HB3 | 1.98 | 0.62 |
| 1:A:556:ASP:CB | 2:B:767:ILE:CD1 | 2.77 | 0.62 |
| 1:A:573:ARG:NH2 | 11:K:87:GLU:OE1 | 2.32 | 0.62 |
| 1:A:1315:THR:HG22 | 1:A:1316:THR:H | 1.65 | 0.62 |
| 1:A:1408:VAL:HG23 | 1:A:1413:GLU:HG3 | 1.81 | 0.62 |
| 9:I:32:GLU:HB2 | 13:M:130:PHE:HB3 | 1.80 | 0.62 |
| 13:M:160:ALA:N | 13:M:173:ILE:HD11 | 2.14 | 0.62 |
| 15:O:222:HIS:CE1 | 15:O:244:ASN:HB3 | 2.35 | 0.62 |
| 15:O:499:THR:CG2 | 16:P:312:PHE:CG | 2.82 | 0.62 |
| 15:O:644:LEU:HD11 | 16:P:310:VAL:HG21 | 1.81 | 0.62 |
| 2:B:756:THR:O | 2:B:941:ASP:N | 2.27 | 0.62 |
| 2:B:757:VAL:HG11 | 2:B:1022:ILE:HD12 | 1.82 | 0.62 |
| 5:E:64:PRO:HD3 | 5:E:77:SER:HA | 1.81 | 0.62 |
| 7:G:126:SER:HB3 | 7:G:139:TYR:HB2 | 1.80 | 0.62 |
| 13:M:111:ARG:NH1 | 13:M:120:GLU:OE1 | 2.33 | 0.62 |
| 1:A:566:HIS:CD2 | 1:A:568:ASP:HB3 | 2.35 | 0.62 |
| 2:B:726:TYR:HE2 | 2:B:1028:LYS:HG3 | 1.65 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:133:HIS:CE1 | 7:G:211:TRP:HB3 | 2.34 | 0.62 |
| 18:R:434:GLU:HA | 18:R:436:LYS:H | 1.64 | 0.62 |
| 20:X:26:DT:H2' | 20:X:27:DT:C6 | 2.34 | 0.62 |
| 2:B:48:LEU:HD22 | 2:B:743:LEU:HD21 | 1.80 | 0.62 |
| 18:R:202:ALA:O | 18:R:205:LEU:HB3 | 1.98 | 0.62 |
| 1:A:432:TYR:OH | 18:R:20:ASN:ND2 | 2.32 | 0.62 |
| 1:A:628:ALA:CB | 1:A:675:HIS:HD2 | 2.12 | 0.62 |
| 1:A:666:LYS:HG2 | 1:A:667:SER:H | 1.65 | 0.62 |
| 1:A:1145:LEU:CD1 | 1:A:1157:VAL:CG2 | 2.54 | 0.62 |
| 2:B:713:ILE:HG13 | 2:B:725:LEU:HD11 | 1.82 | 0.62 |
| 2:B:997:ASN:OD1 | 2:B:998:TYR:N | 2.33 | 0.62 |
| 18:R:196:ILE:O | 18:R:199:VAL:HB | 1.99 | 0.62 |
| 1:A:33:GLU:HG3 | 1:A:83:HIS:NE2 | 2.14 | 0.62 |
| 1:A:974:LEU:HD21 | 1:A:998:TYR:CB | 2.23 | 0.62 |
| 7:G:9:ASP:OD1 | 7:G:10:LEU:N | 2.33 | 0.62 |
| 7:G:207:LEU:HD22 | 7:G:210:TRP:CD1 | 2.35 | 0.62 |
| 18:R:121:ARG:HB2 | 18:R:124:ASN:HD22 | 1.63 | 0.62 |
| 2:B:140:ASN:HD22 | 19:S:394:LYS:HG2 | 1.65 | 0.62 |
| 2:B:546:SER:HB2 | 14:N:391:LEU:HD22 | 1.71 | 0.62 |
| 2:B:833:GLY:N | 2:B:881:ILE:O | 2.29 | 0.62 |
| 18:R:195:LYS:O | 18:R:199:VAL:N | 2.27 | 0.62 |
| 18:R:439:ALA:HA | 18:R:450:THR:H | 1.63 | 0.62 |
| 15:O:316:LEU:O | 15:O:320:GLU:N | 2.32 | 0.62 |
| 1:A:133:ASP:OD1 | 1:A:134:ASN:N | 2.32 | 0.61 |
| 1:A:201:TRP:HB3 | 1:A:205:LEU:HD13 | 1.82 | 0.61 |
| 13:M:160:ALA:HA | 14:N:306:VAL:HG12 | 1.81 | 0.61 |
| 15:O:455:SER:HA | 15:O:458:LYS:HD3 | 1.81 | 0.61 |
| 1:A:1384:LEU:HB2 | 1:A:1413:GLU:OE1 | 1.99 | 0.61 |
| 1:A:1438:GLU:HA | 1:A:1441:LEU:HD13 | 1.82 | 0.61 |
| 7:G:89:ILE:HG13 | 7:G:92:CYS:SG | 2.39 | 0.61 |
| 15:O:356:THR:HB | 15:O:357:PRO:HD3 | 1.81 | 0.61 |
| 15:O:567:ARG:HG2 | 15:O:568:CYS:H | 1.65 | 0.61 |
| 18:R:516:PHE:HB2 | 20:X:13:DA:H5' | 1.82 | 0.61 |
| 10:J:7:CYS:HB2 | 10:J:11:GLY:H | 1.65 | 0.61 |
| 1:A:252:ARG:O | 1:A:254:GLU:N | 2.29 | 0.61 |
| 2:B:109:LYS:CG | 2:B:111:TYR:O | 2.49 | 0.61 |
| 16:P:106:TRP:HE1 | 16:P:145:ARG:HA | 1.65 | 0.61 |
| 19:S:387:ALA:O | 19:S:391:ASN:N | 2.28 | 0.61 |
| 1:A:286:THR:O | 1:A:290:THR:HB | 1.99 | 0.61 |
| 1:A:642:PRO:HB3 | 8:H:103:LYS:NZ | 2.16 | 0.61 |
| 13:M:80:GLY:HA3 | 13:M:261:LYS:HE2 | 1.80 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:395:PRO:HG2 | 1:A:398:VAL:HG22 | 1.83 | 0.61 |
| 1:A:502:GLU:OE1 | 2:B:767:ILE:HG13 | 2.01 | 0.61 |
| 2:B:521:THR:O | 2:B:606:GLY:N | 2.32 | 0.61 |
| 2:B:555:VAL:HG12 | 2:B:564:SER:H | 1.65 | 0.61 |
| 10:J:16:ASP:OD1 | 10:J:17:LYS:N | 2.33 | 0.61 |
| 18:R:28:CYS:SG | 18:R:29:GLY:N | 2.74 | 0.61 |
| 18:R:518:GLY:HA3 | 18:R:532:ILE:O | 2.00 | 0.61 |
| 2:B:201:SER:OG | 2:B:376:ARG:NH1 | 2.33 | 0.61 |
| 8:H:101:ALA:HB2 | 8:H:116:TYR:HE1 | 1.65 | 0.61 |
| 15:O:285:ASP:OD1 | 15:O:286:ARG:N | 2.33 | 0.61 |
| 1:A:1203:GLU:HA | 1:A:1206:ALA:HB3 | 1.83 | 0.61 |
| 2:B:125:TYR:HB3 | 2:B:186:ILE:HG23 | 1.83 | 0.61 |
| 2:B:1003:MET:SD | 3:C:293:ARG:NH2 | 2.73 | 0.61 |
| 2:B:1042:PRO:HD2 | 2:B:1057:ASP:CB | 2.31 | 0.61 |
| 5:E:115:ASN:OD1 | 5:E:116:ILE:N | 2.34 | 0.61 |
| 5:E:141:VAL:HG23 | 5:E:142:VAL:H | 1.66 | 0.61 |
| 8:H:10:PHE:HE2 | 8:H:38:LEU:HD13 | 1.65 | 0.61 |
| 11:K:63:PHE:CD2 | 11:K:117:LEU:HD13 | 2.36 | 0.61 |
| 19:S:381:VAL:HG22 | 19:S:383:ARG:H | 1.65 | 0.61 |
| 1:A:1378:LYS:HG3 | 1:A:1379:MET:N | 2.15 | 0.61 |
| 2:B:234:ILE:HA | 2:B:240:ILE:HA | 1.82 | 0.61 |
| 2:B:612:LEU:HA | 2:B:675:ILE:HG23 | 1.83 | 0.61 |
| 13:M:182:PHE:HD1 | 13:M:183:PHE:H | 1.47 | 0.61 |
| 16:P:33:GLN:NE2 | 19:S:372:MET:SD | 2.74 | 0.61 |
| 19:S:488:ILE:O | 19:S:488:ILE:HG22 | 2.01 | 0.61 |
| 1:A:200:GLU:CB | 15:O:516:LEU:CD2 | 2.78 | 0.61 |
| 1:A:373:VAL:HG21 | 2:B:1062:LEU:HG | 1.82 | 0.61 |
| 1:A:1160:ARG:NH1 | 1:A:1307:ASP:OD2 | 2.31 | 0.61 |
| 2:B:126:SER:OG | 2:B:151:ARG:HB3 | 2.00 | 0.61 |
| 2:B:1080:LEU:O | 2:B:1084:MET:HB3 | 2.01 | 0.61 |
| 5:E:161:LYS:HE2 | 5:E:195:VAL:HG23 | 1.82 | 0.61 |
| 5:E:181:ALA:C | 5:E:182:ASP:O | 2.38 | 0.61 |
| 15:O:292:ARG:HD2 | 15:O:488:LYS:NZ | 2.16 | 0.61 |
| 1:A:117:GLU:HG2 | 1:A:119:ASP:H | 1.64 | 0.60 |
| 2:B:916:HIS:CD2 | 2:B:957:LYS:HB2 | 2.35 | 0.60 |
| 5:E:112:TYR:CG | 5:E:116:ILE:HG12 | 2.36 | 0.60 |
| 1:A:1171:PHE:HD2 | 1:A:1172:TYR:HD2 | 1.50 | 0.60 |
| 2:B:326:ALA:HB3 | 13:M:231:LEU:HD11 | 1.83 | 0.60 |
| 4:D:17:LEU:HD11 | 4:D:63:VAL:HG23 | 1.81 | 0.60 |
| 15:O:188:SER:O | 15:O:190:LEU:N | 2.34 | 0.60 |
| 18:R:87:LEU:CD2 | 18:R:105:PHE:HB2 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:X:6:DA:C6 | 20:X:7:DA:C6 | 2.90 | 0.60 |
| 1:A:269:ARG:HH22 | 1:A:283:ASP:C | 2.05 | 0.60 |
| 1:A:716:ASP:OD1 | 1:A:789:ASN:HB2 | 2.01 | 0.60 |
| 2:B:776:SER:HB2 | 2:B:928:GLN:HE21 | 1.66 | 0.60 |
| 7:G:94:ALA:O | 7:G:128:TRP:NE1 | 2.34 | 0.60 |
| 18:R:464:LYS:NZ | 18:R:605:VAL:O | 2.29 | 0.60 |
| 1:A:714:ILE:O | 1:A:717:VAL:N | 2.34 | 0.60 |
| 1:A:1224:ILE:HG13 | 1:A:1229:ARG:H | 1.67 | 0.60 |
| 2:B:1054:ARG:HG2 | 2:B:1055:SER:H | 1.67 | 0.60 |
| 15:O:338:ASP:H | 15:O:342:ALA:HB2 | 1.66 | 0.60 |
| 18:R:417:ASN:HA | 19:S:437:THR:HG22 | 1.83 | 0.60 |
| 21:Y:47:DC:H2' | 21:Y:48:DT:C4 | 2.37 | 0.60 |
| 1:A:1145:LEU:N | 1:A:1292:GLU:OE1 | 2.30 | 0.60 |
| 2:B:502:THR:HG22 | 2:B:510:LEU:HD11 | 1.83 | 0.60 |
| 5:E:185:ALA:O | 5:E:189:GLY:N | 2.34 | 0.60 |
| 16:P:20:SER:HA | 16:P:23:MET:HG2 | 1.84 | 0.60 |
| 19:S:427:LYS:HB2 | 19:S:446:TYR:OH | 2.00 | 0.60 |
| 1:A:1136:ILE:HG21 | 1:A:1318:HIS:HB3 | 1.84 | 0.60 |
| 2:B:534:TYR:HA | 2:B:538:VAL:HG22 | 1.84 | 0.60 |
| 3:C:248:GLN:HB3 | 3:C:256:ILE:HD11 | 1.84 | 0.60 |
| 5:E:20:LYS:HB3 | 5:E:35:VAL:HG23 | 1.83 | 0.60 |
| 15:O:506:ARG:HH21 | 16:P:246:VAL:HG13 | 1.67 | 0.60 |
| 1:A:331:SER:O | 1:A:351:ARG:NH2 | 2.35 | 0.60 |
| 2:B:643:LEU:HB3 | 2:B:645:LEU:HD13 | 1.84 | 0.60 |
| 13:M:84:SER:HB3 | 13:M:174:GLU:HG2 | 1.84 | 0.60 |
| 1:A:1130:ILE:CG2 | 1:A:1371:ILE:HG13 | 2.30 | 0.60 |
| 3:C:113:LEU:HD11 | 3:C:132:ILE:HD11 | 1.81 | 0.60 |
| 5:E:180:ARG:NH1 | 5:E:190:LEU:O | 2.30 | 0.60 |
| 21:Y:17:DT:H2" | 21:Y:18:DC:C5 | 2.36 | 0.60 |
| 1:A:18:PHE:CE1 | 2:B:1139:PRO:CB | 2.83 | 0.60 |
| 1:A:373:VAL:HG12 | 1:A:374:ASP:N | 2.16 | 0.60 |
| 1:A:1285:ILE:HA | 1:A:1291:ARG:HG2 | 1.82 | 0.60 |
| 2:B:415:GLU:HG2 | 2:B:416:TYR:N | 2.11 | 0.60 |
| 2:B:501:ASP:HB3 | 2:B:703:CYS:HB2 | 1.83 | 0.60 |
| 7:G:119:CYS:HB2 | 7:G:128:TRP:HB3 | 1.84 | 0.60 |
| 14:N:364:ARG:N | 14:N:372:SER:O | 2.34 | 0.60 |
| 16:P:31:PHE:CE2 | 16:P:72:PHE:HB2 | 2.37 | 0.60 |
| 16:P:190:THR:HA | 16:P:215:TYR:CE1 | 2.37 | 0.60 |
| 16:P:253:LEU:HB2 | 16:P:262:ARG:O | 2.02 | 0.60 |
| 16:P:308:GLU:HG2 | 16:P:308:GLU:O | 2.01 | 0.60 |
| 19:S:432:LEU:O | 19:S:476:LYS:NZ | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1125:ARG:HH22 | 1:A:1317:ASN:HB3 | 1.66 | 0.59 |
| 1:A:980:SER:HA | 5:E:163:GLU:HG2 | 1.84 | 0.59 |
| 2:B:354:ARG:NH1 | 2:B:549:LEU:HD13 | 2.17 | 0.59 |
| 2:B:728:MET:SD | 2:B:753:GLN:NE2 | 2.74 | 0.59 |
| 2:B:961:LEU:HD11 | 2:B:1019:PHE:HA | 1.84 | 0.59 |
| 2:B:417:ASP:C | 2:B:419:LEU:H | 2.05 | 0.59 |
| 2:B:1045:VAL:HG23 | 2:B:1046:LEU:N | 2.18 | 0.59 |
| 3:C:218:LYS:HE2 | 12:L:70:ARG:HB3 | 1.85 | 0.59 |
| 5:E:47:CYS:HA | 5:E:53:PRO:HA | 1.83 | 0.59 |
| 13:M:251:THR:OG1 | 13:M:254:GLN:NE2 | 2.35 | 0.59 |
| 15:O:105:LYS:HB3 | 15:O:210:PRO:HG3 | 1.85 | 0.59 |
| 15:O:220:GLU:HG2 | 15:O:221:LYS:H | 1.66 | 0.59 |
| 15:O:634:GLU:O | 15:O:637:VAL:HG12 | 2.01 | 0.59 |
| 18:R:478:PHE:HB3 | 18:R:599:PRO:HA | 1.84 | 0.59 |
| 18:R:583:HIS:NE2 | 18:R:585:LEU:O | 2.35 | 0.59 |
| 2:B:253:ILE:HG22 | 2:B:286:ASN:ND2 | 2.17 | 0.59 |
| 3:C:238:PRO:O | 3:C:239:ILE:HG13 | 2.01 | 0.59 |
| 15:O:496:ILE:O | 15:O:496:ILE:HG22 | 2.02 | 0.59 |
| 18:R:166:LYS:HG2 | 18:R:522:ARG:HH12 | 1.68 | 0.59 |
| 1:A:248:VAL:HG23 | 1:A:248:VAL:O | 2.02 | 0.59 |
| 1:A:786:ASP:OD1 | 1:A:787:ASN:N | 2.35 | 0.59 |
| 2:B:831:GLU:N | 2:B:831:GLU:OE1 | 2.31 | 0.59 |
| 15:O:52:LEU:HD11 | 15:O:131:LEU:HD12 | 1.82 | 0.59 |
| 15:O:506:ARG:HB3 | 16:P:250:ASP:OD1 | 2.03 | 0.59 |
| 2:B:1045:VAL:HG23 | 2:B:1046:LEU:CD1 | 2.25 | 0.59 |
| 15:O:215:TRP:O | 15:O:219:TYR:HB2 | 2.03 | 0.59 |
| 16:P:184:ARG:O | 16:P:187:SER:OG | 2.20 | 0.59 |
| 18:R:213:TRP:CD1 | 18:R:287:PRO:HD3 | 2.32 | 0.59 |
| 1:A:132:VAL:HG13 | 1:A:136:ARG:HB2 | 1.84 | 0.59 |
| 13:M:159:TYR:C | 13:M:173:ILE:HD11 | 2.22 | 0.59 |
| 20:X:7:DA:H4' | 20:X:8:DC:OP1 | 2.03 | 0.59 |
| 1:A:830:ARG:NH1 | 2:B:657:SER:O | 2.36 | 0.59 |
| 2:B:260:CYS:O | 2:B:342:PHE:HB3 | 2.01 | 0.59 |
| 2:B:542:THR:O | 13:M:178:GLN:NE2 | 2.36 | 0.59 |
| 2:B:1042:PRO:HD2 | 2:B:1057:ASP:CG | 2.23 | 0.59 |
| 3:C:255:VAL:HG22 | 3:C:256:ILE:H | 1.68 | 0.59 |
| 4:D:119:GLU:HA | 4:D:122:GLN:HB3 | 1.84 | 0.59 |
| 14:N:394:VAL:HB | 14:N:412:VAL:HB | 1.83 | 0.59 |
| 1:A:164:VAL:HA | 1:A:180:HIS:HB2 | 1.84 | 0.59 |
| 1:A:370:GLY:O | 2:B:1061:ARG:NH1 | 2.36 | 0.59 |
| 1:A:904:VAL:HG13 | 1:A:912:VAL:HG23 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1224:ILE:HG12 | 1:A:1226:GLY:N | 2.18 | 0.59 |
| 2:B:481:ARG:NH2 | 21:Y:21:DG:H2' | 2.17 | 0.59 |
| 2:B:992:VAL:HG23 | 3:C:278:GLU:HG2 | 1.83 | 0.59 |
| 5:E:83:CYS:SG | 5:E:84:ASP:N | 2.75 | 0.59 |
| 19:S:421:THR:HG23 | 19:S:424:GLU:H | 1.67 | 0.59 |
| 1:A:813:VAL:HB | 1:A:848:VAL:HG13 | 1.85 | 0.59 |
| 1:A:1022:LEU:HD22 | 1:A:1060:TYR:HE2 | 1.67 | 0.59 |
| 3:C:77:SER:OG | 3:C:221:PRO:HB3 | 2.03 | 0.59 |
| 7:G:112:GLN:HE22 | 7:G:115:LEU:HD22 | 1.68 | 0.59 |
| 8:H:24:CYS:SG | 8:H:25:ARG:N | 2.76 | 0.59 |
| 8:H:107:VAL:N | 8:H:111:LEU:O | 2.32 | 0.59 |
| 16:P:14:ASN:HB3 | 16:P:51:ILE:HD13 | 1.85 | 0.59 |
| 1:A:327:ILE:CA | 1:A:353:PHE:CE2 | 2.86 | 0.58 |
| 1:A:1380:ARG:HH11 | 1:A:1385:GLN:HE22 | 1.51 | 0.58 |
| 2:B:612:LEU:HD11 | 2:B:649:LEU:HD11 | 1.84 | 0.58 |
| 2:B:822:GLN:HG2 | 2:B:823:SER:H | 1.68 | 0.58 |
| 8:H:5:LEU:HB2 | 8:H:59:ILE:O | 2.03 | 0.58 |
| 11:K:85:ASP:OD2 | 11:K:111:THR:OG1 | 2.21 | 0.58 |
| 13:M:149:LYS:HB3 | 13:M:182:PHE:HE2 | 1.67 | 0.58 |
| 14:N:282:LEU:O | 14:N:286:ASP:HB2 | 2.02 | 0.58 |
| 15:O:128:HIS:NE2 | 15:O:132:TYR:HE2 | 2.00 | 0.58 |
| 16:P:236:THR:HG23 | 16:P:239:ASN:H | 1.68 | 0.58 |
| 19:S:418:ASP:HB3 | 19:S:449:ARG:HH12 | 1.68 | 0.58 |
| 1:A:235:LYS:CD | 1:A:252:ARG:CB | 2.81 | 0.58 |
| 2:B:1038:ARG:HE | 2:B:1041:GLY:H | 1.49 | 0.58 |
| 15:O:584:ASN:HD22 | 15:O:587:ASN:HB2 | 1.68 | 0.58 |
| 15:O:592:LYS:O | 15:O:596:LYS:HG2 | 2.03 | 0.58 |
| 16:P:142:PHE:CZ | 20:X:30:DT:H4' | 2.38 | 0.58 |
| 20:X:60:DA:H2' | 20:X:61:DT:C6 | 2.38 | 0.58 |
| 5:E:155:ARG:NH2 | 5:E:194:GLU:OE2 | 2.36 | 0.58 |
| 1:A:622:VAL:HB | 1:A:624:ILE:HD11 | 1.85 | 0.58 |
| 1:A:1161:VAL:HG22 | 1:A:1275:LEU:HD13 | 1.84 | 0.58 |
| 5:E:55:ARG:HD2 | 5:E:82:PHE:CE2 | 2.38 | 0.58 |
| 14:N:306:VAL:HG23 | 14:N:415:LYS:HD3 | 1.85 | 0.58 |
| 15:O:195:CYS:SG | 15:O:196:GLU:N | 2.76 | 0.58 |
| 19:S:444:GLN:NE2 | 19:S:490:LYS:NZ | 2.51 | 0.58 |
| 1:A:45:ASP:OD1 | 1:A:46:ARG:N | 2.36 | 0.58 |
| 1:A:212:GLU:HG2 | 1:A:213:ARG:H | 1.68 | 0.58 |
| 1:A:975:VAL:HG22 | 1:A:976:ARG:N | 2.10 | 0.58 |
| 2:B:766:ASP:OD1 | 2:B:945:ASN:HB2 | 2.03 | 0.58 |
| 2:B:929:GLU:HG2 | 3:C:72:ILE:CG2 | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:933:PHE:O | 2:B:934:ASN:HB3 | 2.03 | 0.58 |
| 15:O:570:GLU:HA | 15:O:573:SER:HB3 | 1.85 | 0.58 |
| 16:P:206:VAL:HB | 16:P:210:PRO:HG3 | 1.85 | 0.58 |
| 18:R:623:LYS:HE2 | 19:S:435:TRP:HD1 | 1.67 | 0.58 |
| 1:A:31:GLU:HG3 | 1:A:69:THR:HG21 | 1.86 | 0.58 |
| 2:B:235:THR:HG22 | 2:B:236:LYS:HG3 | 1.86 | 0.58 |
| 3:C:227:TYR:HB3 | 3:C:300:PHE:CD1 | 2.38 | 0.58 |
| 3:C:255:VAL:HG13 | 3:C:256:ILE:N | 2.18 | 0.58 |
| 10:J:14:VAL:O | 10:J:17:LYS:N | 2.37 | 0.58 |
| 13:M:94:PRO:HB3 | 14:N:391:LEU:C | 2.23 | 0.58 |
| 14:N:364:ARG:NH1 | 14:N:365:VAL:O | 2.37 | 0.58 |
| 16:P:247:LEU:HB3 | 16:P:253:LEU:HG | 1.85 | 0.58 |
| 18:R:431:ARG:NH1 | 18:R:438:THR:OG1 | 2.35 | 0.58 |
| 2:B:494:PHE:CE1 | 2:B:680:ILE:HD12 | 2.38 | 0.58 |
| 2:B:780:ARG:HH11 | 10:J:6:ARG:HD2 | 1.63 | 0.58 |
| 5:E:181:ALA:HA | 5:E:186:LEU:HG | 1.84 | 0.58 |
| 1:A:197:TRP:CH2 | 15:O:567:ARG:NH1 | 2.71 | 0.58 |
| 1:A:974:LEU:O | 1:A:975:VAL:HG12 | 2.02 | 0.58 |
| 2:B:49:PRO:O | 2:B:53:LYS:N | 2.35 | 0.58 |
| 3:C:240:LYS:HB3 | 3:C:264:GLU:HB3 | 1.85 | 0.58 |
| 7:G:89:ILE:HG23 | 7:G:142:VAL:HG12 | 1.86 | 0.58 |
| 15:O:478:VAL:HG12 | 15:O:479:PRO:O | 2.03 | 0.58 |
| 15:O:620:LEU:HD23 | 15:O:623:GLU:HB2 | 1.86 | 0.58 |
| 21:Y:44:DT:H2" | 21:Y:45:DT:H2' | 1.85 | 0.58 |
| 1:A:106:ILE:HD13 | 1:A:234:ILE:HG12 | 1.85 | 0.58 |
| 1:A:178:ILE:HD11 | 1:A:222:LEU:HB2 | 1.86 | 0.58 |
| 1:A:354:CYS:SG | 1:A:1393:THR:OG1 | 2.58 | 0.58 |
| 1:A:1221:ASP:OD1 | 1:A:1222:VAL:N | 2.36 | 0.58 |
| 2:B:265:ASP:HA | 2:B:268:ILE:HD12 | 1.86 | 0.58 |
| 4:D:72:PHE:O | 7:G:145:LYS:NZ | 2.36 | 0.58 |
| 13:M:226:ARG:HG3 | 13:M:227:LEU:H | 1.69 | 0.58 |
| 15:O:193:GLN:C | 15:O:195:CYS:N | 2.57 | 0.58 |
| 18:R:173:LEU:O | 18:R:175:LEU:N | 2.37 | 0.58 |
| 1:A:116:SER:HB3 | 1:A:155:LEU:HD22 | 1.85 | 0.58 |
| 1:A:501:ASN:O | 1:A:504:VAL:HG22 | 2.04 | 0.58 |
| 1:A:795:ALA:HB1 | 1:A:802:SER:HA | 1.86 | 0.58 |
| 2:B:1012:CYS:SG | 3:C:293:ARG:NH2 | 2.75 | 0.58 |
| 3:C:222:VAL:HG11 | 3:C:225:ALA:CB | 2.28 | 0.58 |
| 15:O:132:TYR:O | 15:O:134:GLY:N | 2.31 | 0.58 |
| 15:O:449:SER:HA | 15:O:456:HIS:CD2 | 2.39 | 0.58 |
| 15:O:495:VAL:HG13 | 15:O:496:ILE:HG13 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:568:ASP:OD1 | 8:H:22:LYS:HG2 | 2.03 | 0.57 |
| 1:A:1126:ILE:HG22 | 1:A:1130:ILE:HD12 | 1.86 | 0.57 |
| 13:M:134:ASP:O | 13:M:138:SER:N | 2.36 | 0.57 |
| 16:P:53:GLN:NE2 | 19:S:363:GLN:HA | 2.19 | 0.57 |
| 18:R:521:TYR:CE2 | 18:R:523:MET:HB2 | 2.39 | 0.57 |
| 1:A:200:GLU:CB | 15:O:516:LEU:HD23 | 2.34 | 0.57 |
| 1:A:752:THR:HA | 1:A:761:THR:HG21 | 1.87 | 0.57 |
| 1:A:1323:PHE:HD1 | 1:A:1328:ILE:H | 1.51 | 0.57 |
| 5:E:46:TYR:CZ | 5:E:58:MET:HA | 2.39 | 0.57 |
| 7:G:126:SER:HG | 7:G:139:TYR:CB | 2.17 | 0.57 |
| 13:M:102:ALA:O | 13:M:103:GLU:HB2 | 2.04 | 0.57 |
| 15:O:104:VAL:N | 15:O:123:ASN:HB2 | 2.18 | 0.57 |
| 18:R:25:CYS:SG | 18:R:28:CYS:CB | 2.92 | 0.57 |
| 18:R:463:ARG:HG3 | 18:R:602:LEU:HD13 | 1.86 | 0.57 |
| 19:S:364:LEU:HB3 | 19:S:374:ILE:HD12 | 1.87 | 0.57 |
| 2:B:1045:VAL:CG2 | 2:B:1046:LEU:HD12 | 2.27 | 0.57 |
| 15:O:110:THR:HG22 | 15:O:116:LYS:CA | 2.26 | 0.57 |
| 15:O:581:LEU:O | 15:O:585:MET:HB2 | 2.04 | 0.57 |
| 19:S:413:ARG:NE | 20:X:12:DT:OP1 | 2.36 | 0.57 |
| 21:Y:55:DT:C4 | 21:Y:56:DG:O6 | 2.57 | 0.57 |
| 1:A:38:ASP:O | 1:A:40:PHE:N | 2.31 | 0.57 |
| 1:A:385:PRO:HG3 | 2:B:764:GLY:HA3 | 1.86 | 0.57 |
| 2:B:914:SER:C | 2:B:916:HIS:H | 2.06 | 0.57 |
| 4:D:127:LEU:HD12 | 4:D:127:LEU:O | 2.04 | 0.57 |
| 9:I:8:CYS:SG | 9:I:29:CYS:HB2 | 2.43 | 0.57 |
| 16:P:31:PHE:HE2 | 16:P:72:PHE:HB2 | 1.69 | 0.57 |
| 1:A:235:LYS:HD2 | 1:A:252:ARG:CB | 2.33 | 0.57 |
| 1:A:1329:GLU:OE2 | 5:E:200:ARG:NH2 | 2.37 | 0.57 |
| 10:J:41:LEU:HD23 | 10:J:47:ARG:HA | 1.87 | 0.57 |
| 15:O:471:THR:OG1 | 15:O:477:TYR:HB3 | 2.04 | 0.57 |
| 21:Y:7:DA:H2" | 21:Y:8:DG:C8 | 2.39 | 0.57 |
| 1:A:485:ILE:O | 1:A:486:LEU:HD12 | 2.05 | 0.57 |
| 1:A:668:VAL:O | 1:A:677:VAL:N | 2.35 | 0.57 |
| 7:G:45:CYS:SG | 7:G:46:ILE:N | 2.77 | 0.57 |
| 1:A:34:VAL:HG13 | 1:A:35:SER:H | 1.70 | 0.57 |
| 1:A:67:CYS:HB3 | 1:A:70:CYS:O | 2.04 | 0.57 |
| 1:A:189:LYS:HE3 | 1:A:191:ALA:HB2 | 1.86 | 0.57 |
| 1:A:1370:GLY:HA2 | 1:A:1375:GLY:CA | 2.35 | 0.57 |
| 2:B:1022:ILE:HG22 | 2:B:1023:TYR:H | 1.69 | 0.57 |
| 6:F:108:PHE:CE2 | 6:F:131:PRO:HG3 | 2.40 | 0.57 |
| 16:P:45:LEU:HD22 | 19:S:366:LEU:HB3 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:P:314:GLU:HB3 | 17:Q:37:PRO:HB3 | 1.85 | 0.57 |
| 18:R:7:CYS:SG | 18:R:28:CYS:CB | 2.76 | 0.57 |
| 1:A:327:ILE:CG2 | 1:A:353:PHE:CE2 | 2.87 | 0.57 |
| 3:C:165:ARG:NH2 | 3:C:190:ASP:OD1 | 2.37 | 0.57 |
| 13:M:90:TYR:O | 14:N:392:GLN:CB | 2.53 | 0.57 |
| 1:A:30:SER:OG | 1:A:82:GLY:HA2 | 2.04 | 0.57 |
| 1:A:649:ASP:OD2 | 1:A:663:VAL:HG13 | 2.04 | 0.57 |
| 2:B:651:VAL:HG23 | 2:B:652:ASN:H | 1.70 | 0.57 |
| 3:C:30:GLU:HG3 | 11:K:84:PRO:HG3 | 1.87 | 0.57 |
| 5:E:28:TYR:CZ | 5:E:78:LEU:HD23 | 2.40 | 0.57 |
| 7:G:13:ILE:HG13 | 7:G:66:SER:HB3 | 1.87 | 0.57 |
| 15:O:467:PHE:CD1 | 15:O:468:LEU:HD13 | 2.39 | 0.57 |
| 15:O:494:TYR:HB2 | 16:P:294:PHE:HZ | 1.69 | 0.57 |
| 18:R:617:GLU:HG2 | 18:R:621:LYS:HE2 | 1.87 | 0.57 |
| 1:A:980:SER:OG | 5:E:160:GLU:HA | 2.05 | 0.57 |
| 6:F:108:PHE:HE2 | 6:F:131:PRO:HG3 | 1.70 | 0.57 |
| 15:O:158:GLU:OE1 | 15:O:161:GLN:NE2 | 2.37 | 0.57 |
| 15:O:159:ILE:O | 15:O:163:VAL:HG23 | 2.05 | 0.57 |
| 15:O:166:LEU:HB3 | 15:O:169:LEU:HD11 | 1.87 | 0.57 |
| 1:A:91:PHE:HE1 | 1:A:227:THR:HG21 | 1.70 | 0.56 |
| 1:A:584:SER:O | 1:A:586:GLY:N | 2.38 | 0.56 |
| 1:A:940:ASP:O | 1:A:943:TYR:N | 2.38 | 0.56 |
| 2:B:554:GLY:O | 2:B:599:VAL:HG12 | 2.05 | 0.56 |
| 2:B:615:VAL:HA | 2:B:620:SER:HA | 1.87 | 0.56 |
| 2:B:818:ILE:O | 2:B:822:GLN:N | 2.37 | 0.56 |
| 7:G:104:ILE:HG12 | 7:G:105:PHE:CD1 | 2.39 | 0.56 |
| 13:M:183:PHE:C | 13:M:185:TYR:H | 2.07 | 0.56 |
| 15:O:498:SER:HB2 | 16:P:296:TYR:HB3 | 1.85 | 0.56 |
| 15:O:554:THR:CG2 | 15:O:561:ARG:HE | 2.14 | 0.56 |
| 18:R:521:TYR:HE2 | 18:R:523:MET:HB2 | 1.69 | 0.56 |
| 1:A:1144:VAL:HG12 | 1:A:1292:GLU:HG3 | 1.88 | 0.56 |
| 2:B:546:SER:HB3 | 14:N:391:LEU:HD21 | 1.86 | 0.56 |
| 1:A:478:PRO:HG3 | 21:Y:23:DG:N3 | 2.19 | 0.56 |
| 1:A:595:PRO:HG2 | 1:A:598:MET:HG2 | 1.87 | 0.56 |
| 1:A:943:TYR:O | 1:A:947:PHE:N | 2.38 | 0.56 |
| 2:B:59:LYS:HE2 | 2:B:519:HIS:CD2 | 2.41 | 0.56 |
| 2:B:539:GLU:HA | 14:N:308:GLN:HE22 | 1.70 | 0.56 |
| 2:B:932:PRO:HB2 | 2:B:1004:LEU:HD13 | 1.85 | 0.56 |
| 3:C:132:ILE:O | 3:C:208:CYS:HB3 | 2.04 | 0.56 |
| 4:D:65:TYR:HA | 4:D:68:ILE:HG22 | 1.87 | 0.56 |
| 8:H:106:GLU:OE1 | 8:H:106:GLU:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:K:99:ASN:O | 11:K:100:LEU:HD12 | 2.06 | 0.56 |
| 13:M:123:ILE:O | 13:M:146:GLN:N | 2.35 | 0.56 |
| 18:R:401:THR:O | 18:R:479:THR:OG1 | 2.20 | 0.56 |
| 18:R:510:SER:N | 18:R:520:ILE:O | 2.34 | 0.56 |
| 1:A:1319:VAL:HG21 | 1:A:1335:ILE:HB | 1.87 | 0.56 |
| 2:B:855:PRO:O | 18:R:106:GLN:NE2 | 2.38 | 0.56 |
| 2:B:905:ARG:O | 2:B:907:GLU:N | 2.38 | 0.56 |
| 3:C:69:ARG:HE | 11:K:71:THR:HG22 | 1.71 | 0.56 |
| 15:O:251:LYS:HA | 15:O:254:ASN:HB2 | 1.88 | 0.56 |
| 16:P:216:SER:OG | 16:P:260:CYS:HA | 2.05 | 0.56 |
| 18:R:397:VAL:O | 18:R:484:GLN:N | 2.37 | 0.56 |
| 1:A:176:LEU:HB3 | 1:A:320:GLN:NE2 | 2.19 | 0.56 |
| 2:B:332:ILE:HG13 | 2:B:333:ALA:H | 1.68 | 0.56 |
| 8:H:93:TYR:HD2 | 8:H:143:LEU:HG | 1.71 | 0.56 |
| 15:O:91:VAL:O | 15:O:95:LEU:CB | 2.52 | 0.56 |
| 15:O:583:TRP:CZ3 | 16:P:315:TRP:HB3 | 2.40 | 0.56 |
| 1:A:496:ARG:HB2 | 2:B:1035:MET:SD | 2.45 | 0.56 |
| 2:B:297:THR:OG1 | 2:B:302:LEU:HG | 2.06 | 0.56 |
| 2:B:961:LEU:HD13 | 2:B:1018:PHE:CE2 | 2.41 | 0.56 |
| 7:G:126:SER:HB3 | 7:G:139:TYR:HB3 | 1.87 | 0.56 |
| 15:O:498:SER:OG | 16:P:296:TYR:HB2 | 2.04 | 0.56 |
| 1:A:11:LYS:HD2 | 2:B:1145:ASP:HA | 1.88 | 0.56 |
| 1:A:830:ARG:NH2 | 1:A:833:PRO:O | 2.37 | 0.56 |
| 1:A:835:PHE:CE2 | 1:A:844:SER:HA | 2.40 | 0.56 |
| 2:B:915:ARG:CD | 2:B:1023:TYR:HB3 | 2.35 | 0.56 |
| 3:C:66:ALA:O | 3:C:70:ILE:HG22 | 2.06 | 0.56 |
| 3:C:86:PHE:O | 3:C:87:ASN:O | 2.23 | 0.56 |
| 3:C:89:THR:CG2 | 3:C:201:GLU:H | 2.18 | 0.56 |
| 15:O:193:GLN:C | 15:O:195:CYS:H | 2.09 | 0.56 |
| 1:A:777:VAL:HG12 | 1:A:811:ALA:HB1 | 1.86 | 0.56 |
| 1:A:816:GLN:HB3 | 1:A:867:SER:HB2 | 1.87 | 0.56 |
| 2:B:461:LEU:HD21 | 2:B:1028:LYS:HD3 | 1.87 | 0.56 |
| 2:B:695:GLN:HG3 | 2:B:697:PRO:HD2 | 1.88 | 0.56 |
| 4:D:110:LEU:HD21 | 4:D:123:ILE:HD11 | 1.88 | 0.56 |
| 5:E:17:ARG:HG3 | 5:E:35:VAL:HG22 | 1.87 | 0.56 |
| 5:E:63:ASN:HA | 5:E:77:SER:HA | 1.88 | 0.56 |
| 7:G:96:GLY:HA2 | 7:G:112:GLN:OE1 | 2.05 | 0.56 |
| 11:K:63:PHE:HD2 | 11:K:117:LEU:HD13 | 1.70 | 0.56 |
| 13:M:107:ILE:HD12 | 13:M:124:PRO:HG3 | 1.87 | 0.56 |
| 13:M:159:TYR:HD1 | 13:M:172:PRO:HA | 1.69 | 0.56 |
| 15:O:46:LEU:HD11 | 15:O:66:GLY:HA2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:O:234:ASP:O | 15:O:238:ARG:N | 2.39 | 0.56 |
| 18:R:6:ASN:HD22 | 18:R:30:VAL:HG21 | 1.70 | 0.56 |
| 1:A:842:PRO:C | 1:A:844:SER:H | 2.09 | 0.56 |
| 2:B:177:CYS:SG | 2:B:714:ALA:HB1 | 2.46 | 0.56 |
| 2:B:541:ILE:HA | 2:B:544:ILE:HD12 | 1.88 | 0.56 |
| 4:D:135:TYR:HA | 4:D:141:CYS:SG | 2.46 | 0.56 |
| 9:I:15:THR:HG22 | 9:I:24:LEU:HA | 1.87 | 0.56 |
| 15:O:555:ALA:HB2 | 15:O:561:ARG:HG3 | 1.88 | 0.56 |
| 15:O:595:LEU:HD12 | 15:O:598:GLU:CG | 2.35 | 0.56 |
| 1:A:329:SER:HA | 1:A:351:ARG:NE | 2.21 | 0.56 |
| 1:A:486:LEU:HD23 | 1:A:537:VAL:HG22 | 1.87 | 0.56 |
| 1:A:628:ALA:CB | 1:A:675:HIS:CD2 | 2.89 | 0.56 |
| 1:A:955:LEU:HB2 | 1:A:958:ALA:HB3 | 1.87 | 0.56 |
| 2:B:109:LYS:HG2 | 2:B:111:TYR:O | 2.05 | 0.56 |
| 2:B:734:PRO:CB | 2:B:915:ARG:NH1 | 2.69 | 0.56 |
| 2:B:1038:ARG:NE | 2:B:1041:GLY:H | 2.03 | 0.56 |
| 18:R:639:GLU:HG3 | 18:R:642:ARG:HE | 1.69 | 0.56 |
| 20:X:56:DC:N3 | 21:Y:8:DG:N1 | 2.53 | 0.56 |
| 1:A:364:PHE:HE2 | 1:A:1387:ALA:C | 2.10 | 0.55 |
| 1:A:890:MET:SD | 2:B:1068:ASP:HB2 | 2.46 | 0.55 |
| 1:A:893:LEU:HD13 | 1:A:1361:VAL:HG21 | 1.86 | 0.55 |
| 1:A:1189:ASP:OD2 | 1:A:1192:THR:N | 2.39 | 0.55 |
| 1:A:1202:ILE:O | 1:A:1205:ILE:HG13 | 2.06 | 0.55 |
| 1:A:1385:GLN:HA | 1:A:1388:SER:HB3 | 1.87 | 0.55 |
| 1:A:321:LEU:O | 1:A:325:MET:CB | 2.54 | 0.55 |
| 1:A:598:MET:HB2 | 8:H:96:VAL:HG21 | 1.87 | 0.55 |
| 1:A:1429:LYS:HD3 | 6:F:137:TYR:CE2 | 2.40 | 0.55 |
| 2:B:658:TYR:CD2 | 2:B:670:MET:HG2 | 2.41 | 0.55 |
| 2:B:754:ASN:O | 10:J:48:ARG:NH1 | 2.40 | 0.55 |
| 2:B:932:PRO:HG2 | 2:B:940:PRO:CG | 2.36 | 0.55 |
| 2:B:933:PHE:HE1 | 2:B:1005:TYR:CD2 | 2.09 | 0.55 |
| 2:B:936:GLN:HB2 | 2:B:938:ILE:HD12 | 1.86 | 0.55 |
| 3:C:31:TRP:CG | 3:C:32:ASN:N | 2.74 | 0.55 |
| 3:C:96:VAL:O | 3:C:99:HIS:HB3 | 2.06 | 0.55 |
| 8:H:8:ASP:OD1 | 8:H:9:ILE:N | 2.38 | 0.55 |
| 18:R:219:ARG:N | 21:Y:54:DA:OP1 | 2.26 | 0.55 |
| 21:Y:39:DA:H1' | 21:Y:40:DA:H5' | 1.88 | 0.55 |
| 2:B:471:THR:HG23 | 2:B:514:LEU:HB2 | 1.88 | 0.55 |
| 13:M:84:SER:C | 13:M:85:LEU:CD1 | 2.71 | 0.55 |
| 13:M:90:TYR:CB | 13:M:179:LEU:HB3 | 2.35 | 0.55 |
| 13:M:183:PHE:C | 13:M:185:TYR:N | 2.57 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:O:307:VAL:HG13 | 15:O:308:THR:H | 1.70 | 0.55 |
| 16:P:14:ASN:HA | 16:P:17:THR:HG22 | 1.88 | 0.55 |
| 1:A:207:HIS:CE1 | 15:O:521:ILE:HG21 | 2.42 | 0.55 |
| 3:C:240:LYS:HB2 | 3:C:261:GLY:O | 2.06 | 0.55 |
| 15:O:193:GLN:O | 15:O:194:LEU:C | 2.42 | 0.55 |
| 15:O:338:ASP:OD1 | 15:O:339:LEU:N | 2.40 | 0.55 |
| 21:Y:10:DC:N3 | 21:Y:11:DA:N6 | 2.54 | 0.55 |
| 1:A:552:ALA:HB3 | 1:A:671:ASP:H | 1.72 | 0.55 |
| 1:A:633:PHE:HZ | 1:A:643:ASN:HB3 | 1.72 | 0.55 |
| 2:B:81:GLN:O | 2:B:94:LYS:HA | 2.07 | 0.55 |
| 2:B:1036:HIS:NE2 | 2:B:1058:GLY:HA2 | 2.20 | 0.55 |
| 15:O:78:GLU:HG2 | 15:O:82:LYS:HZ1 | 1.70 | 0.55 |
| 15:O:135:LEU:HD12 | 15:O:138:ASP:HB3 | 1.87 | 0.55 |
| 15:O:190:LEU:CA | 15:O:193:GLN:HB3 | 2.36 | 0.55 |
| 18:R:219:ARG:NH1 | 18:R:514:GLU:O | 2.39 | 0.55 |
| 19:S:417:THR:HG22 | 19:S:453:GLN:HE21 | 1.72 | 0.55 |
| 19:S:439:PHE:HD1 | 19:S:454:VAL:HG12 | 1.72 | 0.55 |
| 19:S:507:ASN:HA | 19:S:510:LYS:HB3 | 1.87 | 0.55 |
| 1:A:371:LYS:HZ3 | 2:B:1122:PRO:CB | 2.06 | 0.55 |
| 1:A:418:GLU:O | 1:A:421:VAL:HG12 | 2.07 | 0.55 |
| 1:A:523:GLN:HB2 | 2:B:1081:GLU:OE2 | 2.06 | 0.55 |
| 1:A:790:ALA:HB1 | 1:A:794:MET:HE2 | 1.88 | 0.55 |
| 1:A:974:LEU:HD11 | 1:A:998:TYR:CD2 | 2.41 | 0.55 |
| 2:B:521:THR:HG22 | 2:B:605:GLY:HA2 | 1.89 | 0.55 |
| 2:B:931:MET:HG3 | 2:B:932:PRO:HD2 | 1.89 | 0.55 |
| 13:M:164:LYS:HE3 | 13:M:259:ILE:HG13 | 1.88 | 0.55 |
| 15:O:296:LEU:HD22 | 15:O:487:LEU:HD21 | 1.87 | 0.55 |
| 16:P:221:ILE:O | 16:P:225:ILE:HG12 | 2.07 | 0.55 |
| 18:R:96:ILE:HG22 | 18:R:141:HIS:NE2 | 2.21 | 0.55 |
| 18:R:100:ILE:O | 18:R:103:ALA:HB3 | 2.07 | 0.55 |
| 19:S:414:GLY:HA3 | 20:X:11:DA:P | 2.47 | 0.55 |
| 1:A:134:ASN:OD1 | 1:A:1404:LYS:NZ | 2.39 | 0.55 |
| 1:A:484:SER:O | 1:A:508:TYR:HE1 | 1.90 | 0.55 |
| 1:A:1411:VAL:HG13 | 1:A:1412:SER:H | 1.72 | 0.55 |
| 2:B:733:GLN:HG3 | 10:J:54:VAL:HG13 | 1.89 | 0.55 |
| 15:O:647:LEU:O | 15:O:650:VAL:HG12 | 2.07 | 0.55 |
| 1:A:11:LYS:HG3 | 2:B:1117:ILE:HD13 | 1.87 | 0.55 |
| 1:A:520:HIS:HE1 | 2:B:1062:LEU:HD21 | 1.72 | 0.55 |
| 2:B:383:LEU:HB3 | 2:B:442:TRP:CH2 | 2.41 | 0.55 |
| 2:B:611:PRO:HG3 | 2:B:648:TYR:CE1 | 2.41 | 0.55 |
| 2:B:976:GLY:HA2 | 2:B:981:GLY:HA3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:89:GLU:OE1 | 6:F:90:ARG:N | 2.40 | 0.55 |
| 7:G:126:SER:CB | 7:G:139:TYR:CB | 2.85 | 0.55 |
| 1:A:372:ARG:HG2 | 2:B:1050:PRO:HB2 | 1.89 | 0.55 |
| 1:A:715:ASN:HD21 | 2:B:1001:LYS:HD3 | 1.70 | 0.55 |
| 5:E:77:SER:O | 5:E:105:PHE:HB3 | 2.06 | 0.55 |
| 13:M:112:TYR:HD1 | 13:M:119:TRP:NE1 | 2.00 | 0.55 |
| 14:N:287:HIS:NE2 | 14:N:384:LYS:HG3 | 2.22 | 0.55 |
| 15:O:171:VAL:HB | 15:O:276:PRO:HB3 | 1.87 | 0.55 |
| 1:A:164:VAL:HB | 1:A:180:HIS:CB | 2.37 | 0.55 |
| 1:A:308:SER:HA | 15:O:534:ARG:CD | 2.37 | 0.55 |
| 1:A:404:TYR:CZ | 1:A:528:ARG:HD2 | 2.42 | 0.55 |
| 1:A:636:PRO:HG2 | 1:A:643:ASN:HA | 1.89 | 0.55 |
| 1:A:1125:ARG:NH2 | 1:A:1317:ASN:HB3 | 2.22 | 0.55 |
| 2:B:906:PRO:HB3 | 2:B:1026:LYS:HE3 | 1.89 | 0.55 |
| 18:R:11:GLU:N | 18:R:11:GLU:OE1 | 2.40 | 0.55 |
| 18:R:270:LEU:O | 18:R:273:GLN:NE2 | 2.36 | 0.55 |
| 2:B:817:PRO:HB2 | 2:B:822:GLN:HA | 1.89 | 0.54 |
| 5:E:182:ASP:OD1 | 5:E:183:PRO:HD2 | 2.07 | 0.54 |
| 7:G:82:GLY:HA2 | 7:G:150:ILE:O | 2.08 | 0.54 |
| 8:H:93:TYR:CD2 | 8:H:143:LEU:HG | 2.42 | 0.54 |
| 18:R:436:LYS:NZ | 19:S:462:GLU:OE2 | 2.25 | 0.54 |
| 18:R:483:ILE:HG21 | 18:R:486:ILE:HG13 | 1.89 | 0.54 |
| 18:R:627:TRP:O | 18:R:631:ASN:ND2 | 2.32 | 0.54 |
| 1:A:628:ALA:HB2 | 1:A:675:HIS:HD2 | 1.69 | 0.54 |
| 2:B:400:LYS:O | 2:B:403:ILE:HG22 | 2.07 | 0.54 |
| 2:B:566:ARG:NH2 | 14:N:282:LEU:HD23 | 2.22 | 0.54 |
| 2:B:583:LYS:HG2 | 2:B:584:VAL:HG13 | 1.88 | 0.54 |
| 2:B:778:ILE:HG13 | 2:B:906:PRO:HG2 | 1.88 | 0.54 |
| 2:B:904:ARG:NH2 | 2:B:1033:ASP:OD1 | 2.40 | 0.54 |
| 7:G:114:MET:HB3 | 7:G:201:GLN:HB3 | 1.89 | 0.54 |
| 15:O:128:HIS:CE1 | 15:O:652:GLN:HE22 | 2.25 | 0.54 |
| 15:O:132:TYR:C | 15:O:134:GLY:H | 2.10 | 0.54 |
| 15:O:230:SER:O | 15:O:237:LYS:NZ | 2.36 | 0.54 |
| 18:R:165:VAL:HA | 18:R:170:ILE:HD13 | 1.90 | 0.54 |
| 1:A:625:ASN:HD21 | 1:A:941:HIS:HA | 1.72 | 0.54 |
| 1:A:661:SER:HB2 | 8:H:122:LEU:HD11 | 1.89 | 0.54 |
| 2:B:260:CYS:O | 2:B:346:ALA:HB2 | 2.07 | 0.54 |
| 8:H:43:ASN:ND2 | 8:H:46:LEU:HD13 | 2.22 | 0.54 |
| 19:S:429:TYR:HA | 19:S:432:LEU:HD12 | 1.88 | 0.54 |
| 2:B:334:HIS:O | 2:B:337:VAL:N | 2.40 | 0.54 |
| 7:G:126:SER:OG | 7:G:139:TYR:CG | 2.58 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:114:VAL:HG21 | 8:H:130:ARG:NH1 | 2.22 | 0.54 |
| 13:M:163:VAL:HG22 | 13:M:168:VAL:HG22 | 1.89 | 0.54 |
| 1:A:164:VAL:CA | 1:A:180:HIS:HB2 | 2.38 | 0.54 |
| 1:A:675:HIS:CA | 1:A:937:ARG:HH22 | 2.20 | 0.54 |
| 2:B:932:PRO:HG2 | 2:B:940:PRO:HG3 | 1.89 | 0.54 |
| 4:D:61:ASN:ND2 | 7:G:103:GLY:O | 2.41 | 0.54 |
| 15:O:59:GLU:HG3 | 15:O:61:ALA:H | 1.73 | 0.54 |
| 18:R:213:TRP:NE1 | 18:R:287:PRO:HG3 | 2.22 | 0.54 |
| 1:A:66:GLU:HB3 | 1:A:71:HIS:HB2 | 1.90 | 0.54 |
| 1:A:921:LEU:CD2 | 1:A:932:PRO:HG3 | 2.38 | 0.54 |
| 1:A:1193:ILE:HG12 | 1:A:1200:LEU:HD11 | 1.90 | 0.54 |
| 3:C:119:ASN:O | 3:C:120:LEU:CG | 2.51 | 0.54 |
| 3:C:123:ASP:OD1 | 3:C:124:GLU:N | 2.40 | 0.54 |
| 5:E:153:HIS:CE1 | 5:E:184:VAL:HG11 | 2.43 | 0.54 |
| 15:O:623:GLU:O | 15:O:627:LEU:HG | 2.07 | 0.54 |
| 16:P:269:LEU:HD11 | 16:P:296:TYR:OH | 2.07 | 0.54 |
| 2:B:1031:VAL:O | 2:B:1034:LYS:N | 2.41 | 0.54 |
| 3:C:230:LEU:HD13 | 3:C:297:HIS:CE1 | 2.42 | 0.54 |
| 1:A:226:LYS:NZ | 15:O:547:GLU:OE2 | 2.31 | 0.54 |
| 2:B:239:LYS:HG2 | 2:B:241:TYR:CE2 | 2.41 | 0.54 |
| 5:E:2:ASP:O | 5:E:6:GLU:N | 2.41 | 0.54 |
| 7:G:203:ASP:HB3 | 7:G:211:TRP:HE1 | 1.73 | 0.54 |
| 8:H:93:TYR:HD1 | 8:H:145:ARG:HD3 | 1.72 | 0.54 |
| 13:M:122:ASP:HB3 | 13:M:145:VAL:CG2 | 2.37 | 0.54 |
| 13:M:182:PHE:HD1 | 13:M:183:PHE:N | 2.04 | 0.54 |
| 15:O:366:LEU:HD22 | 15:O:368:ARG:HH11 | 1.72 | 0.54 |
| 18:R:610:LEU:HA | 18:R:613:HIS:CD2 | 2.41 | 0.54 |
| 19:S:434:MET:HE3 | 19:S:479:PRO:HB3 | 1.89 | 0.54 |
| 20:X:16:DA:H2' | 20:X:17:DG:C8 | 2.43 | 0.54 |
| 1:A:200:GLU:CB | 15:O:516:LEU:HD21 | 2.38 | 0.54 |
| 1:A:211:LEU:HD22 | 1:A:215:VAL:HG21 | 1.90 | 0.54 |
| 1:A:830:ARG:HD2 | 1:A:837:LYS:HG2 | 1.90 | 0.54 |
| 1:A:869:ARG:NH2 | 2:B:502:THR:HB | 2.22 | 0.54 |
| 1:A:1278:ILE:HG12 | 1:A:1297:GLY:HA3 | 1.88 | 0.54 |
| 2:B:254:ALA:O | 2:B:258:LYS:HG2 | 2.08 | 0.54 |
| 2:B:647:GLU:OE1 | 2:B:647:GLU:N | 2.41 | 0.54 |
| 5:E:112:TYR:CZ | 5:E:116:ILE:HG23 | 2.43 | 0.54 |
| 16:P:295:ASN:HB2 | 16:P:297:PHE:CE1 | 2.43 | 0.54 |
| 18:R:632:ALA:O | 18:R:636:LEU:CB | 2.55 | 0.54 |
| 1:A:516:GLU:OE2 | 2:B:1034:LYS:HD3 | 2.07 | 0.54 |
| 2:B:135:TYR:O | 2:B:142:ILE:HA | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:138:GLY:N | 2:B:141:ILE:HG21 | 2.21 | 0.54 |
| 2:B:330:THR:HA | 2:B:345:LYS:HE3 | 1.90 | 0.54 |
| 2:B:936:GLN:NE2 | 10:J:43:ARG:NH1 | 2.56 | 0.54 |
| 3:C:223:SER:HB2 | 3:C:303:GLU:HB2 | 1.89 | 0.54 |
| 6:F:79:ARG:NH1 | 6:F:145:ASP:H | 2.06 | 0.54 |
| 11:K:123:ASP:O | 11:K:126:ASP:N | 2.40 | 0.54 |
| 13:M:106:PHE:O | 13:M:107:ILE:HG22 | 2.07 | 0.54 |
| 13:M:242:ASN:O | 13:M:243:ILE:HB | 2.08 | 0.54 |
| 18:R:399:THR:HB | 18:R:484:GLN:NE2 | 2.23 | 0.54 |
| 20:X:25:DT:O4 | 21:Y:38:DA:N6 | 2.41 | 0.54 |
| 1:A:379:THR:HG21 | 1:A:497:THR:HA | 1.90 | 0.53 |
| 1:A:891:LYS:HG3 | 1:A:1389:PHE:HD1 | 1.73 | 0.53 |
| 2:B:723:THR:HG23 | 2:B:724:LEU:H | 1.74 | 0.53 |
| 15:O:187:ILE:O | 15:O:189:SER:N | 2.41 | 0.53 |
| 15:O:190:LEU:CD1 | 15:O:194:LEU:HD23 | 2.32 | 0.53 |
| 15:O:190:LEU:CB | 15:O:194:LEU:HG | 2.38 | 0.53 |
| 18:R:437:THR:O | 18:R:465:TYR:OH | 2.26 | 0.53 |
| 1:A:371:LYS:HZ1 | 2:B:1122:PRO:CB | 2.21 | 0.53 |
| 1:A:378:ARG:O | 1:A:379:THR:OG1 | 2.24 | 0.53 |
| 1:A:1024:LYS:HE2 | 1:A:1030:GLY:HA3 | 1.89 | 0.53 |
| 1:A:1028:MET:SD | 1:A:1048:VAL:HG22 | 2.49 | 0.53 |
| 2:B:347:LEU:HB3 | 2:B:541:ILE:HD11 | 1.90 | 0.53 |
| 4:D:14:TYR:CE2 | 4:D:103:PHE:HB2 | 2.44 | 0.53 |
| 18:R:398:ALA:HB3 | 18:R:449:VAL:HB | 1.89 | 0.53 |
| 20:X:3:DT:O4 | 21:Y:60:DA:N6 | 2.41 | 0.53 |
| 1:A:252:ARG:HB3 | 1:A:253:PRO:HD2 | 1.89 | 0.53 |
| 2:B:244:HIS:HB3 | 2:B:247:ILE:HG22 | 1.90 | 0.53 |
| 2:B:552:ASN:OD1 | 2:B:553:TYR:CD2 | 2.61 | 0.53 |
| 5:E:32:GLN:O | 5:E:36:GLU:N | 2.41 | 0.53 |
| 14:N:282:LEU:O | 14:N:286:ASP:CB | 2.57 | 0.53 |
| 16:P:209:ALA:O | 16:P:212:VAL:HG12 | 2.08 | 0.53 |
| 16:P:311:TYR:HA | 17:Q:40:PRO:CA | 2.21 | 0.53 |
| 18:R:395:ASN:H | 18:R:487:VAL:HB | 1.72 | 0.53 |
| 21:Y:7:DA:H2" | 21:Y:8:DG:H8 | 1.73 | 0.53 |
| 21:Y:46:DA:H2" | 21:Y:47:DC:O4' | 2.08 | 0.53 |
| 1:A:287:VAL:O | 1:A:290:THR:HG22 | 2.07 | 0.53 |
| 1:A:302:GLY:C | 1:A:304:ASP:H | 2.12 | 0.53 |
| 1:A:389:ILE:N | 1:A:695:ASN:OD1 | 2.37 | 0.53 |
| 1:A:542:LEU:HD21 | 1:A:679:TYR:HE1 | 1.73 | 0.53 |
| 1:A:624:ILE:HG22 | 1:A:625:ASN:N | 2.24 | 0.53 |
| 3:C:105:PRO:HG3 | 10:J:6:ARG:NH2 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:2:PHE:N | 7:G:77:PHE:HA | 2.22 | 0.53 |
| 13:M:255:PHE:O | 13:M:258:THR:OG1 | 2.25 | 0.53 |
| 18:R:97:PRO:HD2 | 18:R:100:ILE:HD12 | 1.89 | 0.53 |
| 20:X:6:DA:C4 | 20:X:7:DA:C5 | 2.96 | 0.53 |
| 20:X:11:DA:H2" | 20:X:12:DT:C6 | 2.44 | 0.53 |
| 1:A:197:TRP:HZ3 | 15:O:567:ARG:HH11 | 1.51 | 0.53 |
| 1:A:308:SER:N | 1:A:311:ASN:OD1 | 2.41 | 0.53 |
| 1:A:373:VAL:N | 2:B:1050:PRO:HG2 | 2.22 | 0.53 |
| 1:A:628:ALA:O | 1:A:651:PHE:HA | 2.07 | 0.53 |
| 2:B:1022:ILE:HG22 | 2:B:1023:TYR:N | 2.23 | 0.53 |
| 10:J:56:LEU:O | 10:J:59:LYS:N | 2.41 | 0.53 |
| 15:O:267:PRO:HD3 | 15:O:273:ILE:HG22 | 1.91 | 0.53 |
| 1:A:214:TYR:HD2 | 1:A:215:VAL:HG13 | 1.73 | 0.53 |
| 1:A:269:ARG:HH21 | 1:A:286:THR:H | 1.55 | 0.53 |
| 2:B:626:HIS:HA | 2:B:629:LYS:HB3 | 1.89 | 0.53 |
| 3:C:211:GLY:HA3 | 3:C:219:PHE:CE2 | 2.44 | 0.53 |
| 6:F:85:MET:SD | 6:F:153:VAL:HA | 2.49 | 0.53 |
| 15:O:44:PRO:HA | 15:O:582:GLU:HG3 | 1.91 | 0.53 |
| 15:O:496:ILE:HD11 | 15:O:576:PHE:CZ | 2.44 | 0.53 |
| 15:O:584:ASN:OD1 | 16:P:310:VAL:HA | 2.09 | 0.53 |
| 16:P:128:LEU:HA | 16:P:131:GLN:HB2 | 1.91 | 0.53 |
| 18:R:397:VAL:HG12 | 18:R:484:GLN:HB2 | 1.90 | 0.53 |
| 1:A:224:PRO:O | 1:A:227:THR:HG22 | 2.07 | 0.53 |
| 1:A:269:ARG:NH1 | 1:A:285:LEU:HB2 | 2.22 | 0.53 |
| 1:A:482:ARG:HB3 | 1:A:544:PRO:HG3 | 1.91 | 0.53 |
| 1:A:993:GLU:O | 5:E:197:LYS:NZ | 2.42 | 0.53 |
| 1:A:1305:CYS:SG | 5:E:141:VAL:HG11 | 2.49 | 0.53 |
| 9:I:22:TYR:O | 9:I:23:THR:HG22 | 2.07 | 0.53 |
| 9:I:29:CYS:HA | 13:M:183:PHE:CE2 | 2.35 | 0.53 |
| 10:J:43:ARG:NH1 | 10:J:43:ARG:HG2 | 2.24 | 0.53 |
| 15:O:538:ALA:O | 15:O:541:ILE:HG22 | 2.08 | 0.53 |
| 16:P:241:ARG:O | 16:P:245:GLU:HG2 | 2.08 | 0.53 |
| 18:R:521:TYR:HB3 | 18:R:530:LEU:HB2 | 1.89 | 0.53 |
| 1:A:44:LYS:HG3 | 1:A:45:ASP:H | 1.72 | 0.53 |
| 1:A:476:ARG:HG3 | 1:A:477:GLN:HB3 | 1.91 | 0.53 |
| 1:A:678:PHE:CE2 | 1:A:694:MET:HG2 | 2.43 | 0.53 |
| 1:A:968:GLY:O | 1:A:972:GLU:HG2 | 2.09 | 0.53 |
| 5:E:94:LYS:O | 5:E:98:ILE:HG12 | 2.09 | 0.53 |
| 7:G:141:ASP:OD1 | 7:G:142:VAL:N | 2.42 | 0.53 |
| 8:H:97:MET:HB2 | 8:H:142:LEU:HB3 | 1.90 | 0.53 |
| 13:M:125:LEU:HD11 | 13:M:146:GLN:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:389:THR:C | 14:N:391:LEU:H | 2.13 | 0.53 |
| 16:P:106:TRP:CZ3 | 16:P:108:LYS:HB3 | 2.44 | 0.53 |
| 16:P:256:VAL:O | 16:P:260:CYS:HB3 | 2.08 | 0.53 |
| 18:R:516:PHE:CD1 | 18:R:517:PRO:HD2 | 2.43 | 0.53 |
| 1:A:472:VAL:HG11 | 1:A:519:LEU:HG | 1.90 | 0.53 |
| 1:A:896:LEU:HB3 | 1:A:1090:GLY:HA3 | 1.91 | 0.53 |
| 1:A:912:VAL:HG23 | 1:A:913:GLN:H | 1.74 | 0.53 |
| 1:A:995:VAL:HG23 | 1:A:996:ASP:H | 1.74 | 0.53 |
| 2:B:247:ILE:HG13 | 2:B:248:ALA:H | 1.74 | 0.53 |
| 2:B:464:ILE:HD11 | 2:B:746:TYR:CE1 | 2.44 | 0.53 |
| 2:B:529:ILE:HD11 | 2:B:575:PHE:CE1 | 2.42 | 0.53 |
| 2:B:551:LEU:CD1 | 14:N:388:THR:N | 2.68 | 0.53 |
| 3:C:115:TRP:HH2 | 3:C:212:ILE:HB | 1.73 | 0.53 |
| 8:H:13:SER:HB3 | 8:H:27:GLU:O | 2.08 | 0.53 |
| 9:I:30:PRO:CD | 13:M:183:PHE:HZ | 2.21 | 0.53 |
| 14:N:287:HIS:CD2 | 14:N:384:LYS:HG3 | 2.43 | 0.53 |
| 15:O:507:LEU:O | 15:O:511:ILE:HG12 | 2.08 | 0.53 |
| 16:P:98:GLU:HB3 | 16:P:150:LEU:HD21 | 1.89 | 0.53 |
| 18:R:287:PRO:HD2 | 18:R:290:PHE:CE1 | 2.44 | 0.53 |
| 18:R:463:ARG:NH1 | 18:R:598:ASP:O | 2.39 | 0.53 |
| 1:A:45:ASP:O | 1:A:48:PRO:HD3 | 2.10 | 0.53 |
| 1:A:1130:ILE:HA | 1:A:1362:MET:HE1 | 1.91 | 0.53 |
| 2:B:758:ALA:O | 2:B:943:ILE:HD12 | 2.09 | 0.53 |
| 2:B:934:ASN:ND2 | 2:B:1019:PHE:HZ | 2.07 | 0.53 |
| 3:C:7:ILE:HG12 | 3:C:292:GLY:HA2 | 1.90 | 0.53 |
| 3:C:108:VAL:HB | 3:C:184:VAL:HG12 | 1.91 | 0.53 |
| 6:F:101:ILE:HG21 | 6:F:120:ILE:HD11 | 1.91 | 0.53 |
| 13:M:109:ALA:HB3 | 13:M:122:ASP:HB2 | 1.90 | 0.53 |
| 18:R:405:ARG:HG3 | 18:R:443:ALA:O | 2.09 | 0.53 |
| 1:A:1171:PHE:HD2 | 1:A:1172:TYR:CD2 | 2.26 | 0.52 |
| 2:B:167:ASP:C | 2:B:169:SER:H | 2.12 | 0.52 |
| 2:B:337:VAL:HG23 | 2:B:338:GLU:H | 1.73 | 0.52 |
| 2:B:914:SER:OG | 2:B:914:SER:O | 2.19 | 0.52 |
| 5:E:66:GLU:HG3 | 5:E:67:GLU:H | 1.74 | 0.52 |
| 5:E:82:PHE:HZ | 5:E:113:GLN:HB2 | 1.74 | 0.52 |
| 9:I:35:ILE:HD12 | 9:I:36:GLU:HG2 | 1.91 | 0.52 |
| 13:M:90:TYR:C | 14:N:392:GLN:NE2 | 2.62 | 0.52 |
| 13:M:122:ASP:HA | 13:M:146:GLN:O | 2.09 | 0.52 |
| 15:O:332:GLN:HE22 | 15:O:337:GLN:NE2 | 2.07 | 0.52 |
| 1:A:32:VAL:HG11 | 1:A:57:LYS:HD2 | 1.90 | 0.52 |
| 1:A:109:ASN:ND2 | 1:A:159:ALA:CB | 2.64 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1391:LYS:HB2 | 1:A:1395:HIS:CE1 | 2.45 | 0.52 |
| 2:B:289:GLU:O | 2:B:292:LYS:HG2 | 2.09 | 0.52 |
| 2:B:317:LEU:O | 2:B:320:LEU:HG | 2.09 | 0.52 |
| 3:C:172:GLN:N | 3:C:175:GLN:HB3 | 2.16 | 0.52 |
| 3:C:255:VAL:O | 3:C:268:LYS:HB2 | 2.09 | 0.52 |
| 5:E:153:HIS:ND1 | 5:E:184:VAL:HG11 | 2.24 | 0.52 |
| 7:G:115:LEU:H | 7:G:199:SER:HB3 | 1.75 | 0.52 |
| 13:M:171:VAL:CG1 | 13:M:172:PRO:HD2 | 2.39 | 0.52 |
| 18:R:140:HIS:ND1 | 18:R:140:HIS:O | 2.42 | 0.52 |
| 19:S:409:GLY:HA3 | 21:Y:55:DT:H4' | 1.91 | 0.52 |
| 20:X:59:DC:C2 | 20:X:60:DA:N7 | 2.76 | 0.52 |
| 1:A:381:ILE:HD11 | 1:A:517:MET:HG2 | 1.90 | 0.52 |
| 1:A:703:ARG:NH2 | 11:K:93:ILE:O | 2.42 | 0.52 |
| 1:A:1316:THR:OG1 | 1:A:1317:ASN:N | 2.42 | 0.52 |
| 2:B:155:MET:HB2 | 2:B:185:PHE:CE1 | 2.44 | 0.52 |
| 2:B:714:ALA:O | 2:B:717:GLN:HB2 | 2.10 | 0.52 |
| 3:C:100:ARG:HH12 | 10:J:2:ILE:HB | 1.73 | 0.52 |
| 14:N:395:ILE:HD12 | 14:N:411:ARG:HA | 1.92 | 0.52 |
| 15:O:132:TYR:OH | 15:O:291:ARG:NH1 | 2.43 | 0.52 |
| 16:P:106:TRP:HB2 | 16:P:147:ILE:HG22 | 1.90 | 0.52 |
| 18:R:195:LYS:HA | 18:R:198:VAL:HB | 1.92 | 0.52 |
| 1:A:5:VAL:HG22 | 7:G:37:LYS:HB3 | 1.90 | 0.52 |
| 1:A:161:ASN:HB2 | 1:A:180:HIS:CE1 | 2.43 | 0.52 |
| 1:A:606:GLY:HA2 | 1:A:609:VAL:HG12 | 1.90 | 0.52 |
| 2:B:553:TYR:HA | 2:B:597:MET:HB3 | 1.89 | 0.52 |
| 2:B:726:TYR:CE2 | 2:B:1028:LYS:HG3 | 2.44 | 0.52 |
| 2:B:926:VAL:CG1 | 2:B:930:ASP:HB2 | 2.40 | 0.52 |
| 2:B:933:PHE:CE2 | 3:C:226:SER:HB3 | 2.39 | 0.52 |
| 2:B:1038:ARG:NH1 | 2:B:1058:GLY:O | 2.36 | 0.52 |
| 3:C:211:GLY:HA3 | 3:C:219:PHE:CD2 | 2.44 | 0.52 |
| 15:O:110:THR:HG22 | 15:O:115:LYS:O | 2.09 | 0.52 |
| 15:O:163:VAL:HG12 | 15:O:282:ILE:HD11 | 1.91 | 0.52 |
| 15:O:352:VAL:HG13 | 15:O:353:GLU:CD | 2.28 | 0.52 |
| 16:P:135:LYS:HB3 | 16:P:151:TYR:HD1 | 1.74 | 0.52 |
| 18:R:4:CYS:HB3 | 18:R:9:GLY:H | 1.73 | 0.52 |
| 18:R:12:PHE:CD1 | 18:R:25:CYS:HB3 | 2.44 | 0.52 |
| 21:Y:45:DT:H73 | 21:Y:46:DA:N7 | 2.25 | 0.52 |
| 1:A:598:MET:HA | 1:A:602:TYR:HD1 | 1.75 | 0.52 |
| 1:A:1173:VAL:HA | 1:A:1186:VAL:HG12 | 1.91 | 0.52 |
| 2:B:774:ASN:O | 2:B:777:SER:HB2 | 2.10 | 0.52 |
| 2:B:914:SER:HB3 | 2:B:918:GLN:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:933:PHE:O | 2:B:1004:LEU:HD23 | 2.09 | 0.52 |
| 2:B:1057:ASP:CG | 2:B:1058:GLY:N | 2.62 | 0.52 |
| 15:O:36:SER:O | 15:O:40:ARG:HB2 | 2.10 | 0.52 |
| 21:Y:15:DT:H2' | 21:Y:16:DA:C8 | 2.44 | 0.52 |
| 1:A:1431:VAL:HG13 | 7:G:57:GLY:O | 2.10 | 0.52 |
| 2:B:244:HIS:CE1 | 2:B:332:ILE:HD12 | 2.45 | 0.52 |
| 2:B:556:TYR:HE1 | 2:B:561:LEU:HD12 | 1.74 | 0.52 |
| 2:B:911:LYS:HD3 | 2:B:1029:HIS:HB2 | 1.92 | 0.52 |
| 5:E:200:ARG:HD2 | 5:E:208:TYR:CZ | 2.44 | 0.52 |
| 7:G:98:LYS:HA | 7:G:109:PHE:HA | 1.92 | 0.52 |
| 14:N:389:THR:O | 14:N:391:LEU:N | 2.42 | 0.52 |
| 16:P:27:ILE:HB | 16:P:31:PHE:HB2 | 1.91 | 0.52 |
| 18:R:467:ARG:O | 18:R:471:LYS:CB | 2.58 | 0.52 |
| 18:R:502:ALA:HB2 | 18:R:519:LEU:HD11 | 1.90 | 0.52 |
| 19:S:431:ALA:HA | 19:S:434:MET:HB2 | 1.91 | 0.52 |
| 1:A:473:LEU:HD13 | 1:A:485:ILE:HG23 | 1.92 | 0.52 |
| 2:B:296:TYR:HD2 | 13:M:186:ILE:HG13 | 1.73 | 0.52 |
| 2:B:727:LEU:HD21 | 2:B:788:ARG:HE | 1.73 | 0.52 |
| 2:B:884:VAL:HG12 | 2:B:898:VAL:HB | 1.91 | 0.52 |
| 2:B:958:MET:HG3 | 2:B:1018:PHE:CE2 | 2.44 | 0.52 |
| 4:D:1:MET:HG3 | 4:D:2:LYS:H | 1.73 | 0.52 |
| 11:K:68:GLU:HG3 | 11:K:69:ASP:H | 1.74 | 0.52 |
| 18:R:91:SER:HB3 | 18:R:101:THR:HG21 | 1.91 | 0.52 |
| 18:R:418:ALA:HA | 18:R:429:ILE:O | 2.09 | 0.52 |
| 18:R:422:PRO:HB2 | 18:R:634:PHE:CZ | 2.45 | 0.52 |
| 1:A:224:PRO:HA | 1:A:227:THR:HG22 | 1.91 | 0.52 |
| 1:A:624:ILE:H | 1:A:657:SER:HG | 1.55 | 0.52 |
| 5:E:26:ARG:HH22 | 5:E:189:GLY:N | 2.08 | 0.52 |
| 6:F:85:MET:HA | 6:F:151:LEU:HD21 | 1.91 | 0.52 |
| 8:H:101:ALA:HB2 | 8:H:116:TYR:CE1 | 2.44 | 0.52 |
| 15:O:499:THR:HG21 | 16:P:312:PHE:CG | 2.45 | 0.52 |
| 16:P:310:VAL:HB | 17:Q:43:ILE:HD11 | 1.91 | 0.52 |
| 21:Y:18:DC:H2" | 21:Y:19:DT:C5 | 2.45 | 0.52 |
| 1:A:628:ALA:HB1 | 1:A:675:HIS:CD2 | 2.45 | 0.52 |
| 1:A:643:ASN:HB2 | 1:A:651:PHE:CE2 | 2.45 | 0.52 |
| 1:A:1318:HIS:CD2 | 1:A:1321:GLU:HB3 | 2.45 | 0.52 |
| 2:B:736:VAL:HG21 | 2:B:960:GLU:HG3 | 1.91 | 0.52 |
| 2:B:779:ASP:OD2 | 3:C:216:HIS:HB3 | 2.10 | 0.52 |
| 10:J:7:CYS:SG | 10:J:46:CYS:HA | 2.49 | 0.52 |
| 18:R:273:GLN:HB2 | 19:S:277:UNK:N | 2.25 | 0.52 |
| 1:A:235:LYS:HZ3 | 1:A:254:GLU:HG3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:975:VAL:CG2 | 1:A:976:ARG:H | 2.08 | 0.52 |
| 2:B:285:VAL:O | 2:B:288:GLU:HB3 | 2.10 | 0.52 |
| 2:B:621:ARG:HG3 | 2:B:645:LEU:HG | 1.92 | 0.52 |
| 15:O:519:GLU:OE1 | 15:O:519:GLU:N | 2.40 | 0.52 |
| 16:P:63:LEU:HA | 16:P:71:LYS:O | 2.08 | 0.52 |
| 18:R:289:SER:HB2 | 18:R:535:SER:HB3 | 1.92 | 0.52 |
| 18:R:506:GLY:HA2 | 18:R:509:SER:HB2 | 1.92 | 0.52 |
| 1:A:106:ILE:HD11 | 1:A:111:SER:C | 2.29 | 0.51 |
| 1:A:457:GLN:N | 1:A:460:ASP:OD2 | 2.43 | 0.51 |
| 2:B:197:GLN:HE22 | 2:B:451:ARG:HD2 | 1.75 | 0.51 |
| 2:B:464:ILE:HG12 | 2:B:687:LEU:HD11 | 1.93 | 0.51 |
| 5:E:190:LEU:HD23 | 5:E:214:CYS:HB2 | 1.92 | 0.51 |
| 13:M:95:ARG:NH2 | 14:N:413:ASP:O | 2.43 | 0.51 |
| 18:R:467:ARG:HD3 | 18:R:602:LEU:HG | 1.92 | 0.51 |
| 18:R:509:SER:HB3 | 18:R:519:LEU:HD21 | 1.92 | 0.51 |
| 1:A:277:SER:HB3 | 1:A:278:PRO:HD2 | 1.91 | 0.51 |
| 1:A:656:GLY:H | 1:A:944:ASN:HD22 | 1.58 | 0.51 |
| 1:A:1157:VAL:HG11 | 1:A:1308:GLY:HA3 | 1.92 | 0.51 |
| 2:B:529:ILE:HD11 | 2:B:575:PHE:HE1 | 1.74 | 0.51 |
| 5:E:100:ILE:HG21 | 5:E:127:ILE:HG13 | 1.92 | 0.51 |
| 15:O:53:VAL:O | 15:O:58:GLY:N | 2.43 | 0.51 |
| 1:A:413:ARG:O | 1:A:416:LEU:N | 2.43 | 0.51 |
| 1:A:502:GLU:CD | 2:B:767:ILE:HG13 | 2.30 | 0.51 |
| 1:A:925:GLU:CD | 1:A:1081:ALA:HA | 2.30 | 0.51 |
| 1:A:1347:GLY:O | 1:A:1348:MET:HG2 | 2.10 | 0.51 |
| 2:B:666:ILE:HA | 2:B:670:MET:SD | 2.50 | 0.51 |
| 2:B:800:ASN:HA | 2:B:855:PRO:HG3 | 1.92 | 0.51 |
| 2:B:971:GLY:HA2 | 10:J:51:LEU:CD1 | 2.39 | 0.51 |
| 4:D:102:SER:O | 4:D:106:LEU:N | 2.43 | 0.51 |
| 5:E:118:PRO:O | 5:E:122:LYS:N | 2.44 | 0.51 |
| 15:O:190:LEU:HB3 | 15:O:194:LEU:HG | 1.91 | 0.51 |
| 15:O:255:LYS:HB3 | 15:O:256:PRO:HD3 | 1.92 | 0.51 |
| 16:P:106:TRP:NE1 | 16:P:145:ARG:HA | 2.24 | 0.51 |
| 17:Q:38:SER:O | 17:Q:39:ILE:C | 2.49 | 0.51 |
| 18:R:401:THR:HG22 | 18:R:403:GLY:H | 1.76 | 0.51 |
| 18:R:468:ILE:HG13 | 18:R:610:LEU:HD11 | 1.92 | 0.51 |
| 18:R:510:SER:OG | 18:R:512:GLU:OE2 | 2.28 | 0.51 |
| 19:S:425:MET:HG2 | 19:S:429:TYR:CE2 | 2.45 | 0.51 |
| 19:S:444:GLN:HE22 | 19:S:490:LYS:HZ2 | 1.58 | 0.51 |
| 1:A:1145:LEU:HA | 1:A:1309:VAL:HA | 1.93 | 0.51 |
| 3:C:85:PHE:CZ | 3:C:98:ALA:HB2 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:251:PHE:CD2 | 3:C:255:VAL:HG21 | 2.45 | 0.51 |
| 18:R:478:PHE:O | 18:R:599:PRO:HB3 | 2.10 | 0.51 |
| 19:S:506:GLN:O | 19:S:510:LYS:CB | 2.57 | 0.51 |
| 1:A:11:LYS:HG3 | 2:B:1117:ILE:HG21 | 1.93 | 0.51 |
| 1:A:17:GLU:O | 2:B:1139:PRO:C | 2.49 | 0.51 |
| 1:A:329:SER:HA | 1:A:351:ARG:CZ | 2.39 | 0.51 |
| 2:B:383:LEU:HB3 | 2:B:442:TRP:HH2 | 1.75 | 0.51 |
| 2:B:536:LEU:HD22 | 2:B:571:PHE:CD1 | 2.45 | 0.51 |
| 5:E:22:MET:CE | 5:E:26:ARG:HH21 | 2.23 | 0.51 |
| 12:L:53:HIS:CD2 | 12:L:54:ARG:H | 2.28 | 0.51 |
| 13:M:159:TYR:CD1 | 13:M:172:PRO:HA | 2.45 | 0.51 |
| 15:O:188:SER:HG | 15:O:191:PHE:HD1 | 1.55 | 0.51 |
| 1:A:528:ARG:HH12 | 6:F:118:LEU:HB2 | 1.76 | 0.51 |
| 1:A:589:HIS:HA | 11:K:104:ARG:HH21 | 1.74 | 0.51 |
| 1:A:594:PRO:HB3 | 8:H:79:TRP:CD1 | 2.45 | 0.51 |
| 1:A:734:ALA:HB2 | 1:A:773:VAL:HG21 | 1.92 | 0.51 |
| 2:B:832:VAL:HB | 12:L:60:ARG:HA | 1.93 | 0.51 |
| 3:C:33:VAL:HG21 | 11:K:126:ASP:OD2 | 2.11 | 0.51 |
| 3:C:270:ALA:O | 3:C:271:ARG:HG2 | 2.10 | 0.51 |
| 4:D:126:GLN:O | 4:D:127:LEU:CG | 2.49 | 0.51 |
| 7:G:88:TRP:HA | 7:G:146:ILE:HD12 | 1.93 | 0.51 |
| 10:J:53:HIS:ND1 | 10:J:53:HIS:O | 2.44 | 0.51 |
| 18:R:190:ASP:O | 18:R:195:LYS:NZ | 2.43 | 0.51 |
| 21:Y:55:DT:H2" | 21:Y:56:DG:H8 | 1.70 | 0.51 |
| 2:B:279:TYR:OH | 2:B:358:MET:HG2 | 2.11 | 0.51 |
| 2:B:755:ALA:HA | 10:J:48:ARG:HH12 | 1.75 | 0.51 |
| 2:B:758:ALA:HA | 2:B:1019:PHE:HB3 | 1.93 | 0.51 |
| 5:E:41:ASP:HA | 5:E:44:ALA:HB3 | 1.92 | 0.51 |
| 10:J:1:MET:O | 10:J:53:HIS:NE2 | 2.43 | 0.51 |
| 13:M:88:PHE:HB2 | 14:N:395:ILE:HG23 | 1.92 | 0.51 |
| 15:O:590:PHE:O | 15:O:593:GLU:N | 2.44 | 0.51 |
| 16:P:82:LYS:O | 16:P:86:MET:HG2 | 2.10 | 0.51 |
| 18:R:554:GLU:HG2 | 18:R:582:LEU:HD22 | 1.92 | 0.51 |
| 1:A:38:ASP:HB3 | 1:A:290:THR:OG1 | 2.10 | 0.51 |
| 1:A:38:ASP:N | 1:A:38:ASP:OD1 | 2.38 | 0.51 |
| 1:A:327:ILE:CB | 1:A:353:PHE:CE2 | 2.94 | 0.51 |
| 1:A:330:ASP:CG | 1:A:331:SER:H | 2.12 | 0.51 |
| 1:A:1164:THR:OG1 | 1:A:1272:VAL:HG12 | 2.09 | 0.51 |
| 1:A:1382:SER:HA | 1:A:1406:ASP:OD1 | 2.11 | 0.51 |
| 2:B:45:TRP:HA | 2:B:676:GLU:OE2 | 2.11 | 0.51 |
| 2:B:214:GLY:HA3 | 2:B:234:ILE:CG2 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:230:LYS:HD3 | 2:B:334:HIS:HE1 | 1.76 | 0.51 |
| 2:B:767:ILE:HG22 | 2:B:768:GLU:N | 2.26 | 0.51 |
| 5:E:153:HIS:CD2 | 5:E:198:ILE:HG12 | 2.46 | 0.51 |
| 7:G:95:GLU:HG3 | 7:G:96:GLY:H | 1.75 | 0.51 |
| 14:N:290:ILE:HG21 | 14:N:384:LYS:HZ1 | 1.76 | 0.51 |
| 15:O:480:TYR:HA | 15:O:483:LEU:HB3 | 1.92 | 0.51 |
| 15:O:507:LEU:HD21 | 15:O:536:THR:HG23 | 1.91 | 0.51 |
| 15:O:602:LEU:HD11 | 15:O:623:GLU:HG2 | 1.91 | 0.51 |
| 16:P:266:GLU:O | 16:P:269:LEU:HB3 | 2.10 | 0.51 |
| 18:R:104:ALA:HA | 18:R:107:TRP:HD1 | 1.76 | 0.51 |
| 18:R:186:ALA:HA | 18:R:189:LEU:HD12 | 1.93 | 0.51 |
| 1:A:504:VAL:O | 1:A:507:PRO:HD2 | 2.11 | 0.51 |
| 2:B:204:ARG:HH22 | 2:B:602:ALA:HB1 | 1.76 | 0.51 |
| 2:B:558:ASN:HD21 | 2:B:603:THR:HG22 | 1.76 | 0.51 |
| 3:C:32:ASN:O | 3:C:33:VAL:HG23 | 2.10 | 0.51 |
| 4:D:11:LEU:HB3 | 7:G:2:PHE:O | 2.11 | 0.51 |
| 5:E:179:GLN:O | 5:E:180:ARG:C | 2.49 | 0.51 |
| 15:O:267:PRO:HD3 | 15:O:273:ILE:CG2 | 2.40 | 0.51 |
| 15:O:519:GLU:HA | 15:O:522:ILE:HB | 1.93 | 0.51 |
| 18:R:498:LEU:HD13 | 18:R:519:LEU:HB2 | 1.92 | 0.51 |
| 1:A:753:GLN:O | 1:A:755:GLY:N | 2.43 | 0.51 |
| 1:A:1411:VAL:HG21 | 2:B:1071:ILE:HD12 | 1.92 | 0.51 |
| 2:B:780:ARG:CZ | 3:C:217:ALA:CB | 2.85 | 0.51 |
| 2:B:908:LEU:HA | 2:B:922:CYS:SG | 2.51 | 0.51 |
| 7:G:147:ARG:NH2 | 7:G:204:GLY:O | 2.44 | 0.51 |
| 15:O:190:LEU:HD21 | 15:O:199:TYR:CE1 | 2.46 | 0.51 |
| 15:O:353:GLU:HA | 15:O:357:PRO:CD | 2.21 | 0.51 |
| 16:P:81:GLN:O | 16:P:85:THR:OG1 | 2.25 | 0.51 |
| 18:R:191:LEU:HB2 | 18:R:195:LYS:HD3 | 1.92 | 0.51 |
| 1:A:714:ILE:HG13 | 2:B:962:ILE:HD12 | 1.93 | 0.50 |
| 1:A:723:LEU:O | 1:A:727:LYS:HB2 | 2.11 | 0.50 |
| 1:A:934:ASN:ND2 | 1:A:937:ARG:HE | 2.09 | 0.50 |
| 1:A:1146:VAL:HG23 | 1:A:1308:GLY:O | 2.11 | 0.50 |
| 2:B:109:LYS:HG3 | 2:B:111:TYR:O | 2.11 | 0.50 |
| 2:B:771:LEU:O | 2:B:923:GLY:N | 2.35 | 0.50 |
| 8:H:115:TYR:HE1 | 8:H:124:ARG:HG3 | 1.76 | 0.50 |
| 15:O:578:ARG:HA | 15:O:648:TRP:HZ3 | 1.77 | 0.50 |
| 18:R:213:TRP:CD1 | 18:R:287:PRO:HG3 | 2.46 | 0.50 |
| 1:A:98:ALA:O | 1:A:101:GLN:N | 2.45 | 0.50 |
| 1:A:270:PRO:HG3 | 2:B:1046:LEU:CD1 | 2.41 | 0.50 |
| 1:A:407:LYS:HG2 | 1:A:461:VAL:HG22 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:552:ALA:HB3 | 1:A:671:ASP:CB | 2.41 | 0.50 |
| 1:A:773:VAL:O | 1:A:777:VAL:HG23 | 2.11 | 0.50 |
| 1:A:1180:ASN:HB3 | 9:I:21:VAL:H | 1.75 | 0.50 |
| 1:A:1386:LEU:HB3 | 1:A:1395:HIS:CD2 | 2.47 | 0.50 |
| 2:B:97:ASP:OD2 | 2:B:99:ARG:NH1 | 2.45 | 0.50 |
| 2:B:371:TYR:HB2 | 2:B:492:SER:OG | 2.10 | 0.50 |
| 2:B:454:VAL:HG13 | 2:B:455:THR:HG23 | 1.93 | 0.50 |
| 2:B:629:LYS:O | 2:B:635:LEU:HB2 | 2.11 | 0.50 |
| 2:B:849:THR:HG22 | 2:B:865:GLN:O | 2.11 | 0.50 |
| 5:E:152:LYS:HE2 | 5:E:154:ILE:HD11 | 1.94 | 0.50 |
| 15:O:595:LEU:HD12 | 15:O:598:GLU:HG3 | 1.93 | 0.50 |
| 16:P:64:VAL:HB | 16:P:71:LYS:HB2 | 1.92 | 0.50 |
| 1:A:37:ARG:HG2 | 1:A:38:ASP:OD1 | 2.11 | 0.50 |
| 1:A:235:LYS:HE3 | 1:A:254:GLU:HG3 | 1.91 | 0.50 |
| 1:A:548:GLU:OE2 | 1:A:672:GLY:O | 2.28 | 0.50 |
| 1:A:1445:ARG:HG3 | 1:A:1447:LEU:HD12 | 1.93 | 0.50 |
| 2:B:263:LEU:HD11 | 2:B:296:TYR:HA | 1.93 | 0.50 |
| 2:B:279:TYR:HE1 | 2:B:358:MET:HA | 1.75 | 0.50 |
| 2:B:415:GLU:OE1 | 2:B:415:GLU:N | 2.45 | 0.50 |
| 2:B:662:TYR:HE1 | 2:B:677:PRO:HG3 | 1.75 | 0.50 |
| 2:B:731:PRO:HB2 | 2:B:750:PRO:HG2 | 1.92 | 0.50 |
| 2:B:1036:HIS:CE1 | 2:B:1054:ARG:HA | 2.46 | 0.50 |
| 4:D:126:GLN:O | 4:D:127:LEU:O | 2.30 | 0.50 |
| 7:G:53:THR:CG2 | 7:G:71:THR:HG22 | 2.37 | 0.50 |
| 7:G:112:GLN:NE2 | 7:G:115:LEU:HD22 | 2.26 | 0.50 |
| 13:M:135:LYS:O | 13:M:138:SER:OG | 2.20 | 0.50 |
| 15:O:69:VAL:HG22 | 15:O:122:TYR:CG | 2.46 | 0.50 |
| 15:O:251:LYS:O | 15:O:255:LYS:N | 2.38 | 0.50 |
| 18:R:168:LEU:HB2 | 18:R:170:ILE:HD11 | 1.94 | 0.50 |
| 18:R:281:GLU:OE1 | 18:R:281:GLU:N | 2.40 | 0.50 |
| 1:A:200:GLU:HG2 | 15:O:515:LYS:HD3 | 1.93 | 0.50 |
| 1:A:476:ARG:NH1 | 1:A:477:GLN:HB3 | 2.26 | 0.50 |
| 1:A:949:ASN:OD1 | 1:A:950:GLN:N | 2.45 | 0.50 |
| 1:A:1022:LEU:HA | 1:A:1025:SER:HB3 | 1.93 | 0.50 |
| 2:B:1004:LEU:HD21 | 2:B:1019:PHE:HE2 | 1.76 | 0.50 |
| 2:B:1107:CYS:SG | 2:B:1109:THR:HG22 | 2.52 | 0.50 |
| 8:H:81:PRO:HD2 | 11:K:108:TYR:OH | 2.12 | 0.50 |
| 14:N:395:ILE:HD11 | 14:N:408:LEU:HD21 | 1.92 | 0.50 |
| 15:O:483:LEU:O | 15:O:487:LEU:N | 2.44 | 0.50 |
| 15:O:643:ARG:NH2 | 17:Q:51:GLU:OE1 | 2.45 | 0.50 |
| 18:R:523:MET:O | 18:R:527:LYS:HA | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:153:ARG:HG3 | 1:A:160:LEU:HB3 | 1.94 | 0.50 |
| 1:A:224:PRO:HD2 | 1:A:316:TRP:HH2 | 1.76 | 0.50 |
| 1:A:427:HIS:NE2 | 1:A:492:ILE:HG21 | 2.26 | 0.50 |
| 1:A:642:PRO:HB2 | 1:A:644:GLU:H | 1.77 | 0.50 |
| 1:A:705:LEU:HD22 | 2:B:761:SER:HB2 | 1.91 | 0.50 |
| 1:A:733:ILE:HD12 | 1:A:736:HIS:CE1 | 2.47 | 0.50 |
| 1:A:1452:SER:HA | 4:D:120:LYS:NZ | 2.27 | 0.50 |
| 2:B:58:VAL:HA | 2:B:60:GLN:OE1 | 2.12 | 0.50 |
| 2:B:109:LYS:HG3 | 2:B:111:TYR:N | 2.21 | 0.50 |
| 2:B:884:VAL:HG23 | 12:L:58:LYS:HB3 | 1.94 | 0.50 |
| 4:D:65:TYR:OH | 4:D:69:ASN:ND2 | 2.36 | 0.50 |
| 5:E:59:SER:HA | 5:E:81:GLU:HA | 1.94 | 0.50 |
| 14:N:380:MET:SD | 14:N:421:GLN:NE2 | 2.84 | 0.50 |
| 15:O:73:ARG:HD3 | 15:O:121:TYR:OH | 2.11 | 0.50 |
| 16:P:106:TRP:CG | 16:P:107:SER:N | 2.79 | 0.50 |
| 16:P:292:SER:OG | 16:P:293:ILE:N | 2.43 | 0.50 |
| 18:R:287:PRO:HD2 | 18:R:290:PHE:HE1 | 1.76 | 0.50 |
| 1:A:236:SER:H | 1:A:252:ARG:HD2 | 1.76 | 0.50 |
| 1:A:272:VAL:HB | 1:A:281:ASN:HB3 | 1.92 | 0.50 |
| 1:A:354:CYS:HG | 1:A:1393:THR:HG1 | 1.58 | 0.50 |
| 2:B:354:ARG:CZ | 2:B:549:LEU:HD13 | 2.40 | 0.50 |
| 2:B:778:ILE:CD1 | 2:B:906:PRO:HG2 | 2.41 | 0.50 |
| 3:C:14:ASN:ND2 | 3:C:295:ARG:HH12 | 2.08 | 0.50 |
| 4:D:146:ASP:O | 4:D:150:ILE:HG12 | 2.12 | 0.50 |
| 5:E:2:ASP:HA | 5:E:5:ASN:HB2 | 1.94 | 0.50 |
| 7:G:203:ASP:O | 7:G:205:MET:HG2 | 2.11 | 0.50 |
| 18:R:256:GLN:HA | 18:R:259:LEU:HB3 | 1.93 | 0.50 |
| 1:A:746:ASN:OD1 | 1:A:747:LYS:N | 2.45 | 0.50 |
| 2:B:143:MET:CG | 19:S:399:GLU:HB2 | 2.42 | 0.50 |
| 2:B:775:LYS:HG3 | 2:B:925:ILE:HG22 | 1.93 | 0.50 |
| 7:G:54:VAL:HA | 7:G:70:VAL:HG12 | 1.93 | 0.50 |
| 7:G:88:TRP:O | 7:G:99:VAL:HA | 2.12 | 0.50 |
| 13:M:121:ILE:N | 13:M:148:LEU:O | 2.29 | 0.50 |
| 13:M:255:PHE:O | 13:M:259:ILE:HG12 | 2.11 | 0.50 |
| 15:O:282:ILE:H | 15:O:282:ILE:HD12 | 1.77 | 0.50 |
| 16:P:218:THR:HG23 | 16:P:219:GLN:H | 1.77 | 0.50 |
| 1:A:100:ILE:HD11 | 1:A:178:ILE:HG21 | 1.94 | 0.50 |
| 1:A:520:HIS:CE1 | 2:B:1062:LEU:HD21 | 2.47 | 0.50 |
| 1:A:1286:ARG:N | 1:A:1290:LYS:O | 2.44 | 0.50 |
| 2:B:362:ASN:ND2 | 2:B:365:MET:SD | 2.76 | 0.50 |
| 2:B:553:TYR:HD1 | 2:B:597:MET:HA | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:933:PHE:CZ | 2:B:934:ASN:O | 2.64 | 0.50 |
| 10:J:12:LYS:O | 10:J:14:VAL:HG23 | 2.12 | 0.50 |
| 11:K:138:LYS:O | 11:K:142:MET:N | 2.41 | 0.50 |
| 18:R:194:LYS:O | 18:R:197:LYS:HB3 | 2.11 | 0.50 |
| 18:R:468:ILE:O | 18:R:472:ILE:N | 2.43 | 0.50 |
| 18:R:502:ALA:O | 18:R:506:GLY:N | 2.36 | 0.50 |
| 20:X:6:DA:N1 | 20:X:7:DA:C6 | 2.80 | 0.50 |
| 1:A:552:ALA:HB3 | 1:A:671:ASP:HB3 | 1.92 | 0.50 |
| 1:A:1078:TYR:O | 1:A:1081:ALA:N | 2.45 | 0.50 |
| 1:A:1224:ILE:HG12 | 1:A:1226:GLY:H | 1.77 | 0.50 |
| 2:B:760:MET:HE3 | 2:B:762:TYR:HB2 | 1.94 | 0.50 |
| 3:C:61:THR:HA | 3:C:298:PHE:HZ | 1.77 | 0.50 |
| 3:C:209:ILE:HG13 | 3:C:210:LEU:N | 2.26 | 0.50 |
| 7:G:203:ASP:OD1 | 7:G:204:GLY:N | 2.41 | 0.50 |
| 15:O:125:GLU:HB3 | 15:O:128:HIS:HB2 | 1.94 | 0.50 |
| 17:Q:36:PHE:N | 17:Q:37:PRO:HD2 | 2.26 | 0.50 |
| 18:R:172:GLU:HG3 | 18:R:506:GLY:HA3 | 1.94 | 0.50 |
| 18:R:424:ARG:HG2 | 21:Y:46:DA:OP1 | 2.12 | 0.50 |
| 21:Y:59:DG:H1' | 21:Y:60:DA:C8 | 2.46 | 0.50 |
| 1:A:278:PRO:HD3 | 2:B:852:ALA:HB1 | 1.94 | 0.49 |
| 1:A:376:SER:HB2 | 2:B:1060:LEU:HD12 | 1.93 | 0.49 |
| 1:A:424:PRO:HG2 | 1:A:444:LEU:CD2 | 2.41 | 0.49 |
| 2:B:100:VAL:HG12 | 2:B:129:ILE:HD13 | 1.94 | 0.49 |
| 2:B:543:LEU:HD22 | 13:M:158:GLN:NE2 | 2.27 | 0.49 |
| 3:C:70:ILE:HG23 | 3:C:317:SER:OG | 2.12 | 0.49 |
| 3:C:197:ARG:HB3 | 3:C:198:PRO:CD | 2.41 | 0.49 |
| 13:M:117:HIS:HB2 | 13:M:119:TRP:HE1 | 1.76 | 0.49 |
| 13:M:247:TRP:CH2 | 13:M:249:GLU:HB2 | 2.47 | 0.49 |
| 15:O:273:ILE:HG23 | 15:O:274:VAL:O | 2.11 | 0.49 |
| 16:P:298:LYS:HG2 | 16:P:298:LYS:O | 2.11 | 0.49 |
| 18:R:128:SER:OG | 18:R:164:MET:SD | 2.62 | 0.49 |
| 1:A:37:ARG:HG2 | 1:A:38:ASP:H | 1.76 | 0.49 |
| 1:A:73:ASN:OD1 | 1:A:74:LEU:N | 2.45 | 0.49 |
| 1:A:903:THR:HA | 1:A:914:PHE:O | 2.12 | 0.49 |
| 2:B:337:VAL:HG23 | 2:B:345:LYS:NZ | 2.24 | 0.49 |
| 2:B:1019:PHE:HE1 | 10:J:44:TYR:OH | 1.94 | 0.49 |
| 5:E:31:THR:HG23 | 5:E:34:GLU:H | 1.76 | 0.49 |
| 13:M:159:TYR:CD2 | 13:M:170:LEU:HD21 | 2.47 | 0.49 |
| 15:O:95:LEU:HD21 | 15:O:120:TYR:CZ | 2.47 | 0.49 |
| 18:R:398:ALA:HA | 18:R:484:GLN:H | 1.77 | 0.49 |
| 1:A:351:ARG:HD2 | 1:A:355:GLN:HE22 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:733:ILE:O | 1:A:737:LYS:HG3 | 2.11 | 0.49 |
| 1:A:1163:LYS:HG3 | 1:A:1164:THR:N | 2.21 | 0.49 |
| 1:A:1165:LEU:HD22 | 1:A:1198:LEU:HD21 | 1.93 | 0.49 |
| 2:B:141:ILE:HG23 | 2:B:142:ILE:N | 2.26 | 0.49 |
| 2:B:538:VAL:HB | 2:B:563:GLY:HA3 | 1.94 | 0.49 |
| 2:B:724:LEU:HD21 | 2:B:726:TYR:CZ | 2.48 | 0.49 |
| 5:E:96:PHE:O | 5:E:100:ILE:HG12 | 2.12 | 0.49 |
| 5:E:112:TYR:CD2 | 5:E:116:ILE:HG12 | 2.48 | 0.49 |
| 6:F:97:ARG:O | 6:F:101:ILE:HG12 | 2.12 | 0.49 |
| 7:G:21:ASP:OD1 | 7:G:22:THR:N | 2.42 | 0.49 |
| 14:N:276:ALA:HB1 | 14:N:280:LEU:HD23 | 1.94 | 0.49 |
| 19:S:430:LYS:O | 19:S:434:MET:HG2 | 2.13 | 0.49 |
| 19:S:470:GLU:O | 19:S:474:ARG:CB | 2.58 | 0.49 |
| 21:Y:52:DA:H2" | 21:Y:53:DT:O5' | 2.11 | 0.49 |
| 1:A:937:ARG:HG3 | 1:A:938:SER:N | 2.27 | 0.49 |
| 2:B:490:GLN:OE1 | 2:B:490:GLN:N | 2.45 | 0.49 |
| 3:C:33:VAL:C | 3:C:35:LYS:H | 2.16 | 0.49 |
| 9:I:34:PRO:O | 9:I:35:ILE:HG13 | 2.13 | 0.49 |
| 14:N:384:LYS:HA | 14:N:416:ILE:HD11 | 1.93 | 0.49 |
| 15:O:140:ILE:O | 15:O:144:MET:N | 2.42 | 0.49 |
| 16:P:15:ALA:HA | 16:P:55:LEU:HD11 | 1.93 | 0.49 |
| 16:P:211:ASN:OD1 | 16:P:212:VAL:N | 2.46 | 0.49 |
| 18:R:440:LEU:O | 18:R:447:MET:HB2 | 2.12 | 0.49 |
| 1:A:298:LEU:HD21 | 1:A:315:HIS:CE1 | 2.48 | 0.49 |
| 1:A:373:VAL:N | 2:B:1060:LEU:O | 2.38 | 0.49 |
| 1:A:1370:GLY:C | 1:A:1375:GLY:HA3 | 2.33 | 0.49 |
| 1:A:1434:THR:HG23 | 7:G:56:GLU:HA | 1.95 | 0.49 |
| 2:B:454:VAL:HG13 | 2:B:455:THR:H | 1.77 | 0.49 |
| 2:B:529:ILE:HD13 | 2:B:584:VAL:HG11 | 1.94 | 0.49 |
| 2:B:540:ASP:OD1 | 2:B:541:ILE:N | 2.45 | 0.49 |
| 2:B:1004:LEU:HD21 | 2:B:1019:PHE:CE2 | 2.47 | 0.49 |
| 2:B:1126:LYS:O | 2:B:1129:PHE:N | 2.45 | 0.49 |
| 8:H:10:PHE:CE2 | 8:H:38:LEU:HD13 | 2.45 | 0.49 |
| 15:O:288:MET:O | 15:O:291:ARG:HG2 | 2.13 | 0.49 |
| 15:O:554:THR:CG2 | 15:O:561:ARG:NE | 2.74 | 0.49 |
| 18:R:268:ALA:O | 18:R:272:VAL:HB | 2.12 | 0.49 |
| 18:R:290:PHE:CE1 | 18:R:495:PRO:HG3 | 2.47 | 0.49 |
| 1:A:997:GLN:C | 1:A:999:ASP:H | 2.15 | 0.49 |
| 1:A:1217:ILE:HG22 | 1:A:1218:GLN:N | 2.27 | 0.49 |
| 2:B:59:LYS:O | 2:B:63:ASP:N | 2.42 | 0.49 |
| 2:B:615:VAL:HG12 | 2:B:620:SER:HA | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:961:LEU:HD22 | 2:B:1018:PHE:CZ | 2.47 | 0.49 |
| 3:C:75:VAL:HG12 | 3:C:320:ILE:HD12 | 1.95 | 0.49 |
| 3:C:224:THR:CB | 10:J:10:CYS:SG | 2.98 | 0.49 |
| 14:N:364:ARG:HB3 | 14:N:372:SER:HB3 | 1.93 | 0.49 |
| 15:O:260:SER:HB3 | 15:O:264:THR:OG1 | 2.12 | 0.49 |
| 1:A:403:THR:HG21 | 1:A:431:ASN:HD21 | 1.78 | 0.49 |
| 1:A:498:PHE:CE2 | 1:A:519:LEU:HD13 | 2.47 | 0.49 |
| 1:A:1123:VAL:N | 1:A:1124:PRO:HD2 | 2.28 | 0.49 |
| 2:B:251:ILE:HG21 | 2:B:256:VAL:HG23 | 1.94 | 0.49 |
| 3:C:80:ALA:HA | 3:C:208:CYS:HA | 1.94 | 0.49 |
| 5:E:188:LEU:HD23 | 5:E:190:LEU:HD11 | 1.94 | 0.49 |
| 14:N:402:ASP:O | 14:N:405:SER:HB2 | 2.13 | 0.49 |
| 15:O:516:LEU:HA | 15:O:566:PHE:O | 2.13 | 0.49 |
| 17:Q:1072:UNK:O | 17:Q:1074:UNK:N | 2.46 | 0.49 |
| 19:S:451:ARG:HG3 | 19:S:452:LYS:H | 1.78 | 0.49 |
| 21:Y:13:DT:H2" | 21:Y:14:DT:C6 | 2.47 | 0.49 |
| 1:A:214:TYR:CD2 | 1:A:215:VAL:HG13 | 2.48 | 0.49 |
| 1:A:285:LEU:O | 1:A:288:LYS:N | 2.46 | 0.49 |
| 1:A:487:SER:OG | 1:A:536:GLY:HA2 | 2.13 | 0.49 |
| 4:D:14:TYR:HD2 | 4:D:15:GLU:HG2 | 1.77 | 0.49 |
| 13:M:149:LYS:CB | 13:M:182:PHE:HE2 | 2.25 | 0.49 |
| 15:O:595:LEU:HD21 | 15:O:630:VAL:HG23 | 1.94 | 0.49 |
| 18:R:6:ASN:ND2 | 18:R:30:VAL:HG21 | 2.27 | 0.49 |
| 18:R:394:GLN:HB3 | 21:Y:49:DA:H4' | 1.94 | 0.49 |
| 1:A:213:ARG:HA | 1:A:216:LYS:HB2 | 1.95 | 0.49 |
| 1:A:481:HIS:HA | 1:A:1095:GLN:OE1 | 2.13 | 0.49 |
| 1:A:497:THR:HG23 | 1:A:499:ARG:HG3 | 1.95 | 0.49 |
| 1:A:557:PHE:HA | 1:A:701:CYS:SG | 2.53 | 0.49 |
| 1:A:633:PHE:CZ | 1:A:643:ASN:HB3 | 2.48 | 0.49 |
| 2:B:539:GLU:O | 2:B:563:GLY:HA2 | 2.13 | 0.49 |
| 2:B:652:ASN:O | 2:B:655:ASN:HB3 | 2.12 | 0.49 |
| 2:B:936:GLN:HB2 | 2:B:938:ILE:CD1 | 2.42 | 0.49 |
| 2:B:957:LYS:HZ2 | 2:B:1022:ILE:HD13 | 1.77 | 0.49 |
| 2:B:1106:TRP:HE1 | 7:G:162:SER:CA | 2.26 | 0.49 |
| 5:E:64:PRO:HD3 | 5:E:77:SER:CA | 2.42 | 0.49 |
| 7:G:124:GLU:O | 7:G:126:SER:N | 2.44 | 0.49 |
| 18:R:158:GLY:HA3 | 18:R:515:LEU:HD11 | 1.95 | 0.49 |
| 1:A:618:HIS:CE1 | 1:A:619:ASN:OD1 | 2.66 | 0.49 |
| 2:B:546:SER:HB2 | 14:N:391:LEU:HD21 | 1.68 | 0.49 |
| 2:B:671:THR:HG21 | 2:B:672:HIS:HE1 | 1.76 | 0.49 |
| 2:B:1004:LEU:HD12 | 2:B:1017:ILE:HB | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:228:ARG:HH21 | 3:C:299:ILE:HG21 | 1.78 | 0.49 |
| 11:K:85:ASP:OD1 | 11:K:108:TYR:HB2 | 2.12 | 0.49 |
| 13:M:142:GLY:HA2 | 13:M:185:TYR:CZ | 2.48 | 0.49 |
| 18:R:216:GLU:OE2 | 18:R:498:LEU:HB2 | 2.13 | 0.49 |
| 18:R:218:ARG:CZ | 21:Y:53:DT:H5' | 2.43 | 0.49 |
| 20:X:48:DT:C4 | 20:X:49:DA:N6 | 2.81 | 0.49 |
| 2:B:417:ASP:OD1 | 2:B:418:ALA:N | 2.46 | 0.48 |
| 2:B:721:ILE:HG12 | 2:B:899:LEU:HD22 | 1.95 | 0.48 |
| 2:B:821:HIS:CE1 | 2:B:824:LEU:HD22 | 2.48 | 0.48 |
| 3:C:227:TYR:HB3 | 3:C:300:PHE:HD1 | 1.78 | 0.48 |
| 8:H:12:VAL:HG22 | 8:H:26:ILE:HD11 | 1.94 | 0.48 |
| 15:O:285:ASP:O | 15:O:288:MET:HB2 | 2.13 | 0.48 |
| 16:P:173:GLU:HA | 16:P:175:ILE:HD12 | 1.95 | 0.48 |
| 16:P:267:SER:O | 16:P:270:GLN:HB3 | 2.13 | 0.48 |
| 18:R:191:LEU:HD21 | 18:R:239:ARG:HE | 1.77 | 0.48 |
| 1:A:1154:ALA:HB1 | 1:A:1283:ILE:HD12 | 1.95 | 0.48 |
| 2:B:97:ASP:OD1 | 2:B:98:ILE:N | 2.46 | 0.48 |
| 2:B:377:LEU:HD11 | 2:B:520:ILE:HD13 | 1.94 | 0.48 |
| 2:B:501:ASP:OD2 | 2:B:513:ASN:ND2 | 2.46 | 0.48 |
| 2:B:822:GLN:O | 2:B:824:LEU:N | 2.46 | 0.48 |
| 3:C:229:LEU:HB2 | 3:C:293:ARG:NH1 | 2.24 | 0.48 |
| 4:D:132:VAL:HA | 4:D:135:TYR:HB3 | 1.95 | 0.48 |
| 6:F:79:ARG:HH22 | 6:F:145:ASP:HB2 | 1.78 | 0.48 |
| 6:F:125:LEU:HD12 | 6:F:130:ILE:HD12 | 1.94 | 0.48 |
| 7:G:115:LEU:HD21 | 7:G:130:TRP:CZ2 | 2.49 | 0.48 |
| 7:G:157:ASP:OD1 | 7:G:158:VAL:N | 2.40 | 0.48 |
| 15:O:172:GLU:O | 15:O:176:SER:HB2 | 2.12 | 0.48 |
| 15:O:214:LEU:HD11 | 15:O:249:PHE:HE1 | 1.79 | 0.48 |
| 15:O:579:GLN:O | 15:O:583:TRP:N | 2.46 | 0.48 |
| 16:P:240:ILE:HD13 | 16:P:243:LEU:HD22 | 1.95 | 0.48 |
| 18:R:274:LYS:O | 18:R:275:PHE:CG | 2.65 | 0.48 |
| 19:S:381:VAL:HG22 | 19:S:383:ARG:N | 2.27 | 0.48 |
| 20:X:62:DG:N1 | 21:Y:2:DC:N3 | 2.61 | 0.48 |
| 21:Y:9:DT:H2" | 21:Y:10:DC:C6 | 2.47 | 0.48 |
| 1:A:892:SER:O | 1:A:1380:ARG:NH2 | 2.46 | 0.48 |
| 1:A:1384:LEU:HD12 | 1:A:1413:GLU:OE2 | 2.13 | 0.48 |
| 2:B:204:ARG:NH2 | 2:B:558:ASN:HA | 2.28 | 0.48 |
| 7:G:55:GLU:N | 7:G:55:GLU:OE1 | 2.47 | 0.48 |
| 8:H:96:VAL:HG12 | 8:H:143:LEU:CD1 | 2.40 | 0.48 |
| 14:N:400:ALA:HB3 | 14:N:405:SER:HA | 1.94 | 0.48 |
| 16:P:201:GLY:N | 16:P:202:PRO:CD | 2.76 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:191:LEU:HD23 | 18:R:239:ARG:HH21 | 1.78 | 0.48 |
| 18:R:195:LYS:O | 18:R:198:VAL:HB | 2.13 | 0.48 |
| 1:A:96:PHE:O | 1:A:99:THR:N | 2.46 | 0.48 |
| 1:A:362:GLY:O | 1:A:367:ASN:ND2 | 2.47 | 0.48 |
| 1:A:626:LEU:HD23 | 1:A:627:ASP:N | 2.29 | 0.48 |
| 2:B:252:PRO:HD2 | 2:B:255:ILE:HD12 | 1.95 | 0.48 |
| 2:B:554:GLY:HA2 | 2:B:564:SER:HA | 1.94 | 0.48 |
| 2:B:555:VAL:HG12 | 2:B:564:SER:N | 2.27 | 0.48 |
| 2:B:762:TYR:HE2 | 2:B:926:VAL:HG21 | 1.78 | 0.48 |
| 3:C:260:GLU:HB2 | 3:C:263:ASP:HB2 | 1.95 | 0.48 |
| 5:E:41:ASP:O | 5:E:45:LYS:N | 2.46 | 0.48 |
| 7:G:110:ILE:O | 7:G:110:ILE:HG13 | 2.13 | 0.48 |
| 10:J:57:ILE:O | 10:J:61:LEU:HG | 2.13 | 0.48 |
| 13:M:72:GLU:HB2 | 14:N:364:ARG:NE | 2.27 | 0.48 |
| 13:M:113:LYS:HE2 | 13:M:118:LEU:HB2 | 1.95 | 0.48 |
| 14:N:308:GLN:HB2 | 14:N:417:VAL:HG12 | 1.96 | 0.48 |
| 15:O:189:SER:O | 15:O:190:LEU:C | 2.51 | 0.48 |
| 15:O:318:LEU:HD11 | 15:O:368:ARG:HD3 | 1.95 | 0.48 |
| 18:R:214:MET:SD | 18:R:265:THR:HG22 | 2.53 | 0.48 |
| 1:A:368:LEU:O | 1:A:371:LYS:HG3 | 2.13 | 0.48 |
| 1:A:373:VAL:CG1 | 1:A:374:ASP:H | 2.23 | 0.48 |
| 1:A:415:LYS:O | 1:A:419:LEU:N | 2.45 | 0.48 |
| 1:A:543:THR:HB | 1:A:550:ILE:HB | 1.96 | 0.48 |
| 1:A:608:GLN:O | 1:A:611:SER:N | 2.47 | 0.48 |
| 1:A:704:PHE:CZ | 1:A:708:ARG:HD2 | 2.49 | 0.48 |
| 1:A:1064:GLU:O | 1:A:1067:VAL:N | 2.44 | 0.48 |
| 2:B:525:GLU:HG3 | 2:B:526:GLU:H | 1.78 | 0.48 |
| 2:B:848:PRO:HB2 | 2:B:851:SER:HB3 | 1.94 | 0.48 |
| 3:C:218:LYS:HE2 | 12:L:69:ALA:O | 2.14 | 0.48 |
| 4:D:103:PHE:O | 4:D:106:LEU:HB3 | 2.13 | 0.48 |
| 7:G:30:LEU:HB3 | 7:G:48:ILE:HG13 | 1.96 | 0.48 |
| 13:M:90:TYR:O | 14:N:392:GLN:HB2 | 2.13 | 0.48 |
| 18:R:213:TRP:HB3 | 18:R:285:ALA:HB1 | 1.95 | 0.48 |
| 18:R:392:THR:O | 18:R:488:GLY:CA | 2.61 | 0.48 |
| 1:A:636:PRO:HG3 | 1:A:646:SER:N | 2.27 | 0.48 |
| 1:A:714:ILE:HG12 | 2:B:958:MET:HG2 | 1.95 | 0.48 |
| 2:B:415:GLU:CG | 2:B:416:TYR:H | 2.13 | 0.48 |
| 2:B:424:VAL:O | 18:R:92:TYR:OH | 2.25 | 0.48 |
| 2:B:591:TYR:HB2 | 2:B:656:ASP:HB2 | 1.95 | 0.48 |
| 2:B:611:PRO:HG3 | 2:B:648:TYR:HE1 | 1.78 | 0.48 |
| 2:B:914:SER:O | 2:B:915:ARG:CG | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:35:LYS:HD2 | 3:C:35:LYS:HA | 1.45 | 0.48 |
| 5:E:182:ASP:CG | 5:E:183:PRO:HD2 | 2.34 | 0.48 |
| 13:M:113:LYS:HG2 | 13:M:117:HIS:O | 2.14 | 0.48 |
| 13:M:253:GLU:O | 13:M:257:ASP:N | 2.40 | 0.48 |
| 14:N:288:GLN:HE21 | 14:N:292:ARG:HG3 | 1.79 | 0.48 |
| 15:O:352:VAL:O | 15:O:355:LYS:HB3 | 2.14 | 0.48 |
| 15:O:495:VAL:O | 15:O:495:VAL:HG22 | 2.13 | 0.48 |
| 21:Y:43:DA:C4 | 21:Y:44:DT:N3 | 2.81 | 0.48 |
| 21:Y:59:DG:H4' | 21:Y:60:DA:H5' | 1.96 | 0.48 |
| 1:A:18:PHE:CD1 | 2:B:1139:PRO:CA | 2.94 | 0.48 |
| 1:A:493:ARG:HB2 | 1:A:499:ARG:NH2 | 2.28 | 0.48 |
| 2:B:788:ARG:HH22 | 3:C:93:GLN:NE2 | 2.10 | 0.48 |
| 2:B:1053:GLY:O | 2:B:1057:ASP:O | 2.31 | 0.48 |
| 5:E:82:PHE:HD1 | 5:E:111:VAL:HB | 1.77 | 0.48 |
| 7:G:138:LEU:HD12 | 7:G:139:TYR:O | 2.13 | 0.48 |
| 9:I:33:PHE:CD1 | 9:I:34:PRO:HD2 | 2.48 | 0.48 |
| 13:M:83:GLU:O | 13:M:84:SER:O | 2.32 | 0.48 |
| 13:M:148:LEU:HA | 13:M:181:PRO:HA | 1.96 | 0.48 |
| 15:O:599:ASN:O | 15:O:602:LEU:N | 2.46 | 0.48 |
| 18:R:12:PHE:HD1 | 18:R:25:CYS:HB3 | 1.79 | 0.48 |
| 18:R:434:GLU:HA | 18:R:436:LYS:N | 2.28 | 0.48 |
| 18:R:619:ALA:O | 18:R:623:LYS:HB2 | 2.13 | 0.48 |
| 20:X:6:DA:C2 | 20:X:7:DA:C5 | 3.02 | 0.48 |
| 1:A:69:THR:O | 7:G:163:PRO:HB2 | 2.13 | 0.48 |
| 1:A:236:SER:H | 1:A:252:ARG:CD | 2.27 | 0.48 |
| 1:A:284:ASP:OD2 | 1:A:352:GLY:HA3 | 2.14 | 0.48 |
| 1:A:364:PHE:CE2 | 1:A:1387:ALA:C | 2.87 | 0.48 |
| 1:A:1261:GLN:HG3 | 1:A:1265:ARG:HH12 | 1.79 | 0.48 |
| 1:A:1391:LYS:O | 1:A:1395:HIS:ND1 | 2.46 | 0.48 |
| 2:B:112:LEU:HD23 | 2:B:113:THR:H | 1.79 | 0.48 |
| 2:B:517:MET:SD | 2:B:675:ILE:HD11 | 2.54 | 0.48 |
| 3:C:224:THR:HG23 | 3:C:224:THR:O | 2.14 | 0.48 |
| 5:E:1:MET:HG3 | 5:E:4:GLU:H | 1.79 | 0.48 |
| 5:E:19:VAL:O | 5:E:22:MET:HB3 | 2.14 | 0.48 |
| 15:O:650:VAL:HG13 | 15:O:651:PHE:N | 2.29 | 0.48 |
| 16:P:90:GLU:HA | 16:P:93:VAL:HB | 1.96 | 0.48 |
| 18:R:198:VAL:O | 18:R:202:ALA:N | 2.39 | 0.48 |
| 1:A:1187:ARG:HA | 1:A:1228:ASP:O | 2.14 | 0.48 |
| 1:A:1299:GLY:C | 1:A:1301:ARG:H | 2.18 | 0.48 |
| 2:B:236:LYS:O | 2:B:239:LYS:HB3 | 2.13 | 0.48 |
| 2:B:244:HIS:HE1 | 2:B:332:ILE:HB | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:849:THR:HG23 | 2:B:850:ASN:H | 1.78 | 0.48 |
| 2:B:874:ARG:HG2 | 18:R:16:LEU:HD13 | 1.95 | 0.48 |
| 5:E:40:GLU:HG3 | 5:E:41:ASP:H | 1.79 | 0.48 |
| 5:E:82:PHE:HE1 | 5:E:112:TYR:O | 1.96 | 0.48 |
| 13:M:88:PHE:HB2 | 14:N:395:ILE:CG2 | 2.44 | 0.48 |
| 14:N:286:ASP:OD2 | 14:N:385:GLY:N | 2.47 | 0.48 |
| 16:P:308:GLU:OE1 | 16:P:308:GLU:N | 2.46 | 0.48 |
| 20:X:6:DA:C4 | 20:X:7:DA:C8 | 3.02 | 0.48 |
| 1:A:101:GLN:OE1 | 1:A:1402:TYR:OH | 2.30 | 0.48 |
| 1:A:422:ASN:ND2 | 1:A:428:PRO:O | 2.44 | 0.48 |
| 2:B:264:SER:O | 9:I:10:ASN:HA | 2.14 | 0.48 |
| 9:I:7:SER:OG | 9:I:8:CYS:N | 2.45 | 0.48 |
| 13:M:123:ILE:N | 13:M:145:VAL:HG22 | 2.28 | 0.48 |
| 15:O:191:PHE:HD2 | 15:O:192:VAL:HG13 | 1.79 | 0.48 |
| 18:R:492:VAL:HG11 | 18:R:560:LEU:HD13 | 1.94 | 0.48 |
| 19:S:513:MET:HA | 19:S:516:ILE:HD12 | 1.96 | 0.48 |
| 1:A:307:ILE:HB | 1:A:311:ASN:OD1 | 2.14 | 0.47 |
| 1:A:559:THR:HG21 | 2:B:947:HIS:CE1 | 2.49 | 0.47 |
| 1:A:722:ASP:O | 1:A:726:LYS:N | 2.27 | 0.47 |
| 2:B:552:ASN:HD21 | 2:B:568:PRO:N | 2.12 | 0.47 |
| 2:B:635:LEU:HD21 | 2:B:640:PHE:HE1 | 1.79 | 0.47 |
| 2:B:678:PHE:HB3 | 2:B:978:CYS:O | 2.14 | 0.47 |
| 3:C:5:VAL:HG22 | 3:C:293:ARG:O | 2.14 | 0.47 |
| 5:E:89:GLY:HA2 | 5:E:117:THR:HG21 | 1.95 | 0.47 |
| 5:E:185:ALA:HA | 5:E:190:LEU:HD13 | 1.95 | 0.47 |
| 8:H:137:GLN:HB3 | 8:H:139:ASN:OD1 | 2.13 | 0.47 |
| 12:L:29:TYR:CB | 12:L:58:LYS:HA | 2.44 | 0.47 |
| 13:M:87:VAL:HA | 14:N:396:ALA:HA | 1.95 | 0.47 |
| 15:O:478:VAL:HB | 15:O:480:TYR:CZ | 2.49 | 0.47 |
| 18:R:439:ALA:HA | 18:R:450:THR:N | 2.28 | 0.47 |
| 20:X:24:DT:H2" | 20:X:25:DT:O4' | 2.14 | 0.47 |
| 1:A:235:LYS:HD2 | 1:A:252:ARG:NE | 2.29 | 0.47 |
| 1:A:444:LEU:HD21 | 1:A:445:ARG:NH1 | 2.29 | 0.47 |
| 1:A:830:ARG:NH2 | 1:A:835:PHE:O | 2.47 | 0.47 |
| 1:A:1088:ALA:HB2 | 1:A:1423:ILE:HD13 | 1.96 | 0.47 |
| 1:A:1202:ILE:O | 1:A:1205:ILE:N | 2.48 | 0.47 |
| 2:B:1147:PHE:CD2 | 7:G:10:LEU:HD11 | 2.45 | 0.47 |
| 4:D:148:LYS:O | 4:D:152:GLU:HB2 | 2.13 | 0.47 |
| 7:G:126:SER:CB | 7:G:139:TYR:HB2 | 2.42 | 0.47 |
| 13:M:113:LYS:HG3 | 13:M:116:SER:O | 2.14 | 0.47 |
| 17:Q:41:LEU:HB3 | 17:Q:42:PRO:HD2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:24:VAL:HG23 | 18:R:30:VAL:O | 2.13 | 0.47 |
| 19:S:453:GLN:O | 19:S:457:LYS:CB | 2.62 | 0.47 |
| 1:A:106:ILE:CD1 | 1:A:234:ILE:HG12 | 2.44 | 0.47 |
| 1:A:1267:LEU:C | 1:A:1269:ASP:H | 2.17 | 0.47 |
| 1:A:1425:THR:HG23 | 6:F:92:ARG:HB2 | 1.97 | 0.47 |
| 2:B:301:ALA:O | 2:B:305:ILE:HG12 | 2.14 | 0.47 |
| 2:B:659:ILE:HG12 | 2:B:672:HIS:HB2 | 1.95 | 0.47 |
| 2:B:776:SER:HB3 | 3:C:217:ALA:HB2 | 1.95 | 0.47 |
| 3:C:32:ASN:OD1 | 3:C:33:VAL:N | 2.48 | 0.47 |
| 14:N:287:HIS:CD2 | 14:N:384:LYS:HE2 | 2.49 | 0.47 |
| 15:O:499:THR:HG23 | 16:P:312:PHE:CG | 2.49 | 0.47 |
| 18:R:511:TYR:CE2 | 18:R:513:PRO:HG3 | 2.49 | 0.47 |
| 21:Y:42:DT:H2" | 21:Y:43:DA:C8 | 2.50 | 0.47 |
| 1:A:226:LYS:HD3 | 15:O:547:GLU:HG3 | 1.96 | 0.47 |
| 1:A:974:LEU:O | 1:A:975:VAL:CG1 | 2.63 | 0.47 |
| 1:A:1166:LEU:HD21 | 1:A:1268:PRO:HA | 1.96 | 0.47 |
| 2:B:120:LEU:HD23 | 2:B:885:MET:SD | 2.53 | 0.47 |
| 2:B:201:SER:HB2 | 2:B:374:ASN:O | 2.14 | 0.47 |
| 2:B:306:GLY:HA3 | 2:B:324:ILE:HG23 | 1.96 | 0.47 |
| 3:C:122:ASP:OD1 | 3:C:123:ASP:N | 2.47 | 0.47 |
| 3:C:152:ASP:HB2 | 3:C:155:GLU:CG | 2.42 | 0.47 |
| 5:E:1:MET:HB3 | 5:E:4:GLU:HG2 | 1.96 | 0.47 |
| 15:O:121:TYR:CE1 | 15:O:210:PRO:HG2 | 2.49 | 0.47 |
| 18:R:387:SER:HA | 18:R:579:PRO:HA | 1.97 | 0.47 |
| 18:R:496:ILE:HD12 | 18:R:536:GLY:HA2 | 1.97 | 0.47 |
| 1:A:15:GLY:HA2 | 1:A:1407:ALA:HA | 1.96 | 0.47 |
| 1:A:106:ILE:HG13 | 1:A:112:ALA:O | 2.15 | 0.47 |
| 1:A:327:ILE:O | 1:A:354:CYS:HB2 | 2.14 | 0.47 |
| 1:A:483:LEU:HD13 | 1:A:550:ILE:HG21 | 1.95 | 0.47 |
| 1:A:649:ASP:HB3 | 1:A:662:GLY:HA2 | 1.96 | 0.47 |
| 1:A:919:ASP:OD1 | 1:A:921:LEU:HD13 | 2.14 | 0.47 |
| 2:B:140:ASN:ND2 | 19:S:394:LYS:HG2 | 2.28 | 0.47 |
| 2:B:192:LYS:O | 2:B:193:VAL:HG23 | 2.15 | 0.47 |
| 2:B:424:VAL:HA | 18:R:93:ALA:HB2 | 1.95 | 0.47 |
| 2:B:543:LEU:HD22 | 13:M:158:GLN:HE22 | 1.79 | 0.47 |
| 2:B:776:SER:CB | 2:B:928:GLN:HE21 | 2.27 | 0.47 |
| 13:M:160:ALA:H | 13:M:173:ILE:HG13 | 1.79 | 0.47 |
| 15:O:125:GLU:HB3 | 15:O:128:HIS:CB | 2.45 | 0.47 |
| 15:O:362:ASN:O | 15:O:477:TYR:HD1 | 1.97 | 0.47 |
| 16:P:33:GLN:HB2 | 16:P:72:PHE:HE2 | 1.78 | 0.47 |
| 16:P:142:PHE:HZ | 20:X:30:DT:H4' | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:498:LEU:HD22 | 18:R:519:LEU:HD13 | 1.96 | 0.47 |
| 19:S:418:ASP:HB3 | 19:S:449:ARG:NH1 | 2.29 | 0.47 |
| 21:Y:2:DC:H2" | 21:Y:3:DA:N7 | 2.30 | 0.47 |
| 1:A:1155:ARG:HA | 1:A:1158:LYS:HB3 | 1.96 | 0.47 |
| 2:B:77:ILE:CD1 | 2:B:98:ILE:HG12 | 2.44 | 0.47 |
| 2:B:217:GLN:HE21 | 2:B:232:TYR:HB3 | 1.79 | 0.47 |
| 2:B:694:ASN:HD21 | 2:B:916:HIS:CE1 | 2.31 | 0.47 |
| 4:D:130:ASN:OD1 | 4:D:133:HIS:ND1 | 2.47 | 0.47 |
| 5:E:81:GLU:O | 5:E:110:PHE:HA | 2.14 | 0.47 |
| 15:O:78:GLU:O | 15:O:82:LYS:NZ | 2.45 | 0.47 |
| 15:O:171:VAL:O | 15:O:175:LEU:HB3 | 2.14 | 0.47 |
| 16:P:27:ILE:HG21 | 16:P:35:GLU:HG3 | 1.97 | 0.47 |
| 17:Q:64:THR:O | 17:Q:68:GLY:N | 2.47 | 0.47 |
| 18:R:25:CYS:SG | 18:R:28:CYS:HB3 | 2.55 | 0.47 |
| 18:R:91:SER:O | 18:R:96:ILE:HG12 | 2.15 | 0.47 |
| 18:R:247:VAL:O | 18:R:249:HIS:ND1 | 2.42 | 0.47 |
| 18:R:555:ALA:O | 18:R:558:PRO:HD2 | 2.15 | 0.47 |
| 1:A:29:GLN:HE21 | 2:B:1100:LEU:HD13 | 1.80 | 0.47 |
| 1:A:114:LEU:HD12 | 1:A:115:LEU:N | 2.29 | 0.47 |
| 1:A:372:ARG:C | 2:B:1050:PRO:HD2 | 2.35 | 0.47 |
| 1:A:476:ARG:HD3 | 1:A:510:ALA:HB2 | 1.95 | 0.47 |
| 1:A:591:ASP:OD1 | 1:A:591:ASP:N | 2.47 | 0.47 |
| 1:A:1026:ARG:HH12 | 8:H:110:ASP:HB3 | 1.79 | 0.47 |
| 1:A:1150:ASP:OD1 | 1:A:1291:ARG:HD2 | 2.14 | 0.47 |
| 2:B:235:THR:HB | 2:B:239:LYS:HZ2 | 1.79 | 0.47 |
| 2:B:263:LEU:HD21 | 2:B:296:TYR:CD1 | 2.49 | 0.47 |
| 2:B:490:GLN:H | 2:B:490:GLN:CD | 2.18 | 0.47 |
| 3:C:94:ASP:OD1 | 3:C:94:ASP:N | 2.46 | 0.47 |
| 3:C:173:GLY:C | 3:C:175:GLN:H | 2.16 | 0.47 |
| 5:E:96:PHE:CZ | 5:E:100:ILE:HD11 | 2.50 | 0.47 |
| 9:I:5:CYS:SG | 9:I:9:ASN:N | 2.88 | 0.47 |
| 13:M:112:TYR:HA | 13:M:119:TRP:CD1 | 2.49 | 0.47 |
| 13:M:136:ALA:HA | 13:M:140:TRP:O | 2.15 | 0.47 |
| 15:O:92:LYS:NZ | 17:Q:1082:UNK:HA | 2.29 | 0.47 |
| 15:O:484:MET:HB2 | 15:O:485:PRO:HD3 | 1.95 | 0.47 |
| 16:P:219:GLN:NE2 | 16:P:222:LEU:HD12 | 2.29 | 0.47 |
| 18:R:122:SER:N | 20:X:25:DT:OP1 | 2.47 | 0.47 |
| 18:R:155:TYR:CE1 | 20:X:12:DT:H3' | 2.50 | 0.47 |
| 18:R:200:LYS:HG2 | 18:R:276:ARG:NH2 | 2.25 | 0.47 |
| 18:R:501:LEU:HA | 18:R:563:PHE:CE2 | 2.49 | 0.47 |
| 19:S:444:GLN:HE22 | 19:S:490:LYS:HZ1 | 1.61 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:33:GLU:HB3 | 1:A:35:SER:OG | 2.15 | 0.47 |
| 1:A:197:TRP:HH2 | 15:O:549:GLN:NE2 | 2.13 | 0.47 |
| 1:A:565:SER:HB2 | 1:A:664:MET:HE2 | 1.96 | 0.47 |
| 2:B:698:ARG:NH2 | 2:B:952:ARG:HG2 | 2.28 | 0.47 |
| 3:C:225:ALA:HB2 | 3:C:302:VAL:HG23 | 1.96 | 0.47 |
| 9:I:6:PRO:C | 9:I:7:SER:HG | 2.18 | 0.47 |
| 15:O:132:TYR:CD1 | 15:O:645:LEU:HD11 | 2.50 | 0.47 |
| 15:O:338:ASP:HB3 | 15:O:342:ALA:H | 1.79 | 0.47 |
| 16:P:304:LYS:HG3 | 16:P:305:HIS:CD2 | 2.50 | 0.47 |
| 20:X:26:DT:H2' | 20:X:27:DT:H71 | 1.97 | 0.47 |
| 21:Y:25:DC:H2" | 21:Y:26:DA:C8 | 2.49 | 0.47 |
| 1:A:566:HIS:HD2 | 1:A:568:ASP:HB3 | 1.80 | 0.47 |
| 1:A:919:ASP:OD2 | 1:A:1353:ARG:NH2 | 2.48 | 0.47 |
| 1:A:1202:ILE:CD1 | 1:A:1224:ILE:HD12 | 2.43 | 0.47 |
| 1:A:1369:LEU:CD2 | 1:A:1374:PHE:CD2 | 2.92 | 0.47 |
| 2:B:351:MET:HE1 | 2:B:549:LEU:HD21 | 1.97 | 0.47 |
| 2:B:1105:GLY:O | 2:B:1116:ILE:HD12 | 2.14 | 0.47 |
| 9:I:30:PRO:HD2 | 13:M:183:PHE:HZ | 1.79 | 0.47 |
| 15:O:480:TYR:O | 15:O:483:LEU:HB3 | 2.15 | 0.47 |
| 16:P:118:GLN:HA | 16:P:121:VAL:HG22 | 1.96 | 0.47 |
| 18:R:587:THR:O | 18:R:590:THR:OG1 | 2.28 | 0.47 |
| 1:A:1118:ASN:O | 1:A:1138:THR:OG1 | 2.28 | 0.47 |
| 1:A:1275:LEU:O | 1:A:1277:ASP:N | 2.39 | 0.47 |
| 2:B:232:TYR:CE1 | 2:B:253:ILE:HD13 | 2.50 | 0.47 |
| 2:B:454:VAL:HG13 | 2:B:455:THR:N | 2.30 | 0.47 |
| 2:B:531:LYS:O | 2:B:535:VAL:HG23 | 2.15 | 0.47 |
| 2:B:675:ILE:HG13 | 2:B:676:GLU:N | 2.29 | 0.47 |
| 2:B:929:GLU:HB3 | 3:C:69:ARG:HG2 | 1.97 | 0.47 |
| 3:C:78:VAL:HG23 | 3:C:209:ILE:O | 2.15 | 0.47 |
| 4:D:126:GLN:HE21 | 7:G:85:VAL:HA | 1.81 | 0.47 |
| 13:M:134:ASP:HA | 13:M:137:GLU:HB2 | 1.97 | 0.47 |
| 15:O:80:VAL:HG21 | 15:O:87:ASP:OD1 | 2.14 | 0.47 |
| 19:S:425:MET:O | 19:S:428:PHE:HB3 | 2.14 | 0.47 |
| 1:A:62:SER:OG | 1:A:63:SER:N | 2.48 | 0.46 |
| 1:A:424:PRO:HG3 | 1:A:431:ASN:HA | 1.97 | 0.46 |
| 1:A:560:GLY:HA2 | 1:A:705:LEU:HD12 | 1.95 | 0.46 |
| 1:A:653:ILE:O | 1:A:660:LEU:HB2 | 2.16 | 0.46 |
| 1:A:667:SER:OG | 1:A:668:VAL:N | 2.41 | 0.46 |
| 1:A:976:ARG:CG | 1:A:1002:ARG:NH2 | 2.76 | 0.46 |
| 1:A:1166:LEU:HD23 | 1:A:1166:LEU:C | 2.35 | 0.46 |
| 2:B:296:TYR:CE2 | 13:M:183:PHE:HD2 | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:936:GLN:NE2 | 10:J:43:ARG:HH11 | 2.12 | 0.46 |
| 5:E:82:PHE:CD1 | 5:E:111:VAL:HB | 2.50 | 0.46 |
| 8:H:100:THR:OG1 | 8:H:138:GLU:HA | 2.15 | 0.46 |
| 15:O:468:LEU:HG | 15:O:478:VAL:CG1 | 2.44 | 0.46 |
| 15:O:553:ARG:NH1 | 15:O:554:THR:HB | 2.30 | 0.46 |
| 18:R:147:SER:O | 18:R:150:LEU:N | 2.33 | 0.46 |
| 18:R:610:LEU:HA | 18:R:613:HIS:HB2 | 1.97 | 0.46 |
| 1:A:48:PRO:C | 1:A:49:LYS:HG2 | 2.35 | 0.46 |
| 1:A:1317:ASN:O | 1:A:1318:HIS:ND1 | 2.48 | 0.46 |
| 2:B:399:PHE:CE1 | 2:B:422:ILE:HG22 | 2.49 | 0.46 |
| 5:E:106:GLN:O | 5:E:131:THR:N | 2.43 | 0.46 |
| 7:G:58:GLN:N | 7:G:67:TYR:O | 2.48 | 0.46 |
| 8:H:130:ARG:NH2 | 8:H:134:ASN:OD1 | 2.48 | 0.46 |
| 13:M:227:LEU:HG | 13:M:232:LEU:HA | 1.98 | 0.46 |
| 15:O:190:LEU:HB3 | 15:O:194:LEU:N | 2.31 | 0.46 |
| 15:O:350:GLU:OE1 | 15:O:482:LYS:HG3 | 2.14 | 0.46 |
| 16:P:59:ASN:CG | 16:P:80:ALA:HB1 | 2.35 | 0.46 |
| 20:X:7:DA:H2" | 20:X:8:DC:C6 | 2.50 | 0.46 |
| 1:A:239:CYS:SG | 1:A:240:GLU:OE1 | 2.61 | 0.46 |
| 1:A:704:PHE:HZ | 1:A:708:ARG:HD2 | 1.80 | 0.46 |
| 1:A:800:LYS:HB3 | 2:B:951:SER:OG | 2.15 | 0.46 |
| 1:A:1130:ILE:HG22 | 1:A:1371:ILE:HG21 | 1.96 | 0.46 |
| 2:B:140:ASN:HD22 | 19:S:394:LYS:HA | 1.81 | 0.46 |
| 2:B:191:GLU:OE1 | 2:B:191:GLU:N | 2.48 | 0.46 |
| 2:B:757:VAL:HA | 2:B:942:ILE:O | 2.16 | 0.46 |
| 2:B:775:LYS:HA | 2:B:778:ILE:HG22 | 1.97 | 0.46 |
| 5:E:181:ALA:HA | 5:E:186:LEU:CG | 2.45 | 0.46 |
| 7:G:114:MET:HG3 | 7:G:149:ARG:NH2 | 2.30 | 0.46 |
| 7:G:156:VAL:O | 7:G:193:ALA:HA | 2.16 | 0.46 |
| 13:M:125:LEU:HD23 | 13:M:131:TYR:HE1 | 1.79 | 0.46 |
| 15:O:45:ASP:N | 15:O:582:GLU:OE2 | 2.48 | 0.46 |
| 18:R:122:SER:OG | 20:X:25:DT:H5' | 2.15 | 0.46 |
| 18:R:623:LYS:HE2 | 19:S:435:TRP:CD1 | 2.50 | 0.46 |
| 1:A:356:ARG:HE | 1:A:363:ARG:HH12 | 1.62 | 0.46 |
| 1:A:598:MET:HB2 | 8:H:96:VAL:CG2 | 2.46 | 0.46 |
| 1:A:974:LEU:HD11 | 1:A:998:TYR:CG | 2.50 | 0.46 |
| 1:A:1217:ILE:HG22 | 1:A:1218:GLN:H | 1.80 | 0.46 |
| 2:B:778:ILE:HA | 2:B:782:PHE:HB3 | 1.97 | 0.46 |
| 2:B:944:MET:HG2 | 2:B:945:ASN:N | 2.27 | 0.46 |
| 3:C:33:VAL:HG12 | 3:C:34:GLU:N | 2.29 | 0.46 |
| 3:C:334:THR:HG23 | 11:K:48:LYS:HG3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:20:LYS:O | 5:E:23:VAL:HG12 | 2.15 | 0.46 |
| 8:H:1:MET:HG3 | 8:H:3:ASN:H | 1.81 | 0.46 |
| 13:M:77:LYS:HA | 14:N:360:VAL:HG22 | 1.96 | 0.46 |
| 16:P:79:GLU:HA | 16:P:82:LYS:HE3 | 1.97 | 0.46 |
| 18:R:198:VAL:HA | 18:R:201:ASP:HB2 | 1.98 | 0.46 |
| 18:R:249:HIS:HD2 | 19:S:406:TYR:CE2 | 2.33 | 0.46 |
| 19:S:465:ARG:HB3 | 19:S:468:LEU:HD13 | 1.97 | 0.46 |
| 1:A:577:THR:HG21 | 11:K:89:CYS:H | 1.80 | 0.46 |
| 1:A:642:PRO:HB3 | 8:H:103:LYS:HZ2 | 1.80 | 0.46 |
| 1:A:652:VAL:HB | 1:A:668:VAL:HG11 | 1.97 | 0.46 |
| 1:A:818:ILE:HG22 | 1:A:867:SER:HA | 1.96 | 0.46 |
| 1:A:892:SER:HB2 | 1:A:1376:LEU:HD11 | 1.97 | 0.46 |
| 1:A:985:LYS:O | 1:A:987:GLU:HG3 | 2.15 | 0.46 |
| 2:B:800:ASN:HD22 | 2:B:851:SER:HA | 1.79 | 0.46 |
| 13:M:85:LEU:HG | 14:N:398:SER:HB2 | 1.98 | 0.46 |
| 15:O:576:PHE:O | 15:O:579:GLN:HG2 | 2.16 | 0.46 |
| 18:R:467:ARG:O | 18:R:471:LYS:HB2 | 2.16 | 0.46 |
| 18:R:500:GLY:HA2 | 18:R:503:PHE:HB3 | 1.96 | 0.46 |
| 19:S:451:ARG:HG3 | 19:S:452:LYS:N | 2.31 | 0.46 |
| 21:Y:43:DA:C8 | 21:Y:43:DA:H5' | 2.50 | 0.46 |
| 1:A:666:LYS:C | 1:A:667:SER:HG | 2.18 | 0.46 |
| 1:A:1325:VAL:HG23 | 1:A:1326:LEU:H | 1.81 | 0.46 |
| 2:B:122:ASP:HA | 2:B:189:GLY:CA | 2.44 | 0.46 |
| 2:B:166:ALA:HB3 | 2:B:171:MET:HE3 | 1.96 | 0.46 |
| 2:B:325:GLU:O | 2:B:328:ALA:N | 2.49 | 0.46 |
| 2:B:1093:ASP:HB2 | 2:B:1102:GLY:O | 2.16 | 0.46 |
| 3:C:85:PHE:CE2 | 3:C:94:ASP:HB2 | 2.50 | 0.46 |
| 5:E:2:ASP:O | 5:E:6:GLU:HG2 | 2.16 | 0.46 |
| 13:M:125:LEU:HD13 | 13:M:144:ASN:O | 2.16 | 0.46 |
| 13:M:230:SER:C | 13:M:234:HIS:HD1 | 2.18 | 0.46 |
| 19:S:461:GLU:OE1 | 19:S:465:ARG:NH2 | 2.46 | 0.46 |
| 21:Y:55:DT:C2' | 21:Y:56:DG:C8 | 2.98 | 0.46 |
| 1:A:481:HIS:CD2 | 1:A:483:LEU:H | 2.34 | 0.46 |
| 1:A:642:PRO:HB3 | 8:H:103:LYS:HZ3 | 1.80 | 0.46 |
| 1:A:827:PHE:HB3 | 2:B:655:ASN:OD1 | 2.16 | 0.46 |
| 1:A:827:PHE:CE2 | 1:A:833:PRO:HG3 | 2.44 | 0.46 |
| 1:A:974:LEU:C | 1:A:975:VAL:HG12 | 2.36 | 0.46 |
| 1:A:1131:ASN:OD1 | 1:A:1372:THR:OG1 | 2.30 | 0.46 |
| 2:B:232:TYR:HD1 | 2:B:242:LEU:HD23 | 1.79 | 0.46 |
| 2:B:327:ILE:HG12 | 13:M:231:LEU:HD22 | 1.98 | 0.46 |
| 2:B:421:SER:O | 2:B:424:VAL:HB | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:501:ASP:HB3 | 2:B:703:CYS:CB | 2.46 | 0.46 |
| 2:B:721:ILE:HG12 | 2:B:899:LEU:CD2 | 2.45 | 0.46 |
| 2:B:1013:LEU:HD13 | 2:B:1017:ILE:HD11 | 1.98 | 0.46 |
| 5:E:26:ARG:HH12 | 5:E:189:GLY:HA3 | 1.81 | 0.46 |
| 8:H:3:ASN:O | 8:H:5:LEU:HD12 | 2.16 | 0.46 |
| 12:L:32:ALA:HB3 | 12:L:53:HIS:CE1 | 2.51 | 0.46 |
| 12:L:38:LEU:HD22 | 12:L:48:CYS:HA | 1.98 | 0.46 |
| 15:O:134:GLY:O | 15:O:137:ILE:HB | 2.15 | 0.46 |
| 15:O:136:ILE:HG21 | 15:O:164:ILE:HD11 | 1.97 | 0.46 |
| 18:R:288:PRO:HA | 18:R:291:VAL:HB | 1.98 | 0.46 |
| 18:R:467:ARG:HB3 | 18:R:610:LEU:HD13 | 1.98 | 0.46 |
| 19:S:422:VAL:O | 19:S:426:ILE:N | 2.48 | 0.46 |
| 1:A:233:GLN:HG2 | 15:O:575:ASN:HD21 | 1.80 | 0.46 |
| 1:A:392:VAL:HG23 | 1:A:488:HIS:CG | 2.51 | 0.46 |
| 1:A:476:ARG:HG3 | 1:A:477:GLN:OE1 | 2.16 | 0.46 |
| 1:A:550:ILE:HG23 | 1:A:551:ILE:HG23 | 1.98 | 0.46 |
| 1:A:600:PRO:HB2 | 8:H:46:LEU:HD23 | 1.97 | 0.46 |
| 1:A:921:LEU:HA | 1:A:1082:ARG:HA | 1.98 | 0.46 |
| 1:A:1177:TYR:OH | 1:A:1260:MET:HG2 | 2.16 | 0.46 |
| 2:B:112:LEU:HD22 | 2:B:162:ILE:HG12 | 1.97 | 0.46 |
| 2:B:636:ASP:OD1 | 2:B:637:PHE:N | 2.49 | 0.46 |
| 2:B:785:CYS:SG | 2:B:1026:LYS:NZ | 2.64 | 0.46 |
| 2:B:849:THR:HG23 | 2:B:850:ASN:N | 2.31 | 0.46 |
| 5:E:200:ARG:HD2 | 5:E:208:TYR:OH | 2.16 | 0.46 |
| 15:O:144:MET:HE2 | 15:O:153:LYS:HD2 | 1.98 | 0.46 |
| 16:P:53:GLN:NE2 | 19:S:362:ILE:O | 2.38 | 0.46 |
| 16:P:82:LYS:HE2 | 16:P:133:TYR:CE1 | 2.50 | 0.46 |
| 18:R:155:TYR:HE1 | 20:X:13:DA:P | 2.38 | 0.46 |
| 1:A:423:GLY:HA3 | 1:A:449:ARG:NH1 | 2.30 | 0.46 |
| 1:A:506:THR:OG1 | 1:A:507:PRO:HD3 | 2.16 | 0.46 |
| 2:B:177:CYS:SG | 2:B:179:LEU:N | 2.84 | 0.46 |
| 2:B:493:GLN:HG3 | 2:B:497:LEU:HB2 | 1.98 | 0.46 |
| 2:B:691:PRO:HD2 | 2:B:978:CYS:HA | 1.98 | 0.46 |
| 2:B:840:GLN:O | 2:B:872:ILE:HG23 | 2.15 | 0.46 |
| 7:G:111:PRO:HD2 | 7:G:198:GLY:H | 1.81 | 0.46 |
| 8:H:110:ASP:O | 8:H:128:ASN:HA | 2.16 | 0.46 |
| 13:M:159:TYR:O | 14:N:307:PHE:N | 2.35 | 0.46 |
| 15:O:47:PHE:HZ | 15:O:590:PHE:HE2 | 1.62 | 0.46 |
| 16:P:108:LYS:HA | 16:P:111:LYS:HD3 | 1.98 | 0.46 |
| 1:A:646:SER:OG | 1:A:649:ASP:O | 2.26 | 0.46 |
| 1:A:1119:VAL:HA | 1:A:1138:THR:HG21 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1186:VAL:HG22 | 1:A:1230:ILE:HD13 | 1.98 | 0.46 |
| 1:A:1202:ILE:HD12 | 1:A:1228:ASP:HA | 1.97 | 0.46 |
| 1:A:1363:THR:OG1 | 1:A:1368:VAL:HG22 | 2.16 | 0.46 |
| 2:B:140:ASN:HA | 19:S:394:LYS:HB3 | 1.98 | 0.46 |
| 2:B:210:ASP:OD1 | 2:B:211:GLU:N | 2.49 | 0.46 |
| 2:B:574:GLN:HE22 | 14:N:422:ILE:HG12 | 1.81 | 0.46 |
| 3:C:85:PHE:HE1 | 3:C:204:LEU:HD22 | 1.80 | 0.46 |
| 5:E:200:ARG:NH2 | 5:E:210:SER:OG | 2.49 | 0.46 |
| 7:G:4:LEU:HD21 | 7:G:73:ARG:HE | 1.80 | 0.46 |
| 21:Y:11:DA:H2' | 21:Y:12:DT:H71 | 1.98 | 0.46 |
| 1:A:622:VAL:HA | 1:A:685:TYR:CE2 | 2.51 | 0.45 |
| 1:A:813:VAL:HG12 | 1:A:814:GLY:N | 2.31 | 0.45 |
| 2:B:1112:SER:OG | 2:B:1113:ALA:N | 2.49 | 0.45 |
| 3:C:80:ALA:HB3 | 3:C:102:GLY:HA2 | 1.97 | 0.45 |
| 3:C:278:GLU:N | 3:C:278:GLU:OE1 | 2.50 | 0.45 |
| 13:M:91:ALA:CA | 14:N:392:GLN:CD | 2.83 | 0.45 |
| 15:O:516:LEU:HD13 | 15:O:565:LEU:HD23 | 1.97 | 0.45 |
| 15:O:580:ASN:HA | 15:O:583:TRP:HB2 | 1.97 | 0.45 |
| 16:P:96:TYR:OH | 16:P:113:ARG:HG3 | 2.16 | 0.45 |
| 16:P:216:SER:OG | 16:P:217:THR:N | 2.49 | 0.45 |
| 16:P:309:VAL:HG21 | 16:P:311:TYR:CZ | 2.51 | 0.45 |
| 1:A:26:ILE:HD13 | 1:A:262:PRO:HD3 | 1.99 | 0.45 |
| 1:A:123:PHE:CG | 1:A:144:ILE:HD13 | 2.51 | 0.45 |
| 1:A:216:LYS:HG3 | 1:A:217:ARG:H | 1.81 | 0.45 |
| 1:A:574:ALA:HA | 11:K:81:MET:HE3 | 1.96 | 0.45 |
| 1:A:805:ASN:HD21 | 2:B:951:SER:HA | 1.81 | 0.45 |
| 1:A:1127:LYS:O | 1:A:1131:ASN:CB | 2.65 | 0.45 |
| 1:A:1225:ILE:N | 1:A:1229:ARG:HE | 2.11 | 0.45 |
| 2:B:92:TYR:N | 2:B:136:THR:OG1 | 2.40 | 0.45 |
| 2:B:230:LYS:HD3 | 2:B:334:HIS:CE1 | 2.50 | 0.45 |
| 2:B:254:ALA:HB3 | 2:B:290:SER:HB2 | 1.98 | 0.45 |
| 2:B:1039:ALA:HB3 | 18:R:20:ASN:OD1 | 2.14 | 0.45 |
| 15:O:470:GLU:HB2 | 15:O:479:PRO:HD3 | 1.98 | 0.45 |
| 16:P:263:VAL:HG12 | 16:P:265:LEU:H | 1.81 | 0.45 |
| 18:R:121:ARG:NH2 | 20:X:23:DC:O3' | 2.49 | 0.45 |
| 19:S:413:ARG:NH1 | 20:X:11:DA:H3' | 2.31 | 0.45 |
| 20:X:6:DA:N6 | 20:X:7:DA:N6 | 2.64 | 0.45 |
| 20:X:47:DA:H2" | 20:X:48:DT:H5' | 1.98 | 0.45 |
| 1:A:38:ASP:C | 1:A:40:PHE:H | 2.18 | 0.45 |
| 1:A:232:LYS:HD3 | 16:P:315:TRP:CH2 | 2.51 | 0.45 |
| 1:A:328:ASN:O | 1:A:351:ARG:NE | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1203:GLU:O | 1:A:1207:VAL:HG12 | 2.16 | 0.45 |
| 1:A:1272:VAL:HG13 | 1:A:1273:LYS:N | 2.28 | 0.45 |
| 2:B:109:LYS:HD2 | 2:B:110:ASP:H | 1.82 | 0.45 |
| 2:B:134:GLU:HA | 2:B:144:HIS:HB3 | 1.98 | 0.45 |
| 2:B:412:ARG:HH22 | 18:R:151:GLN:HB2 | 1.81 | 0.45 |
| 2:B:958:MET:HG3 | 2:B:1018:PHE:CZ | 2.51 | 0.45 |
| 2:B:1088:ASP:OD1 | 2:B:1088:ASP:N | 2.49 | 0.45 |
| 3:C:255:VAL:HG13 | 3:C:256:ILE:H | 1.80 | 0.45 |
| 4:D:17:LEU:HB2 | 4:D:66:LEU:HD23 | 1.97 | 0.45 |
| 4:D:149:THR:O | 4:D:153:MET:HG3 | 2.16 | 0.45 |
| 5:E:171:LYS:H | 5:E:174:GLN:NE2 | 2.13 | 0.45 |
| 6:F:84:TYR:HD1 | 6:F:152:ILE:HG23 | 1.82 | 0.45 |
| 7:G:112:GLN:OE1 | 7:G:115:LEU:HD13 | 2.15 | 0.45 |
| 10:J:1:MET:HB3 | 10:J:2:ILE:HD12 | 1.98 | 0.45 |
| 13:M:254:GLN:OE1 | 14:N:409:LEU:HG | 2.15 | 0.45 |
| 15:O:551:VAL:O | 15:O:562:ALA:HB1 | 2.15 | 0.45 |
| 15:O:634:GLU:O | 15:O:637:VAL:N | 2.50 | 0.45 |
| 16:P:190:THR:HA | 16:P:215:TYR:HE1 | 1.81 | 0.45 |
| 1:A:49:LYS:HD2 | 1:A:54:LEU:CB | 2.40 | 0.45 |
| 1:A:195:ASP:O | 1:A:198:VAL:HG12 | 2.17 | 0.45 |
| 1:A:777:VAL:O | 1:A:781:CYS:HB2 | 2.16 | 0.45 |
| 2:B:649:LEU:HD22 | 2:B:653:GLU:OE1 | 2.17 | 0.45 |
| 2:B:723:THR:HG23 | 2:B:724:LEU:N | 2.31 | 0.45 |
| 2:B:755:ALA:HB2 | 2:B:782:PHE:HE1 | 1.82 | 0.45 |
| 2:B:791:THR:HG22 | 2:B:842:TYR:HE2 | 1.81 | 0.45 |
| 3:C:278:GLU:O | 3:C:281:ARG:HG2 | 2.16 | 0.45 |
| 14:N:373:VAL:HB | 14:N:381:ASP:O | 2.16 | 0.45 |
| 15:O:205:LYS:HG3 | 15:O:206:LEU:N | 2.32 | 0.45 |
| 15:O:353:GLU:HB2 | 15:O:481:SER:HG | 1.80 | 0.45 |
| 15:O:369:HIS:CG | 15:O:370:LEU:H | 2.35 | 0.45 |
| 15:O:454:ASN:O | 15:O:457:LEU:HB3 | 2.15 | 0.45 |
| 16:P:118:GLN:OE1 | 21:Y:35:DG:H5" | 2.16 | 0.45 |
| 18:R:213:TRP:CD1 | 18:R:287:PRO:CD | 2.99 | 0.45 |
| 18:R:434:GLU:CA | 18:R:436:LYS:H | 2.30 | 0.45 |
| 1:A:3:GLU:O | 7:G:37:LYS:HG3 | 2.15 | 0.45 |
| 1:A:34:VAL:HG13 | 1:A:35:SER:N | 2.31 | 0.45 |
| 1:A:90:VAL:HG21 | 1:A:320:GLN:HA | 1.97 | 0.45 |
| 1:A:114:LEU:HD21 | 1:A:148:CYS:HB2 | 1.97 | 0.45 |
| 1:A:781:CYS:O | 1:A:785:LEU:HB2 | 2.16 | 0.45 |
| 1:A:903:THR:O | 1:A:905:ARG:HG3 | 2.16 | 0.45 |
| 1:A:1170:ALA:HA | 1:A:1188:ILE:CG1 | 2.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1411:VAL:HG13 | 1:A:1412:SER:N | 2.30 | 0.45 |
| 2:B:112:LEU:HD23 | 2:B:113:THR:N | 2.30 | 0.45 |
| 2:B:178:PRO:HD3 | 10:J:63:TYR:OH | 2.16 | 0.45 |
| 2:B:242:LEU:HD12 | 2:B:256:VAL:HG21 | 1.99 | 0.45 |
| 2:B:298:GLN:HA | 2:B:302:LEU:HD12 | 1.98 | 0.45 |
| 2:B:552:ASN:OD1 | 2:B:553:TYR:N | 2.50 | 0.45 |
| 2:B:698:ARG:HE | 2:B:952:ARG:HB3 | 1.82 | 0.45 |
| 3:C:229:LEU:HD23 | 3:C:295:ARG:HA | 1.98 | 0.45 |
| 4:D:157:ILE:O | 4:D:161:ALA:N | 2.49 | 0.45 |
| 9:I:5:CYS:HB3 | 9:I:10:ASN:H | 1.82 | 0.45 |
| 15:O:623:GLU:OE1 | 15:O:624:LEU:HD12 | 2.16 | 0.45 |
| 16:P:151:TYR:OH | 18:R:647:ALA:HB1 | 2.17 | 0.45 |
| 18:R:431:ARG:HH12 | 21:Y:48:DT:P | 2.40 | 0.45 |
| 1:A:134:ASN:HD21 | 1:A:1404:LYS:HD3 | 1.82 | 0.45 |
| 1:A:179:ILE:HG23 | 1:A:220:ASP:O | 2.17 | 0.45 |
| 1:A:200:GLU:HG2 | 15:O:515:LYS:CD | 2.47 | 0.45 |
| 1:A:436:ARG:N | 1:A:460:ASP:OD1 | 2.49 | 0.45 |
| 2:B:44:LYS:NZ | 2:B:663:GLU:HB2 | 2.32 | 0.45 |
| 2:B:273:CYS:O | 2:B:354:ARG:NH1 | 2.50 | 0.45 |
| 2:B:832:VAL:HG13 | 2:B:882:ASP:O | 2.17 | 0.45 |
| 2:B:932:PRO:O | 2:B:940:PRO:CD | 2.60 | 0.45 |
| 2:B:944:MET:CG | 2:B:945:ASN:H | 2.26 | 0.45 |
| 2:B:991:LEU:O | 2:B:994:GLN:N | 2.47 | 0.45 |
| 3:C:112:MET:C | 3:C:113:LEU:HD12 | 2.37 | 0.45 |
| 3:C:231:PRO:HB3 | 3:C:275:VAL:CG2 | 2.41 | 0.45 |
| 15:O:310:GLN:NE2 | 15:O:313:LYS:HD3 | 2.31 | 0.45 |
| 18:R:267:ALA:O | 18:R:271:SER:OG | 2.24 | 0.45 |
| 1:A:152:ARG:HH12 | 21:Y:9:DT:P | 2.39 | 0.45 |
| 1:A:269:ARG:CZ | 1:A:286:THR:H | 2.30 | 0.45 |
| 1:A:315:HIS:O | 1:A:318:TYR:N | 2.49 | 0.45 |
| 1:A:1373:ARG:HB2 | 1:A:1390:GLU:HG2 | 1.97 | 0.45 |
| 2:B:884:VAL:CG2 | 12:L:58:LYS:HB3 | 2.47 | 0.45 |
| 2:B:1004:LEU:HD12 | 2:B:1017:ILE:HD12 | 1.99 | 0.45 |
| 3:C:31:TRP:HE3 | 11:K:82:LYS:HD2 | 1.81 | 0.45 |
| 5:E:112:TYR:O | 5:E:137:GLU:HB2 | 2.17 | 0.45 |
| 7:G:15:PRO:HA | 7:G:18:PHE:CZ | 2.51 | 0.45 |
| 14:N:284:ASN:O | 14:N:287:HIS:N | 2.49 | 0.45 |
| 15:O:259:LEU:HD23 | 15:O:261:GLN:H | 1.81 | 0.45 |
| 15:O:366:LEU:HD22 | 15:O:368:ARG:NH1 | 2.31 | 0.45 |
| 20:X:50:DA:H2 | 21:Y:15:DT:O2 | 2.00 | 0.45 |
| 21:Y:42:DT:N3 | 21:Y:43:DA:N6 | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:283:ASP:OD1 | 1:A:284:ASP:N | 2.43 | 0.45 |
| 1:A:760:GLN:HA | 1:A:763:GLU:HB3 | 1.99 | 0.45 |
| 1:A:1364:TYR:HE2 | 1:A:1379:MET:SD | 2.40 | 0.45 |
| 2:B:239:LYS:HZ3 | 2:B:241:TYR:HE2 | 1.64 | 0.45 |
| 5:E:112:TYR:CD1 | 5:E:116:ILE:HG12 | 2.51 | 0.45 |
| 5:E:123:LEU:HD21 | 5:E:126:SER:HB2 | 1.99 | 0.45 |
| 11:K:132:GLU:O | 11:K:136:THR:HG22 | 2.17 | 0.45 |
| 12:L:29:TYR:HB3 | 12:L:59:ALA:H | 1.82 | 0.45 |
| 18:R:425:PHE:HB2 | 21:Y:46:DA:OP1 | 2.17 | 0.45 |
| 18:R:492:VAL:HB | 18:R:494:PHE:CE2 | 2.52 | 0.45 |
| 18:R:602:LEU:O | 18:R:606:ASP:N | 2.50 | 0.45 |
| 20:X:47:DA:C8 | 20:X:48:DT:H72 | 2.52 | 0.45 |
| 21:Y:1:DC:H1' | 21:Y:2:DC:C2 | 2.51 | 0.45 |
| 1:A:891:LYS:HG3 | 1:A:1389:PHE:CD1 | 2.52 | 0.45 |
| 1:A:1286:ARG:H | 1:A:1291:ARG:HA | 1.81 | 0.45 |
| 1:A:1315:THR:HG22 | 1:A:1316:THR:N | 2.29 | 0.45 |
| 1:A:1339:ILE:HD13 | 1:A:1339:ILE:HA | 1.84 | 0.45 |
| 2:B:536:LEU:HD23 | 2:B:536:LEU:O | 2.17 | 0.45 |
| 2:B:766:ASP:O | 2:B:770:ALA:HB3 | 2.16 | 0.45 |
| 4:D:109:LYS:HB2 | 4:D:156:ILE:HD11 | 1.99 | 0.45 |
| 5:E:9:ILE:HG22 | 5:E:53:PRO:CG | 2.47 | 0.45 |
| 7:G:126:SER:OG | 7:G:139:TYR:CB | 2.65 | 0.45 |
| 12:L:25:ALA:N | 12:L:37:LYS:HE2 | 2.32 | 0.45 |
| 15:O:69:VAL:HG22 | 15:O:122:TYR:CD1 | 2.51 | 0.45 |
| 15:O:197:MET:HG3 | 15:O:286:ARG:HB3 | 1.97 | 0.45 |
| 15:O:221:LYS:N | 15:O:224:LYS:HB3 | 2.32 | 0.45 |
| 21:Y:58:DT:H4' | 21:Y:59:DG:H5' | 1.99 | 0.45 |
| 2:B:62:LEU:HA | 2:B:155:MET:HE3 | 1.98 | 0.45 |
| 2:B:130:TYR:CE1 | 2:B:148:GLU:HG3 | 2.52 | 0.45 |
| 3:C:31:TRP:HB2 | 11:K:82:LYS:HG3 | 1.99 | 0.45 |
| 3:C:71:MET:HE1 | 3:C:314:PHE:HD1 | 1.82 | 0.45 |
| 5:E:46:TYR:O | 5:E:54:GLN:N | 2.49 | 0.45 |
| 9:I:29:CYS:CA | 13:M:183:PHE:HE2 | 2.25 | 0.45 |
| 14:N:304:PHE:HB2 | 14:N:411:ARG:O | 2.17 | 0.45 |
| 14:N:365:VAL:HG13 | 14:N:370:LYS:O | 2.16 | 0.45 |
| 15:O:484:MET:O | 15:O:488:LYS:N | 2.39 | 0.45 |
| 15:O:590:PHE:O | 15:O:591:LYS:C | 2.54 | 0.45 |
| 18:R:408:LEU:HD13 | 18:R:427:ALA:HA | 1.99 | 0.45 |
| 18:R:425:PHE:HE2 | 18:R:427:ALA:HB3 | 1.82 | 0.45 |
| 20:X:25:DT:H2' | 20:X:26:DT:H6 | 1.78 | 0.45 |
| 1:A:103:LEU:HD21 | 1:A:222:LEU:HD22 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:442:ARG:HA | 18:R:29:GLY:O | 2.17 | 0.44 |
| 1:A:645:MET:CE | 8:H:124:ARG:HB2 | 2.42 | 0.44 |
| 1:A:716:ASP:CG | 1:A:789:ASN:HB2 | 2.38 | 0.44 |
| 1:A:1206:ALA:O | 1:A:1209:ILE:HB | 2.17 | 0.44 |
| 1:A:1332:ARG:HA | 1:A:1335:ILE:HG22 | 1.99 | 0.44 |
| 1:A:1447:LEU:HB3 | 1:A:1450:SER:HB3 | 1.98 | 0.44 |
| 2:B:660:ALA:HB2 | 2:B:670:MET:SD | 2.57 | 0.44 |
| 3:C:195:LYS:HD2 | 10:J:57:ILE:HG21 | 1.98 | 0.44 |
| 3:C:255:VAL:HG22 | 3:C:256:ILE:N | 2.32 | 0.44 |
| 6:F:143:PHE:O | 6:F:144:GLU:HB2 | 2.17 | 0.44 |
| 13:M:94:PRO:HA | 14:N:392:GLN:CA | 2.42 | 0.44 |
| 13:M:123:ILE:HB | 13:M:146:GLN:HB3 | 2.00 | 0.44 |
| 15:O:364:ILE:HA | 15:O:476:TYR:OH | 2.17 | 0.44 |
| 16:P:311:TYR:CD1 | 17:Q:40:PRO:HB3 | 2.52 | 0.44 |
| 19:S:523:ALA:HA | 19:S:526:GLU:HB3 | 1.99 | 0.44 |
| 21:Y:15:DT:O4 | 21:Y:16:DA:N6 | 2.50 | 0.44 |
| 1:A:173:SER:HB2 | 1:A:334:PRO:HB2 | 1.99 | 0.44 |
| 1:A:326:TYR:CD2 | 1:A:327:ILE:HG23 | 2.53 | 0.44 |
| 1:A:378:ARG:NE | 1:A:516:GLU:OE1 | 2.49 | 0.44 |
| 1:A:802:SER:OG | 1:A:803:THR:N | 2.49 | 0.44 |
| 1:A:919:ASP:OD2 | 1:A:921:LEU:HB2 | 2.17 | 0.44 |
| 1:A:1329:GLU:OE2 | 5:E:200:ARG:NE | 2.46 | 0.44 |
| 2:B:84:LEU:HG | 2:B:85:SER:O | 2.18 | 0.44 |
| 2:B:259:ALA:HB1 | 2:B:302:LEU:HD23 | 1.99 | 0.44 |
| 2:B:971:GLY:CA | 10:J:51:LEU:HD11 | 2.43 | 0.44 |
| 4:D:102:SER:HA | 4:D:105:GLU:HB2 | 1.99 | 0.44 |
| 7:G:4:LEU:HD12 | 7:G:74:ALA:O | 2.17 | 0.44 |
| 13:M:104:HIS:CB | 13:M:105:PRO:HD2 | 2.43 | 0.44 |
| 15:O:267:PRO:HG2 | 15:O:270:SER:HB2 | 1.99 | 0.44 |
| 18:R:414:HIS:HD2 | 18:R:615:LEU:O | 2.01 | 0.44 |
| 1:A:16:LEU:HD11 | 1:A:1417:LEU:HD11 | 2.00 | 0.44 |
| 1:A:373:VAL:CA | 2:B:1050:PRO:HG2 | 2.48 | 0.44 |
| 1:A:726:LYS:O | 1:A:730:LEU:HG | 2.17 | 0.44 |
| 1:A:1023:ARG:O | 1:A:1028:MET:HB2 | 2.17 | 0.44 |
| 2:B:93:LEU:HD12 | 2:B:135:TYR:HB3 | 1.99 | 0.44 |
| 2:B:493:GLN:CG | 2:B:497:LEU:HB2 | 2.48 | 0.44 |
| 2:B:842:TYR:CE1 | 2:B:873:TYR:HB2 | 2.52 | 0.44 |
| 3:C:32:ASN:CG | 3:C:33:VAL:H | 2.21 | 0.44 |
| 3:C:59:ILE:HD11 | 3:C:64:ALA:HB2 | 1.99 | 0.44 |
| 3:C:239:ILE:HG22 | 3:C:288:LYS:HD2 | 2.00 | 0.44 |
| 4:D:14:TYR:CD2 | 4:D:15:GLU:HG2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:126:GLN:NE2 | 7:G:85:VAL:HA | 2.32 | 0.44 |
| 5:E:9:ILE:HG22 | 5:E:53:PRO:HG3 | 1.99 | 0.44 |
| 7:G:189:GLU:HG3 | 7:G:191:PRO:HD3 | 2.00 | 0.44 |
| 8:H:9:ILE:O | 8:H:31:THR:HG22 | 2.18 | 0.44 |
| 11:K:63:PHE:CZ | 11:K:114:VAL:HG12 | 2.52 | 0.44 |
| 13:M:253:GLU:HA | 13:M:256:LYS:HB2 | 1.99 | 0.44 |
| 14:N:371:LEU:HD22 | 14:N:384:LYS:CD | 2.46 | 0.44 |
| 20:X:58:DC:C4 | 20:X:59:DC:C4 | 3.05 | 0.44 |
| 1:A:483:LEU:HD21 | 1:A:540:ASN:HB3 | 1.99 | 0.44 |
| 1:A:1188:ILE:HB | 1:A:1228:ASP:HB3 | 1.99 | 0.44 |
| 1:A:1302:ASP:N | 1:A:1302:ASP:OD1 | 2.48 | 0.44 |
| 2:B:128:PRO:HA | 2:B:151:ARG:HG2 | 1.99 | 0.44 |
| 2:B:263:LEU:HD21 | 2:B:296:TYR:CE1 | 2.52 | 0.44 |
| 2:B:427:ASN:HA | 2:B:430:THR:H | 1.82 | 0.44 |
| 2:B:591:TYR:CZ | 2:B:600:HIS:HB2 | 2.51 | 0.44 |
| 2:B:696:SER:OG | 2:B:697:PRO:HD3 | 2.17 | 0.44 |
| 2:B:747:ASP:O | 10:J:54:VAL:HG11 | 2.18 | 0.44 |
| 2:B:791:THR:O | 2:B:791:THR:HG23 | 2.17 | 0.44 |
| 8:H:104:PHE:HE1 | 8:H:114:VAL:HG13 | 1.81 | 0.44 |
| 13:M:257:ASP:O | 13:M:261:LYS:HG3 | 2.17 | 0.44 |
| 14:N:388:THR:HG23 | 14:N:390:PHE:CD2 | 2.53 | 0.44 |
| 15:O:288:MET:SD | 15:O:326:ILE:HG21 | 2.57 | 0.44 |
| 16:P:202:PRO:O | 16:P:203:LYS:HG2 | 2.17 | 0.44 |
| 18:R:229:LEU:HB2 | 18:R:244:ILE:HD13 | 1.98 | 0.44 |
| 21:Y:14:DT:H2' | 21:Y:14:DT:OP2 | 2.17 | 0.44 |
| 21:Y:53:DT:H2" | 21:Y:54:DA:H5" | 2.00 | 0.44 |
| 1:A:235:LYS:HZ3 | 1:A:254:GLU:CG | 2.30 | 0.44 |
| 1:A:372:ARG:O | 2:B:1050:PRO:CD | 2.64 | 0.44 |
| 1:A:379:THR:HG22 | 1:A:380:VAL:N | 2.32 | 0.44 |
| 1:A:474:PHE:CZ | 1:A:517:MET:HG3 | 2.52 | 0.44 |
| 1:A:524:THR:N | 2:B:1081:GLU:OE2 | 2.40 | 0.44 |
| 1:A:598:MET:O | 1:A:600:PRO:HD2 | 2.18 | 0.44 |
| 1:A:704:PHE:O | 1:A:707:ASN:N | 2.51 | 0.44 |
| 1:A:733:ILE:HA | 1:A:736:HIS:NE2 | 2.32 | 0.44 |
| 1:A:815:GLN:HA | 1:A:846:GLY:O | 2.18 | 0.44 |
| 1:A:869:ARG:NH1 | 2:B:502:THR:HB | 2.29 | 0.44 |
| 2:B:240:ILE:CG1 | 2:B:286:ASN:HD22 | 2.31 | 0.44 |
| 2:B:969:LEU:HB3 | 2:B:994:GLN:OE1 | 2.17 | 0.44 |
| 3:C:21:PRO:HD3 | 3:C:30:GLU:HA | 1.98 | 0.44 |
| 3:C:260:GLU:O | 3:C:264:GLU:N | 2.50 | 0.44 |
| 4:D:27:HIS:NE2 | 4:D:53:PRO:HG3 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:159:TYR:CG | 13:M:170:LEU:HD21 | 2.53 | 0.44 |
| 15:O:307:VAL:HG13 | 15:O:308:THR:N | 2.32 | 0.44 |
| 18:R:120:ARG:HE | 21:Y:42:DT:H4' | 1.81 | 0.44 |
| 18:R:633:ASP:O | 18:R:636:LEU:HB3 | 2.18 | 0.44 |
| 1:A:625:ASN:N | 1:A:625:ASN:OD1 | 2.51 | 0.44 |
| 1:A:785:LEU:HD21 | 1:A:789:ASN:HD21 | 1.82 | 0.44 |
| 2:B:77:ILE:HG21 | 2:B:98:ILE:HD11 | 2.00 | 0.44 |
| 2:B:320:LEU:HA | 2:B:324:ILE:HG13 | 1.98 | 0.44 |
| 2:B:592:SER:N | 2:B:656:ASP:OD2 | 2.29 | 0.44 |
| 2:B:658:TYR:HE2 | 2:B:670:MET:HG2 | 1.81 | 0.44 |
| 9:I:32:GLU:HG3 | 13:M:132:ASN:HB2 | 2.00 | 0.44 |
| 13:M:125:LEU:HD22 | 13:M:142:GLY:O | 2.18 | 0.44 |
| 15:O:241:ALA:O | 15:O:245:ALA:N | 2.34 | 0.44 |
| 18:R:116:PHE:CE2 | 18:R:164:MET:HB3 | 2.52 | 0.44 |
| 18:R:399:THR:O | 18:R:481:PHE:HA | 2.18 | 0.44 |
| 18:R:522:ARG:HD3 | 18:R:529:VAL:HG22 | 2.00 | 0.44 |
| 20:X:61:DT:H3 | 21:Y:4:DT:H3 | 1.64 | 0.44 |
| 1:A:477:GLN:HG2 | 1:A:478:PRO:N | 2.32 | 0.44 |
| 1:A:1157:VAL:HG12 | 1:A:1160:ARG:HD2 | 1.98 | 0.44 |
| 3:C:89:THR:HG23 | 3:C:200:GLN:HA | 1.98 | 0.44 |
| 7:G:116:PHE:HZ | 7:G:203:ASP:HA | 1.83 | 0.44 |
| 8:H:80:ARG:HG3 | 11:K:108:TYR:CZ | 2.52 | 0.44 |
| 14:N:384:LYS:HD2 | 14:N:416:ILE:HD11 | 1.99 | 0.44 |
| 15:O:164:ILE:HG12 | 15:O:282:ILE:HD13 | 1.99 | 0.44 |
| 15:O:203:ILE:HG13 | 15:O:203:ILE:O | 2.18 | 0.44 |
| 15:O:248:ASP:O | 15:O:252:ILE:HG12 | 2.18 | 0.44 |
| 15:O:471:THR:HA | 15:O:477:TYR:HD2 | 1.81 | 0.44 |
| 18:R:96:ILE:HD11 | 18:R:101:THR:HG22 | 2.00 | 0.44 |
| 18:R:630:LEU:HD11 | 19:S:444:GLN:HG3 | 1.99 | 0.44 |
| 20:X:51:DA:H2" | 20:X:52:DA:C8 | 2.52 | 0.44 |
| 21:Y:55:DT:C2 | 21:Y:56:DG:C5 | 3.05 | 0.44 |
| 1:A:476:ARG:HA | 1:A:517:MET:SD | 2.58 | 0.44 |
| 1:A:890:MET:O | 1:A:893:LEU:N | 2.50 | 0.44 |
| 1:A:1399:ALA:HA | 1:A:1404:LYS:HD2 | 1.99 | 0.44 |
| 2:B:208:GLU:O | 2:B:215:ILE:HA | 2.17 | 0.44 |
| 2:B:552:ASN:HD21 | 2:B:568:PRO:CA | 2.31 | 0.44 |
| 8:H:112:ILE:O | 8:H:126:GLU:HA | 2.18 | 0.44 |
| 10:J:2:ILE:HD12 | 10:J:2:ILE:H | 1.82 | 0.44 |
| 15:O:56:HIS:CG | 15:O:130:LEU:HD23 | 2.53 | 0.44 |
| 15:O:488:LYS:HD3 | 15:O:488:LYS:HA | 1.64 | 0.44 |
| 17:Q:54:LEU:O | 17:Q:58:TYR:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:S:453:GLN:O | 19:S:457:LYS:HB3 | 2.17 | 0.44 |
| 20:X:10:DT:C4 | 20:X:11:DA:N6 | 2.86 | 0.44 |
| 1:A:57:LYS:HA | 1:A:68:ALA:HB3 | 2.00 | 0.44 |
| 1:A:323:VAL:O | 1:A:326:TYR:HB3 | 2.18 | 0.44 |
| 1:A:427:HIS:HB3 | 1:A:428:PRO:HD3 | 2.00 | 0.44 |
| 1:A:727:LYS:HA | 1:A:730:LEU:HD12 | 1.98 | 0.44 |
| 1:A:1213:SER:OG | 1:A:1217:ILE:HB | 2.18 | 0.44 |
| 2:B:778:ILE:CG1 | 2:B:906:PRO:HG2 | 2.47 | 0.44 |
| 3:C:75:VAL:HG23 | 3:C:221:PRO:HG3 | 2.00 | 0.44 |
| 4:D:106:LEU:HG | 4:D:110:LEU:HD22 | 2.00 | 0.44 |
| 8:H:98:TYR:HD1 | 8:H:141:TYR:CE2 | 2.34 | 0.44 |
| 14:N:386:ALA:HB2 | 14:N:416:ILE:HA | 1.99 | 0.44 |
| 15:O:221:LYS:H | 15:O:224:LYS:HB3 | 1.83 | 0.44 |
| 19:S:509:HIS:HA | 19:S:512:HIS:HB3 | 2.00 | 0.44 |
| 20:X:3:DT:H2" | 20:X:4:DT:H71 | 1.99 | 0.44 |
| 21:Y:55:DT:C4 | 21:Y:56:DG:C6 | 3.06 | 0.44 |
| 1:A:445:ARG:NH2 | 18:R:17:SER:OG | 2.51 | 0.43 |
| 1:A:501:ASN:OD1 | 1:A:502:GLU:N | 2.52 | 0.43 |
| 1:A:976:ARG:HH21 | 1:A:994:TYR:HB2 | 1.83 | 0.43 |
| 2:B:191:GLU:HG2 | 2:B:192:LYS:N | 2.32 | 0.43 |
| 2:B:626:HIS:CD2 | 2:B:645:LEU:HD21 | 2.53 | 0.43 |
| 3:C:100:ARG:NH1 | 10:J:2:ILE:HB | 2.33 | 0.43 |
| 7:G:87:GLY:HA3 | 7:G:148:PHE:CE2 | 2.45 | 0.43 |
| 10:J:43:ARG:HH11 | 10:J:43:ARG:CG | 2.25 | 0.43 |
| 13:M:72:GLU:OE1 | 14:N:364:ARG:NH2 | 2.50 | 0.43 |
| 13:M:174:GLU:HB3 | 13:M:175:ARG:H | 1.65 | 0.43 |
| 15:O:132:TYR:CE1 | 15:O:645:LEU:HD21 | 2.53 | 0.43 |
| 15:O:352:VAL:HG13 | 15:O:353:GLU:H | 1.83 | 0.43 |
| 18:R:195:LYS:O | 18:R:199:VAL:HG23 | 2.18 | 0.43 |
| 18:R:213:TRP:CD1 | 18:R:213:TRP:O | 2.70 | 0.43 |
| 18:R:420:TYR:HB2 | 18:R:428:VAL:HG22 | 2.00 | 0.43 |
| 20:X:45:DA:H2" | 20:X:46:DG:C8 | 2.53 | 0.43 |
| 20:X:60:DA:N6 | 21:Y:4:DT:C4 | 2.86 | 0.43 |
| 21:Y:8:DG:H2' | 21:Y:9:DT:H71 | 1.99 | 0.43 |
| 1:A:78:HIS:ND1 | 2:B:1090:PHE:HZ | 2.16 | 0.43 |
| 1:A:232:LYS:HG2 | 1:A:254:GLU:OE2 | 2.19 | 0.43 |
| 1:A:332:VAL:HG13 | 1:A:333:ASN:N | 2.27 | 0.43 |
| 1:A:432:TYR:CD1 | 1:A:443:ASN:HB3 | 2.53 | 0.43 |
| 1:A:436:ARG:HH11 | 1:A:459:GLY:HA3 | 1.83 | 0.43 |
| 1:A:666:LYS:HA | 1:A:670:GLY:CA | 2.46 | 0.43 |
| 1:A:715:ASN:OD1 | 1:A:716:ASP:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:792:LEU:O | 1:A:796:THR:N | 2.50 | 0.43 |
| 1:A:818:ILE:HD11 | 1:A:823:VAL:HA | 2.00 | 0.43 |
| 1:A:916:TYR:O | 1:A:920:GLY:N | 2.48 | 0.43 |
| 1:A:921:LEU:HD23 | 1:A:932:PRO:HG3 | 1.99 | 0.43 |
| 1:A:1079:ARG:HG2 | 6:F:84:TYR:HE2 | 1.83 | 0.43 |
| 1:A:1083:LEU:HA | 1:A:1083:LEU:HD23 | 1.60 | 0.43 |
| 1:A:1222:VAL:HA | 1:A:1231:ALA:O | 2.17 | 0.43 |
| 1:A:1370:GLY:O | 1:A:1371:ILE:O | 2.36 | 0.43 |
| 2:B:719:LYS:NZ | 10:J:65:PRO:HG3 | 2.33 | 0.43 |
| 2:B:759:VAL:HG12 | 2:B:946:PRO:HG3 | 2.00 | 0.43 |
| 2:B:911:LYS:HA | 2:B:920:GLY:O | 2.18 | 0.43 |
| 5:E:147:HIS:ND1 | 5:E:148:GLU:N | 2.66 | 0.43 |
| 8:H:123:MET:HE2 | 8:H:125:LEU:HD23 | 1.99 | 0.43 |
| 13:M:94:PRO:CA | 14:N:392:GLN:HA | 2.40 | 0.43 |
| 15:O:32:MET:C | 15:O:34:ILE:H | 2.21 | 0.43 |
| 16:P:253:LEU:HA | 16:P:263:VAL:HA | 2.00 | 0.43 |
| 1:A:161:ASN:HB2 | 1:A:180:HIS:HE1 | 1.82 | 0.43 |
| 1:A:733:ILE:HD12 | 1:A:736:HIS:NE2 | 2.33 | 0.43 |
| 1:A:1415:ILE:HG22 | 2:B:1079:LEU:HD21 | 2.00 | 0.43 |
| 2:B:269:MET:HE1 | 2:B:280:GLN:HG2 | 2.00 | 0.43 |
| 2:B:619:GLN:OE1 | 2:B:619:GLN:N | 2.52 | 0.43 |
| 2:B:855:PRO:N | 18:R:106:GLN:HE22 | 2.17 | 0.43 |
| 4:D:68:ILE:O | 4:D:72:PHE:N | 2.41 | 0.43 |
| 4:D:127:LEU:HB2 | 4:D:133:HIS:HB3 | 1.99 | 0.43 |
| 7:G:49:TYR:HB2 | 7:G:75:VAL:HG23 | 2.00 | 0.43 |
| 8:H:116:TYR:HB2 | 8:H:123:MET:HB3 | 2.00 | 0.43 |
| 13:M:159:TYR:C | 13:M:173:ILE:CD1 | 2.86 | 0.43 |
| 14:N:361:GLY:HA3 | 14:N:374:LYS:O | 2.19 | 0.43 |
| 15:O:53:VAL:O | 15:O:57:LEU:N | 2.50 | 0.43 |
| 15:O:347:ASP:HA | 15:O:350:GLU:CG | 2.48 | 0.43 |
| 18:R:519:LEU:HB3 | 18:R:532:ILE:HB | 2.00 | 0.43 |
| 18:R:528:ILE:HG12 | 18:R:543:ALA:HB2 | 2.00 | 0.43 |
| 1:A:216:LYS:HG3 | 1:A:217:ARG:N | 2.33 | 0.43 |
| 1:A:538:LYS:HB3 | 1:A:687:PRO:HB2 | 2.01 | 0.43 |
| 1:A:590:PHE:O | 11:K:106:GLN:NE2 | 2.51 | 0.43 |
| 1:A:694:MET:O | 1:A:697:MET:HB3 | 2.18 | 0.43 |
| 1:A:1235:PHE:HB2 | 1:A:1236:PRO:HD2 | 1.99 | 0.43 |
| 1:A:1265:ARG:NH2 | 2:B:285:VAL:HG22 | 2.34 | 0.43 |
| 1:A:1378:LYS:CG | 1:A:1379:MET:N | 2.82 | 0.43 |
| 2:B:108:THR:HG22 | 2:B:109:LYS:N | 2.26 | 0.43 |
| 2:B:525:GLU:HG3 | 2:B:528:PRO:HD2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:726:TYR:O | 2:B:727:LEU:HB3 | 2.18 | 0.43 |
| 5:E:156:LEU:HD11 | 5:E:195:VAL:HB | 2.00 | 0.43 |
| 7:G:15:PRO:HA | 7:G:18:PHE:CE2 | 2.53 | 0.43 |
| 11:K:110:GLU:OE2 | 11:K:111:THR:HG23 | 2.18 | 0.43 |
| 11:K:120:GLY:O | 11:K:123:ASP:HB2 | 2.19 | 0.43 |
| 14:N:366:HIS:H | 14:N:370:LYS:HB2 | 1.84 | 0.43 |
| 14:N:366:HIS:CG | 14:N:367:LYS:H | 2.36 | 0.43 |
| 15:O:170:THR:HG22 | 15:O:279:SER:HA | 2.00 | 0.43 |
| 15:O:364:ILE:HA | 15:O:476:TYR:CZ | 2.54 | 0.43 |
| 18:R:99:TYR:HD2 | 18:R:100:ILE:HG13 | 1.82 | 0.43 |
| 18:R:413:LEU:HB3 | 18:R:620:SER:OG | 2.19 | 0.43 |
| 1:A:172:GLY:HA3 | 1:A:331:SER:CB | 2.38 | 0.43 |
| 1:A:313:MET:SD | 15:O:548:ILE:HD13 | 2.59 | 0.43 |
| 1:A:713:GLY:HA2 | 2:B:1018:PHE:CG | 2.54 | 0.43 |
| 1:A:753:GLN:HE22 | 1:A:765:LYS:HE2 | 1.83 | 0.43 |
| 1:A:943:TYR:HA | 1:A:946:THR:HG22 | 2.01 | 0.43 |
| 2:B:136:THR:HG22 | 2:B:142:ILE:HG22 | 2.01 | 0.43 |
| 2:B:269:MET:CE | 2:B:280:GLN:HG2 | 2.49 | 0.43 |
| 2:B:417:ASP:C | 2:B:419:LEU:N | 2.70 | 0.43 |
| 2:B:556:TYR:HD1 | 2:B:561:LEU:HA | 1.84 | 0.43 |
| 2:B:933:PHE:CD1 | 2:B:933:PHE:C | 2.91 | 0.43 |
| 2:B:938:ILE:HG23 | 10:J:45:CYS:HB3 | 2.00 | 0.43 |
| 7:G:41:ASN:HA | 7:G:155:PHE:CD2 | 2.54 | 0.43 |
| 7:G:114:MET:HB2 | 7:G:199:SER:HB2 | 1.98 | 0.43 |
| 8:H:99:GLY:HA3 | 8:H:118:PHE:HD1 | 1.83 | 0.43 |
| 10:J:48:ARG:O | 10:J:52:THR:N | 2.22 | 0.43 |
| 13:M:75:PRO:HA | 14:N:362:SER:OG | 2.19 | 0.43 |
| 18:R:143:LEU:HD11 | 18:R:157:ILE:HG22 | 1.99 | 0.43 |
| 18:R:607:ASP:C | 18:R:609:GLU:H | 2.22 | 0.43 |
| 1:A:14:LYS:O | 2:B:1142:ARG:HB2 | 2.19 | 0.43 |
| 1:A:153:ARG:NH2 | 15:O:338:ASP:HA | 2.33 | 0.43 |
| 1:A:270:PRO:HG3 | 2:B:1046:LEU:HD12 | 1.99 | 0.43 |
| 1:A:388:SER:OG | 1:A:389:ILE:N | 2.51 | 0.43 |
| 1:A:629:LYS:HE3 | 1:A:633:PHE:CD2 | 2.53 | 0.43 |
| 1:A:642:PRO:HB2 | 1:A:644:GLU:CG | 2.42 | 0.43 |
| 1:A:777:VAL:CG1 | 1:A:811:ALA:HB1 | 2.49 | 0.43 |
| 1:A:813:VAL:HG12 | 1:A:814:GLY:H | 1.84 | 0.43 |
| 1:A:1166:LEU:CA | 1:A:1169:VAL:HG22 | 2.37 | 0.43 |
| 1:A:1335:ILE:HG23 | 1:A:1336:ILE:H | 1.84 | 0.43 |
| 2:B:630:LEU:HD12 | 2:B:635:LEU:HB3 | 2.00 | 0.43 |
| 2:B:888:VAL:CG1 | 12:L:54:ARG:HD3 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:954:THR:HG23 | 2:B:954:THR:O | 2.19 | 0.43 |
| 5:E:121:MET:HA | 5:E:124:VAL:HB | 2.00 | 0.43 |
| 16:P:235:LEU:HD23 | 16:P:236:THR:O | 2.19 | 0.43 |
| 18:R:75:SER:OG | 20:X:27:DT:H2' | 2.18 | 0.43 |
| 18:R:604:ASP:OD1 | 18:R:605:VAL:N | 2.50 | 0.43 |
| 21:Y:6:DG:C6 | 21:Y:7:DA:C6 | 3.07 | 0.43 |
| 21:Y:26:DA:H2" | 21:Y:27:DC:H5" | 2.00 | 0.43 |
| 1:A:302:GLY:O | 1:A:304:ASP:N | 2.50 | 0.43 |
| 1:A:541:LEU:HD22 | 1:A:682:LEU:HD22 | 1.99 | 0.43 |
| 1:A:573:ARG:O | 1:A:577:THR:CB | 2.67 | 0.43 |
| 1:A:738:CYS:SG | 1:A:842:PRO:HD3 | 2.59 | 0.43 |
| 1:A:975:VAL:O | 1:A:976:ARG:HG3 | 2.19 | 0.43 |
| 1:A:1335:ILE:HG23 | 1:A:1336:ILE:N | 2.34 | 0.43 |
| 2:B:137:ARG:HB3 | 2:B:417:ASP:HA | 2.01 | 0.43 |
| 2:B:300:GLN:HE22 | 13:M:186:ILE:HG22 | 1.83 | 0.43 |
| 3:C:97:LEU:HD12 | 3:C:194:ALA:HB2 | 2.00 | 0.43 |
| 3:C:324:LYS:HD3 | 11:K:68:GLU:OE2 | 2.19 | 0.43 |
| 8:H:5:LEU:HG | 8:H:133:ASN:HB3 | 2.01 | 0.43 |
| 8:H:93:TYR:HB2 | 8:H:143:LEU:HD11 | 2.00 | 0.43 |
| 8:H:107:VAL:O | 8:H:111:LEU:HB2 | 2.18 | 0.43 |
| 10:J:37:SER:OG | 10:J:47:ARG:NH2 | 2.52 | 0.43 |
| 15:O:183:MET:CB | 15:O:186:THR:HB | 2.48 | 0.43 |
| 15:O:499:THR:O | 17:Q:39:ILE:HD13 | 2.18 | 0.43 |
| 15:O:555:ALA:HB2 | 15:O:561:ARG:CG | 2.48 | 0.43 |
| 18:R:238:ARG:HB3 | 19:S:289:UNK:O | 2.18 | 0.43 |
| 1:A:209:PRO:O | 1:A:212:GLU:HB2 | 2.18 | 0.43 |
| 1:A:450:MET:O | 1:A:454:LYS:HG2 | 2.18 | 0.43 |
| 1:A:1343:MET:HE1 | 1:A:1355:ILE:HD11 | 2.01 | 0.43 |
| 1:A:1378:LYS:CG | 1:A:1379:MET:H | 2.29 | 0.43 |
| 1:A:1380:ARG:NH1 | 1:A:1385:GLN:HE22 | 2.14 | 0.43 |
| 2:B:169:SER:O | 2:B:172:ALA:N | 2.51 | 0.43 |
| 2:B:586:GLU:HG2 | 2:B:587:PHE:N | 2.34 | 0.43 |
| 5:E:23:VAL:HG22 | 5:E:28:TYR:HB2 | 2.00 | 0.43 |
| 5:E:146:HIS:O | 5:E:146:HIS:ND1 | 2.51 | 0.43 |
| 5:E:194:GLU:O | 5:E:213:ILE:HG13 | 2.19 | 0.43 |
| 7:G:95:GLU:HG3 | 7:G:96:GLY:N | 2.33 | 0.43 |
| 11:K:106:GLN:HG3 | 11:K:106:GLN:O | 2.18 | 0.43 |
| 13:M:112:TYR:OH | 13:M:114:PRO:HA | 2.18 | 0.43 |
| 16:P:135:LYS:NZ | 16:P:153:LEU:O | 2.42 | 0.43 |
| 17:Q:55:ALA:O | 17:Q:58:TYR:HB3 | 2.19 | 0.43 |
| 18:R:99:TYR:CD2 | 18:R:100:ILE:HG13 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:X:59:DC:N3 | 20:X:60:DA:N6 | 2.67 | 0.43 |
| 1:A:869:ARG:HH12 | 2:B:502:THR:CB | 2.29 | 0.43 |
| 1:A:1408:VAL:HG23 | 1:A:1413:GLU:CG | 2.48 | 0.43 |
| 2:B:296:TYR:CD2 | 13:M:186:ILE:HG13 | 2.52 | 0.43 |
| 2:B:909:GLY:HA2 | 2:B:921:VAL:HG13 | 2.01 | 0.43 |
| 7:G:105:PHE:HD2 | 7:G:107:ASP:H | 1.66 | 0.43 |
| 13:M:91:ALA:HA | 14:N:392:GLN:OE1 | 2.19 | 0.43 |
| 15:O:125:GLU:HB3 | 15:O:128:HIS:CG | 2.54 | 0.43 |
| 15:O:547:GLU:O | 15:O:548:ILE:HG13 | 2.18 | 0.43 |
| 16:P:238:SER:HA | 16:P:241:ARG:CZ | 2.49 | 0.43 |
| 18:R:22:ASP:CG | 18:R:23:LEU:N | 2.71 | 0.43 |
| 18:R:274:LYS:HB3 | 18:R:275:PHE:H | 1.74 | 0.43 |
| 19:S:277:UNK:O | 19:S:279:UNK:N | 2.52 | 0.43 |
| 19:S:367:ASN:HB3 | 19:S:370:GLY:O | 2.19 | 0.43 |
| 20:X:29:DC:C6 | 20:X:30:DT:H72 | 2.53 | 0.43 |
| 1:A:373:VAL:HG11 | 2:B:1082:ARG:HD2 | 2.01 | 0.43 |
| 1:A:585:ASP:N | 1:A:585:ASP:OD1 | 2.51 | 0.43 |
| 2:B:137:ARG:C | 2:B:415:GLU:HB2 | 2.39 | 0.43 |
| 2:B:217:GLN:HB3 | 2:B:356:VAL:CG1 | 2.49 | 0.43 |
| 2:B:1008:ILE:HD11 | 11:K:70:HIS:NE2 | 2.34 | 0.43 |
| 3:C:73:SER:HA | 3:C:213:GLY:HA3 | 2.01 | 0.43 |
| 4:D:10:PHE:HA | 7:G:3:ILE:HG22 | 2.01 | 0.43 |
| 9:I:5:CYS:O | 9:I:9:ASN:HA | 2.19 | 0.43 |
| 11:K:88:PHE:HB3 | 11:K:106:GLN:HG3 | 1.95 | 0.43 |
| 13:M:104:HIS:CB | 13:M:105:PRO:CD | 2.89 | 0.43 |
| 18:R:286:ARG:HA | 18:R:290:PHE:CZ | 2.54 | 0.43 |
| 18:R:610:LEU:HA | 18:R:613:HIS:HD2 | 1.81 | 0.43 |
| 1:A:16:LEU:HD23 | 2:B:1139:PRO:HB2 | 2.01 | 0.42 |
| 2:B:338:GLU:H | 2:B:345:LYS:HZ3 | 1.67 | 0.42 |
| 2:B:732:GLN:O | 2:B:750:PRO:HB2 | 2.19 | 0.42 |
| 2:B:834:MET:CE | 12:L:63:ARG:HD2 | 2.48 | 0.42 |
| 5:E:26:ARG:HH22 | 5:E:189:GLY:CA | 2.32 | 0.42 |
| 13:M:76:LEU:HB3 | 13:M:168:VAL:HB | 2.01 | 0.42 |
| 13:M:155:ASN:OD1 | 13:M:155:ASN:N | 2.51 | 0.42 |
| 16:P:141:LYS:HG2 | 16:P:142:PHE:H | 1.84 | 0.42 |
| 16:P:216:SER:CB | 16:P:260:CYS:HA | 2.49 | 0.42 |
| 18:R:73:LEU:HD22 | 21:Y:32:DA:N7 | 2.34 | 0.42 |
| 19:S:527:ASP:O | 19:S:531:GLN:HG3 | 2.19 | 0.42 |
| 20:X:55:DA:H1' | 20:X:56:DC:H5' | 2.01 | 0.42 |
| 21:Y:60:DA:H2" | 21:Y:61:DA:H8 | 1.84 | 0.42 |
| 1:A:9:THR:O | 1:A:11:LYS:HG2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:185:TRP:O | 1:A:189:LYS:HE2 | 2.19 | 0.42 |
| 1:A:321:LEU:HD22 | 1:A:336:MET:HG2 | 2.02 | 0.42 |
| 1:A:383:PRO:HG3 | 1:A:512:PHE:CE2 | 2.54 | 0.42 |
| 1:A:583:MET:HG3 | 1:A:700:LEU:HB2 | 2.01 | 0.42 |
| 1:A:705:LEU:HD22 | 2:B:761:SER:CB | 2.48 | 0.42 |
| 1:A:869:ARG:NH2 | 2:B:502:THR:O | 2.52 | 0.42 |
| 2:B:417:ASP:O | 2:B:419:LEU:N | 2.52 | 0.42 |
| 2:B:552:ASN:ND2 | 2:B:565:ILE:O | 2.50 | 0.42 |
| 2:B:556:TYR:HD2 | 2:B:600:HIS:CE1 | 2.37 | 0.42 |
| 2:B:778:ILE:HD11 | 2:B:906:PRO:HG2 | 2.00 | 0.42 |
| 5:E:180:ARG:C | 5:E:182:ASP:H | 2.19 | 0.42 |
| 7:G:97:ILE:HG21 | 7:G:140:PHE:HZ | 1.85 | 0.42 |
| 11:K:107:THR:HG23 | 11:K:108:TYR:O | 2.20 | 0.42 |
| 13:M:72:GLU:OE1 | 14:N:364:ARG:NE | 2.50 | 0.42 |
| 13:M:113:LYS:O | 13:M:117:HIS:HA | 2.19 | 0.42 |
| 13:M:160:ALA:N | 13:M:173:ILE:CD1 | 2.81 | 0.42 |
| 15:O:205:LYS:HG3 | 15:O:206:LEU:H | 1.84 | 0.42 |
| 15:O:325:LYS:HE3 | 15:O:484:MET:SD | 2.59 | 0.42 |
| 15:O:499:THR:HG21 | 16:P:312:PHE:CD1 | 2.54 | 0.42 |
| 1:A:67:CYS:H | 1:A:71:HIS:HA | 1.84 | 0.42 |
| 1:A:152:ARG:HE | 1:A:184:ARG:NE | 2.17 | 0.42 |
| 1:A:916:TYR:HB3 | 1:A:920:GLY:HA2 | 2.02 | 0.42 |
| 2:B:140:ASN:HB3 | 19:S:395:GLU:H | 1.82 | 0.42 |
| 2:B:199:GLN:HG3 | 2:B:477:PHE:CE2 | 2.54 | 0.42 |
| 2:B:364:LYS:HG3 | 2:B:365:MET:N | 2.25 | 0.42 |
| 2:B:475:SER:CB | 2:B:510:LEU:O | 2.64 | 0.42 |
| 3:C:8:GLU:HG3 | 3:C:11:ARG:CZ | 2.48 | 0.42 |
| 3:C:52:ALA:HB2 | 3:C:310:PRO:HG2 | 2.01 | 0.42 |
| 3:C:256:ILE:HG22 | 3:C:267:VAL:HA | 2.01 | 0.42 |
| 7:G:207:LEU:HD23 | 7:G:209:SER:H | 1.84 | 0.42 |
| 15:O:262:ILE:O | 15:O:274:VAL:HA | 2.19 | 0.42 |
| 15:O:484:MET:HA | 15:O:487:LEU:HB3 | 2.01 | 0.42 |
| 15:O:517:VAL:HG11 | 15:O:522:ILE:HD11 | 2.01 | 0.42 |
| 15:O:573:SER:O | 15:O:576:PHE:CD2 | 2.72 | 0.42 |
| 18:R:142:MET:HG3 | 18:R:144:ILE:HG22 | 2.01 | 0.42 |
| 18:R:144:ILE:HB | 19:S:408:TYR:CE1 | 2.54 | 0.42 |
| 1:A:155:LEU:HD11 | 1:A:156:HIS:HD2 | 1.83 | 0.42 |
| 1:A:1373:ARG:CG | 1:A:1374:PHE:N | 2.83 | 0.42 |
| 1:A:1449:GLU:OE2 | 4:D:10:PHE:N | 2.52 | 0.42 |
| 2:B:149:ILE:HD12 | 2:B:429:ILE:HG21 | 2.01 | 0.42 |
| 2:B:338:GLU:OE1 | 2:B:339:ALA:N | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:350:ALA:O | 2:B:353:THR:N | 2.52 | 0.42 |
| 2:B:837:GLN:OE1 | 2:B:837:GLN:N | 2.52 | 0.42 |
| 2:B:1088:ASP:OD2 | 2:B:1123:TYR:N | 2.53 | 0.42 |
| 9:I:35:ILE:HB | 9:I:36:GLU:H | 1.59 | 0.42 |
| 15:O:106:TYR:OH | 17:Q:1079:UNK:N | 2.52 | 0.42 |
| 15:O:242:LYS:O | 15:O:246:LYS:N | 2.40 | 0.42 |
| 16:P:202:PRO:O | 16:P:204:LYS:N | 2.48 | 0.42 |
| 18:R:491:ASP:HB2 | 18:R:537:LYS:HG2 | 2.02 | 0.42 |
| 20:X:19:DA:H4' | 20:X:20:DA:OP1 | 2.19 | 0.42 |
| 20:X:62:DG:O6 | 21:Y:2:DC:N4 | 2.53 | 0.42 |
| 1:A:269:ARG:HH22 | 1:A:284:ASP:N | 2.17 | 0.42 |
| 1:A:768:GLY:O | 1:A:772:LYS:HB2 | 2.20 | 0.42 |
| 1:A:862:LEU:HD22 | 2:B:494:PHE:HB2 | 2.01 | 0.42 |
| 2:B:539:GLU:OE1 | 2:B:539:GLU:N | 2.53 | 0.42 |
| 5:E:62:ALA:O | 5:E:78:LEU:N | 2.49 | 0.42 |
| 7:G:52:LEU:O | 7:G:53:THR:HG22 | 2.20 | 0.42 |
| 15:O:507:LEU:HD12 | 15:O:508:SER:N | 2.35 | 0.42 |
| 18:R:2:PRO:HG2 | 18:R:12:PHE:HE2 | 1.83 | 0.42 |
| 18:R:188:LYS:HB2 | 18:R:247:VAL:HG11 | 2.01 | 0.42 |
| 18:R:199:VAL:O | 18:R:203:VAL:HG23 | 2.19 | 0.42 |
| 18:R:213:TRP:O | 18:R:213:TRP:CG | 2.72 | 0.42 |
| 21:Y:38:DA:C6 | 21:Y:39:DA:C6 | 3.07 | 0.42 |
| 1:A:223:ASN:O | 1:A:226:LYS:HB3 | 2.20 | 0.42 |
| 1:A:541:LEU:HD13 | 1:A:682:LEU:HD22 | 2.02 | 0.42 |
| 1:A:842:PRO:C | 1:A:844:SER:N | 2.73 | 0.42 |
| 1:A:916:TYR:CZ | 1:A:1089:ILE:HG21 | 2.55 | 0.42 |
| 1:A:1141:ILE:HB | 1:A:1295:VAL:HB | 1.99 | 0.42 |
| 1:A:1338:GLU:O | 1:A:1342:THR:HG22 | 2.19 | 0.42 |
| 1:A:1370:GLY:HA2 | 1:A:1375:GLY:HA2 | 2.01 | 0.42 |
| 1:A:1395:HIS:O | 1:A:1399:ALA:HB2 | 2.20 | 0.42 |
| 2:B:38:ILE:HG13 | 2:B:43:ASP:HB3 | 2.00 | 0.42 |
| 2:B:230:LYS:HD2 | 2:B:242:LEU:HD22 | 2.01 | 0.42 |
| 2:B:354:ARG:O | 2:B:358:MET:HG3 | 2.20 | 0.42 |
| 2:B:846:SER:OG | 2:B:866:TYR:HB3 | 2.19 | 0.42 |
| 2:B:1025:GLN:O | 2:B:1027:LEU:HD12 | 2.19 | 0.42 |
| 8:H:104:PHE:CE1 | 8:H:114:VAL:HG13 | 2.55 | 0.42 |
| 9:I:33:PHE:CE2 | 9:I:35:ILE:HA | 2.55 | 0.42 |
| 13:M:131:TYR:HE2 | 13:M:133:LYS:HA | 1.84 | 0.42 |
| 15:O:132:TYR:CZ | 15:O:291:ARG:NH1 | 2.88 | 0.42 |
| 15:O:189:SER:O | 15:O:190:LEU:O | 2.38 | 0.42 |
| 16:P:135:LYS:HB3 | 16:P:151:TYR:CD1 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:P:218:THR:HG23 | 16:P:219:GLN:N | 2.34 | 0.42 |
| 1:A:957:TYR:CD2 | 1:A:1035:PRO:HD3 | 2.54 | 0.42 |
| 1:A:1382:SER:HB2 | 1:A:1385:GLN:HG2 | 2.01 | 0.42 |
| 2:B:732:GLN:HB3 | 10:J:52:THR:CG2 | 2.50 | 0.42 |
| 2:B:790:LYS:HA | 2:B:898:VAL:O | 2.19 | 0.42 |
| 2:B:988:SER:HB2 | 2:B:998:TYR:HB2 | 2.00 | 0.42 |
| 3:C:100:ARG:HH21 | 10:J:5:VAL:HG13 | 1.84 | 0.42 |
| 4:D:1:MET:HG3 | 4:D:2:LYS:N | 2.33 | 0.42 |
| 8:H:47:PHE:CZ | 8:H:146:ARG:HG3 | 2.55 | 0.42 |
| 13:M:140:TRP:CD1 | 13:M:185:TYR:HB3 | 2.55 | 0.42 |
| 15:O:126:GLY:C | 15:O:128:HIS:N | 2.72 | 0.42 |
| 15:O:190:LEU:HB2 | 15:O:194:LEU:HG | 2.01 | 0.42 |
| 15:O:471:THR:OG1 | 15:O:472:LYS:N | 2.53 | 0.42 |
| 15:O:561:ARG:HD2 | 15:O:561:ARG:HA | 1.41 | 0.42 |
| 15:O:599:ASN:ND2 | 15:O:630:VAL:HG11 | 2.34 | 0.42 |
| 16:P:21:GLN:O | 16:P:26:GLY:N | 2.50 | 0.42 |
| 18:R:241:HIS:HD2 | 18:R:255:LEU:HD23 | 1.85 | 0.42 |
| 18:R:509:SER:OG | 18:R:521:TYR:HD1 | 2.03 | 0.42 |
| 19:S:291:UNK:O | 19:S:293:UNK:N | 2.53 | 0.42 |
| 1:A:81:PHE:CD1 | 1:A:265:PRO:HD3 | 2.55 | 0.42 |
| 1:A:297:SER:HA | 1:A:300:LYS:HB3 | 2.02 | 0.42 |
| 1:A:475:ASN:OD1 | 1:A:476:ARG:N | 2.48 | 0.42 |
| 1:A:730:LEU:O | 1:A:733:ILE:HG22 | 2.19 | 0.42 |
| 1:A:739:ASP:O | 1:A:743:THR:HG22 | 2.19 | 0.42 |
| 1:A:991:LYS:HG3 | 1:A:993:GLU:HG2 | 2.01 | 0.42 |
| 2:B:306:GLY:HA2 | 2:B:325:GLU:HB2 | 2.01 | 0.42 |
| 2:B:681:LEU:HD23 | 2:B:685:ALA:HB1 | 2.00 | 0.42 |
| 2:B:1036:HIS:CE1 | 2:B:1057:ASP:O | 2.73 | 0.42 |
| 3:C:260:GLU:HB2 | 3:C:263:ASP:H | 1.84 | 0.42 |
| 8:H:16:ASP:O | 8:H:18:GLY:N | 2.51 | 0.42 |
| 9:I:4:PHE:O | 9:I:12:LEU:HD11 | 2.20 | 0.42 |
| 15:O:135:LEU:HB3 | 15:O:287:PHE:HZ | 1.85 | 0.42 |
| 15:O:156:VAL:CG1 | 15:O:189:SER:CB | 2.87 | 0.42 |
| 15:O:160:VAL:O | 15:O:163:VAL:N | 2.53 | 0.42 |
| 15:O:271:LEU:HD23 | 15:O:272:ARG:N | 2.34 | 0.42 |
| 19:S:363:GLN:HB2 | 19:S:378:THR:HG21 | 2.02 | 0.42 |
| 21:Y:40:DA:H1' | 21:Y:41:DG:O4' | 2.19 | 0.42 |
| 1:A:95:TYR:O | 1:A:98:ALA:HB3 | 2.20 | 0.42 |
| 1:A:134:ASN:O | 1:A:137:ARG:HB2 | 2.19 | 0.42 |
| 1:A:235:LYS:HB3 | 1:A:252:ARG:CZ | 2.49 | 0.42 |
| 1:A:912:VAL:HG23 | 1:A:913:GLN:N | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1095:CYS:O | 2:B:1099:GLY:HA2 | 2.20 | 0.42 |
| 4:D:11:LEU:H | 7:G:3:ILE:HA | 1.85 | 0.42 |
| 4:D:64:ASN:HD22 | 7:G:102:LEU:HD22 | 1.85 | 0.42 |
| 15:O:76:VAL:HG23 | 15:O:120:TYR:HE1 | 1.85 | 0.42 |
| 15:O:190:LEU:HD13 | 15:O:194:LEU:CD2 | 2.40 | 0.42 |
| 15:O:347:ASP:OD1 | 15:O:348:GLU:N | 2.53 | 0.42 |
| 16:P:170:LEU:HD23 | 16:P:171:ASP:N | 2.34 | 0.42 |
| 18:R:470:GLN:HG2 | 18:R:475:ALA:O | 2.20 | 0.42 |
| 18:R:486:ILE:N | 18:R:543:ALA:O | 2.52 | 0.42 |
| 19:S:458:PHE:O | 19:S:462:GLU:HB3 | 2.17 | 0.42 |
| 19:S:484:TYR:CE1 | 19:S:488:ILE:HD13 | 2.55 | 0.42 |
| 1:A:176:LEU:HB3 | 1:A:320:GLN:HE21 | 1.85 | 0.42 |
| 1:A:235:LYS:HD3 | 1:A:252:ARG:HB3 | 2.02 | 0.42 |
| 2:B:300:GLN:O | 2:B:304:TYR:N | 2.37 | 0.42 |
| 2:B:465:SER:C | 2:B:468:GLY:H | 2.23 | 0.42 |
| 2:B:552:ASN:OD1 | 2:B:553:TYR:HD2 | 2.02 | 0.42 |
| 2:B:690:TYR:N | 2:B:691:PRO:HD3 | 2.35 | 0.42 |
| 2:B:713:ILE:O | 2:B:749:LEU:HD13 | 2.19 | 0.42 |
| 2:B:842:TYR:HB2 | 2:B:881:ILE:HD11 | 2.02 | 0.42 |
| 2:B:909:GLY:HA2 | 2:B:921:VAL:CG1 | 2.49 | 0.42 |
| 3:C:78:VAL:HG11 | 3:C:108:VAL:HG13 | 2.01 | 0.42 |
| 3:C:195:LYS:HD2 | 10:J:57:ILE:CG2 | 2.50 | 0.42 |
| 10:J:48:ARG:HG3 | 10:J:49:MET:N | 2.35 | 0.42 |
| 13:M:164:LYS:HG3 | 14:N:300:LYS:HD3 | 2.01 | 0.42 |
| 15:O:488:LYS:HD2 | 15:O:654:ALA:HB1 | 2.02 | 0.42 |
| 1:A:15:GLY:N | 1:A:1408:VAL:HG12 | 2.14 | 0.41 |
| 1:A:163:VAL:C | 1:A:180:HIS:CD2 | 2.83 | 0.41 |
| 1:A:805:ASN:ND2 | 2:B:951:SER:HA | 2.35 | 0.41 |
| 1:A:882:THR:O | 1:A:885:MET:HB3 | 2.20 | 0.41 |
| 1:A:1165:LEU:C | 1:A:1167:SER:N | 2.73 | 0.41 |
| 2:B:206:ILE:HD13 | 2:B:374:ASN:ND2 | 2.35 | 0.41 |
| 2:B:495:GLY:HA3 | 2:B:610:ARG:NH1 | 2.35 | 0.41 |
| 2:B:949:PHE:O | 2:B:953:MET:N | 2.52 | 0.41 |
| 2:B:1038:ARG:HD2 | 2:B:1057:ASP:OD2 | 2.20 | 0.41 |
| 3:C:110:PRO:O | 3:C:111:ASP:HB2 | 2.19 | 0.41 |
| 3:C:256:ILE:HG22 | 3:C:267:VAL:HG22 | 2.01 | 0.41 |
| 6:F:99:LEU:O | 6:F:102:SER:OG | 2.26 | 0.41 |
| 13:M:84:SER:O | 13:M:85:LEU:CD1 | 2.23 | 0.41 |
| 13:M:113:LYS:HD3 | 13:M:241:ALA:HA | 2.01 | 0.41 |
| 15:O:74:LEU:HG | 15:O:79:LEU:HD12 | 2.02 | 0.41 |
| 15:O:488:LYS:HA | 15:O:491:VAL:HG23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:O:597:GLN:OE1 | 15:O:597:GLN:N | 2.53 | 0.41 |
| 16:P:297:PHE:C | 16:P:299:MET:H | 2.23 | 0.41 |
| 18:R:467:ARG:CG | 18:R:610:LEU:HD22 | 2.49 | 0.41 |
| 1:A:86:LEU:HD21 | 1:A:319:LEU:HD21 | 2.01 | 0.41 |
| 1:A:533:ASN:ND2 | 6:F:94:LEU:HD22 | 2.35 | 0.41 |
| 2:B:93:LEU:CD1 | 2:B:133:ILE:HG21 | 2.49 | 0.41 |
| 2:B:217:GLN:CG | 2:B:232:TYR:HB3 | 2.50 | 0.41 |
| 2:B:767:ILE:HD12 | 2:B:767:ILE:HG23 | 1.80 | 0.41 |
| 2:B:1009:THR:O | 11:K:74:ASN:ND2 | 2.53 | 0.41 |
| 14:N:385:GLY:O | 14:N:416:ILE:HA | 2.21 | 0.41 |
| 15:O:47:PHE:HB3 | 15:O:582:GLU:OE1 | 2.21 | 0.41 |
| 15:O:67:MET:HG2 | 15:O:83:ILE:HD11 | 2.01 | 0.41 |
| 15:O:472:LYS:CG | 15:O:473:PRO:HD2 | 2.50 | 0.41 |
| 15:O:560:SER:O | 15:O:560:SER:OG | 2.31 | 0.41 |
| 16:P:69:GLU:HG3 | 16:P:70:LEU:N | 2.28 | 0.41 |
| 18:R:455:GLU:HB3 | 18:R:592:LEU:HD23 | 2.02 | 0.41 |
| 20:X:57:DT:H2" | 20:X:58:DC:C5 | 2.55 | 0.41 |
| 1:A:43:GLU:OE1 | 1:A:44:LYS:HG2 | 2.19 | 0.41 |
| 1:A:194:LYS:O | 1:A:197:TRP:HB3 | 2.20 | 0.41 |
| 1:A:261:LEU:HD12 | 1:A:262:PRO:HD2 | 2.02 | 0.41 |
| 1:A:602:TYR:N | 3:C:23:PHE:O | 2.54 | 0.41 |
| 1:A:712:ILE:HG13 | 2:B:946:PRO:HB3 | 2.02 | 0.41 |
| 1:A:896:LEU:HD11 | 1:A:912:VAL:HG21 | 2.02 | 0.41 |
| 1:A:1328:ILE:O | 1:A:1331:ALA:N | 2.53 | 0.41 |
| 2:B:1006:SER:O | 2:B:1010:GLY:N | 2.53 | 0.41 |
| 3:C:91:VAL:HG21 | 10:J:61:LEU:HD23 | 2.01 | 0.41 |
| 9:I:6:PRO:O | 9:I:8:CYS:N | 2.53 | 0.41 |
| 16:P:202:PRO:C | 16:P:203:LYS:HG2 | 2.41 | 0.41 |
| 19:S:420:TRP:CD1 | 19:S:457:LYS:HD2 | 2.55 | 0.41 |
| 1:A:200:GLU:HB3 | 15:O:516:LEU:HD21 | 1.96 | 0.41 |
| 1:A:235:LYS:HD3 | 1:A:252:ARG:CB | 2.50 | 0.41 |
| 1:A:705:LEU:HD23 | 1:A:705:LEU:C | 2.40 | 0.41 |
| 1:A:918:GLY:HA3 | 5:E:208:TYR:CD1 | 2.56 | 0.41 |
| 1:A:1053:LYS:O | 1:A:1056:VAL:N | 2.52 | 0.41 |
| 2:B:224:THR:HG1 | 2:B:225:HIS:N | 2.18 | 0.41 |
| 2:B:390:ASP:OD2 | 2:B:444:LEU:HG | 2.20 | 0.41 |
| 2:B:883:GLN:HB3 | 2:B:899:LEU:HD21 | 2.03 | 0.41 |
| 2:B:961:LEU:HD22 | 2:B:1018:PHE:CE1 | 2.55 | 0.41 |
| 5:E:128:PRO:N | 5:E:129:PRO:HD2 | 2.35 | 0.41 |
| 5:E:143:ASN:OD1 | 5:E:143:ASN:N | 2.52 | 0.41 |
| 7:G:129:ILE:HG23 | 7:G:138:LEU:HA | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:104:HIS:CE1 | 14:N:395:ILE:CD1 | 2.91 | 0.41 |
| 15:O:581:LEU:HB2 | 15:O:648:TRP:CH2 | 2.55 | 0.41 |
| 15:O:630:VAL:O | 15:O:633:ARG:HB3 | 2.21 | 0.41 |
| 18:R:425:PHE:CE2 | 18:R:427:ALA:HB3 | 2.55 | 0.41 |
| 1:A:152:ARG:HH21 | 1:A:184:ARG:HE | 1.69 | 0.41 |
| 1:A:308:SER:HB3 | 1:A:311:ASN:ND2 | 2.36 | 0.41 |
| 1:A:833:PRO:CB | 2:B:659:ILE:HD12 | 2.50 | 0.41 |
| 1:A:925:GLU:OE2 | 1:A:1081:ALA:HA | 2.20 | 0.41 |
| 1:A:1026:ARG:NH2 | 8:H:129:TYR:OH | 2.53 | 0.41 |
| 1:A:1451:LEU:O | 4:D:111:ASN:ND2 | 2.52 | 0.41 |
| 2:B:232:TYR:CD1 | 2:B:242:LEU:HD23 | 2.55 | 0.41 |
| 2:B:306:GLY:CA | 2:B:325:GLU:HB2 | 2.50 | 0.41 |
| 2:B:351:MET:HE3 | 2:B:351:MET:HB3 | 1.89 | 0.41 |
| 2:B:806:ILE:H | 2:B:806:ILE:HG13 | 1.64 | 0.41 |
| 2:B:1028:LYS:HG2 | 2:B:1029:HIS:N | 2.33 | 0.41 |
| 3:C:33:VAL:C | 3:C:35:LYS:N | 2.72 | 0.41 |
| 4:D:28:LEU:HD13 | 4:D:56:GLN:HG3 | 2.02 | 0.41 |
| 4:D:131:MET:H | 4:D:154:LEU:HD11 | 1.85 | 0.41 |
| 5:E:55:ARG:HB3 | 5:E:82:PHE:HD2 | 1.85 | 0.41 |
| 7:G:105:PHE:HD2 | 7:G:107:ASP:N | 2.19 | 0.41 |
| 13:M:131:TYR:CE2 | 13:M:133:LYS:HA | 2.55 | 0.41 |
| 13:M:251:THR:HG21 | 13:M:255:PHE:CD2 | 2.56 | 0.41 |
| 15:O:472:LYS:O | 15:O:474:GLY:N | 2.53 | 0.41 |
| 16:P:29:ALA:O | 16:P:71:LYS:HD3 | 2.21 | 0.41 |
| 18:R:537:LYS:HD3 | 21:Y:52:DA:P | 2.61 | 0.41 |
| 20:X:6:DA:H2" | 20:X:7:DA:H8 | 1.84 | 0.41 |
| 1:A:191:ALA:HB3 | 1:A:194:LYS:HB3 | 2.02 | 0.41 |
| 1:A:385:PRO:HG3 | 2:B:764:GLY:CA | 2.51 | 0.41 |
| 1:A:624:ILE:N | 1:A:657:SER:OG | 2.42 | 0.41 |
| 1:A:738:CYS:O | 1:A:742:ILE:HG22 | 2.21 | 0.41 |
| 2:B:84:LEU:HD22 | 2:B:91:PHE:O | 2.20 | 0.41 |
| 2:B:587:PHE:CE1 | 2:B:607:ARG:HD3 | 2.56 | 0.41 |
| 2:B:623:LYS:O | 2:B:625:ILE:N | 2.53 | 0.41 |
| 2:B:667:VAL:HG12 | 2:B:669:SER:H | 1.85 | 0.41 |
| 2:B:710:ILE:HG12 | 2:B:1026:LYS:O | 2.19 | 0.41 |
| 2:B:916:HIS:NE2 | 2:B:957:LYS:N | 2.68 | 0.41 |
| 2:B:933:PHE:CE2 | 2:B:937:GLY:CA | 2.94 | 0.41 |
| 2:B:936:GLN:CB | 2:B:938:ILE:HD12 | 2.51 | 0.41 |
| 4:D:8:ASN:HB3 | 7:G:4:LEU:O | 2.20 | 0.41 |
| 5:E:60:PHE:CZ | 5:E:80:VAL:HG11 | 2.56 | 0.41 |
| 7:G:203:ASP:HB3 | 7:G:211:TRP:NE1 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:O:573:SER:HA | 15:O:576:PHE:CD2 | 2.56 | 0.41 |
| 18:R:213:TRP:HD1 | 18:R:287:PRO:CD | 2.22 | 0.41 |
| 1:A:64:SER:OG | 1:A:65:LEU:N | 2.53 | 0.41 |
| 1:A:305:LYS:HA | 15:O:535:SER:OG | 2.20 | 0.41 |
| 1:A:466:LEU:HD12 | 1:A:466:LEU:HA | 1.91 | 0.41 |
| 1:A:1205:ILE:HA | 1:A:1208:ALA:HB3 | 2.02 | 0.41 |
| 1:A:1299:GLY:O | 1:A:1301:ARG:N | 2.52 | 0.41 |
| 2:B:531:LYS:HA | 2:B:534:TYR:HD2 | 1.86 | 0.41 |
| 2:B:756:THR:H | 10:J:48:ARG:HH12 | 1.68 | 0.41 |
| 3:C:106:LEU:HD12 | 3:C:208:CYS:SG | 2.60 | 0.41 |
| 3:C:140:CYS:HB2 | 3:C:196:LEU:HD13 | 2.01 | 0.41 |
| 5:E:90:VAL:HG23 | 5:E:119:SER:OG | 2.21 | 0.41 |
| 6:F:144:GLU:HG3 | 6:F:145:ASP:N | 2.36 | 0.41 |
| 14:N:290:ILE:O | 14:N:294:LEU:HB3 | 2.19 | 0.41 |
| 15:O:132:TYR:C | 15:O:134:GLY:N | 2.73 | 0.41 |
| 16:P:139:SER:OG | 16:P:140:VAL:N | 2.53 | 0.41 |
| 18:R:467:ARG:O | 18:R:471:LYS:HB3 | 2.21 | 0.41 |
| 1:A:543:THR:OG1 | 1:A:544:PRO:HD2 | 2.21 | 0.41 |
| 1:A:719:PRO:HD3 | 1:A:810:VAL:HG13 | 2.02 | 0.41 |
| 1:A:896:LEU:HD23 | 1:A:1357:LEU:HD21 | 2.02 | 0.41 |
| 1:A:975:VAL:O | 1:A:1002:ARG:NH2 | 2.47 | 0.41 |
| 2:B:180:ASP:OD2 | 2:B:184:TYR:OH | 2.29 | 0.41 |
| 2:B:464:ILE:HD11 | 2:B:746:TYR:HE1 | 1.84 | 0.41 |
| 2:B:797:ARG:NH1 | 18:R:137:GLU:OE1 | 2.54 | 0.41 |
| 2:B:1045:VAL:CG2 | 2:B:1046:LEU:N | 2.83 | 0.41 |
| 5:E:27:GLY:O | 5:E:65:THR:HG22 | 2.20 | 0.41 |
| 5:E:82:PHE:CG | 5:E:83:CYS:N | 2.89 | 0.41 |
| 8:H:15:VAL:HG13 | 8:H:24:CYS:SG | 2.61 | 0.41 |
| 13:M:77:LYS:HG2 | 14:N:360:VAL:N | 2.36 | 0.41 |
| 13:M:227:LEU:O | 13:M:232:LEU:HB2 | 2.20 | 0.41 |
| 15:O:94:THR:HA | 15:O:97:SER:HB2 | 2.02 | 0.41 |
| 15:O:570:GLU:OE1 | 15:O:570:GLU:N | 2.40 | 0.41 |
| 1:A:33:GLU:HG3 | 1:A:83:HIS:HE2 | 1.84 | 0.41 |
| 1:A:228:LEU:HD12 | 1:A:257:ILE:HD11 | 2.03 | 0.41 |
| 1:A:322:THR:O | 1:A:326:TYR:N | 2.47 | 0.41 |
| 1:A:404:TYR:HD2 | 1:A:464:ARG:HH21 | 1.68 | 0.41 |
| 1:A:541:LEU:HG | 1:A:551:ILE:CD1 | 2.47 | 0.41 |
| 1:A:665:ASP:OD2 | 1:A:797:CYS:HA | 2.21 | 0.41 |
| 1:A:792:LEU:O | 1:A:796:THR:HB | 2.20 | 0.41 |
| 1:A:975:VAL:HG13 | 1:A:976:ARG:N | 2.35 | 0.41 |
| 1:A:1448:PHE:CZ | 4:D:16:VAL:HG23 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:98:ILE:CD1 | 2:B:131:VAL:HG12 | 2.51 | 0.41 |
| 2:B:112:LEU:HD22 | 2:B:162:ILE:CG1 | 2.51 | 0.41 |
| 2:B:239:LYS:NZ | 2:B:241:TYR:HE2 | 2.19 | 0.41 |
| 2:B:622:VAL:O | 2:B:626:HIS:HD2 | 2.04 | 0.41 |
| 2:B:625:ILE:HD11 | 2:B:628:ARG:HH21 | 1.86 | 0.41 |
| 2:B:738:THR:HA | 2:B:976:GLY:O | 2.21 | 0.41 |
| 2:B:738:THR:H | 2:B:741:ILE:HD13 | 1.86 | 0.41 |
| 2:B:800:ASN:OD1 | 2:B:855:PRO:HB3 | 2.21 | 0.41 |
| 2:B:889:SER:OG | 2:B:891:ASN:OD1 | 2.36 | 0.41 |
| 2:B:1077:GLN:O | 2:B:1081:GLU:HB2 | 2.20 | 0.41 |
| 3:C:33:VAL:O | 3:C:34:GLU:CB | 2.47 | 0.41 |
| 4:D:157:ILE:HG13 | 4:D:161:ALA:HB3 | 2.03 | 0.41 |
| 5:E:181:ALA:O | 5:E:186:LEU:HG | 2.21 | 0.41 |
| 7:G:44:LEU:HD21 | 7:G:105:PHE:CE1 | 2.56 | 0.41 |
| 7:G:46:ILE:N | 7:G:75:VAL:O | 2.51 | 0.41 |
| 7:G:126:SER:CB | 7:G:139:TYR:HB3 | 2.49 | 0.41 |
| 7:G:152:ARG:HB3 | 7:G:197:LEU:HD11 | 2.03 | 0.41 |
| 13:M:236:VAL:O | 13:M:240:GLU:N | 2.51 | 0.41 |
| 15:O:172:GLU:O | 15:O:176:SER:CB | 2.69 | 0.41 |
| 15:O:547:GLU:HG2 | 15:O:548:ILE:N | 2.22 | 0.41 |
| 15:O:595:LEU:HD22 | 15:O:633:ARG:CZ | 2.51 | 0.41 |
| 15:O:639:ALA:O | 15:O:643:ARG:HG3 | 2.21 | 0.41 |
| 16:P:25:LYS:HG3 | 16:P:26:GLY:N | 2.36 | 0.41 |
| 16:P:96:TYR:OH | 16:P:113:ARG:NH1 | 2.54 | 0.41 |
| 17:Q:48:THR:HG23 | 17:Q:51:GLU:H | 1.86 | 0.41 |
| 18:R:172:GLU:HG2 | 18:R:502:ALA:O | 2.21 | 0.41 |
| 18:R:249:HIS:CD2 | 19:S:406:TYR:CE2 | 3.09 | 0.41 |
| 18:R:471:LYS:HD3 | 18:R:614:LEU:HD23 | 2.02 | 0.41 |
| 18:R:508:PHE:O | 18:R:522:ARG:N | 2.28 | 0.41 |
| 19:S:491:ASN:OD1 | 19:S:492:ILE:N | 2.53 | 0.41 |
| 20:X:60:DA:C6 | 21:Y:4:DT:C4 | 3.09 | 0.41 |
| 1:A:87:ALA:O | 1:A:88:LEU:HB2 | 2.21 | 0.41 |
| 1:A:565:SER:OG | 1:A:663:VAL:HA | 2.21 | 0.41 |
| 1:A:570:PHE:CE1 | 1:A:605:THR:HG22 | 2.56 | 0.41 |
| 1:A:660:LEU:HG | 8:H:117:SER:OG | 2.21 | 0.41 |
| 1:A:773:VAL:O | 1:A:776:GLU:HB3 | 2.21 | 0.41 |
| 1:A:792:LEU:HG | 1:A:796:THR:OG1 | 2.21 | 0.41 |
| 1:A:1072:GLU:O | 1:A:1076:PHE:HB2 | 2.21 | 0.41 |
| 2:B:184:TYR:HB3 | 2:B:470:MET:HE1 | 2.02 | 0.41 |
| 2:B:225:HIS:CD2 | 2:B:226:GLU:HG2 | 2.56 | 0.41 |
| 2:B:521:THR:HG21 | 2:B:587:PHE:CD2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:930:ASP:O | 2:B:931:MET:HB3 | 2.20 | 0.41 |
| 2:B:938:ILE:CG1 | 10:J:45:CYS:SG | 3.09 | 0.41 |
| 2:B:1093:ASP:OD1 | 2:B:1118:LYS:HG2 | 2.21 | 0.41 |
| 4:D:133:HIS:HE1 | 7:G:212:GLU:H | 1.68 | 0.41 |
| 5:E:3:GLN:O | 5:E:6:GLU:HB2 | 2.21 | 0.41 |
| 5:E:93:MET:HE1 | 5:E:124:VAL:HA | 2.03 | 0.41 |
| 6:F:81:THR:HG22 | 6:F:82:THR:N | 2.35 | 0.41 |
| 13:M:184:LYS:HD2 | 13:M:184:LYS:HA | 1.70 | 0.41 |
| 15:O:174:TYR:O | 15:O:178:VAL:HG23 | 2.21 | 0.41 |
| 15:O:340:GLU:O | 15:O:343:LYS:N | 2.51 | 0.41 |
| 17:Q:52:ARG:O | 17:Q:55:ALA:N | 2.54 | 0.41 |
| 18:R:231:ALA:HA | 18:R:234:MET:HB3 | 2.03 | 0.41 |
| 18:R:420:TYR:CZ | 18:R:422:PRO:HG3 | 2.56 | 0.41 |
| 18:R:528:ILE:HG23 | 18:R:541:THR:O | 2.21 | 0.41 |
| 1:A:201:TRP:CD1 | 1:A:216:LYS:NZ | 2.90 | 0.40 |
| 1:A:424:PRO:HG2 | 1:A:444:LEU:HD23 | 2.03 | 0.40 |
| 1:A:502:GLU:OE2 | 2:B:767:ILE:HG13 | 2.20 | 0.40 |
| 1:A:535:MET:HG3 | 2:B:1073:TYR:CD1 | 2.57 | 0.40 |
| 1:A:630:ASN:ND2 | 1:A:663:VAL:O | 2.55 | 0.40 |
| 1:A:717:VAL:O | 1:A:810:VAL:HG22 | 2.20 | 0.40 |
| 1:A:794:MET:SD | 2:B:947:HIS:ND1 | 2.93 | 0.40 |
| 1:A:913:GLN:HG2 | 1:A:915:THR:O | 2.21 | 0.40 |
| 1:A:921:LEU:HG | 1:A:1081:ALA:O | 2.21 | 0.40 |
| 2:B:251:ILE:CG2 | 2:B:256:VAL:HG23 | 2.51 | 0.40 |
| 2:B:526:GLU:O | 2:B:529:ILE:HG22 | 2.21 | 0.40 |
| 6:F:76:LYS:HD3 | 6:F:79:ARG:HH21 | 1.86 | 0.40 |
| 8:H:128:ASN:CG | 8:H:129:TYR:H | 2.24 | 0.40 |
| 10:J:52:THR:HG22 | 10:J:53:HIS:N | 2.32 | 0.40 |
| 13:M:91:ALA:N | 14:N:392:GLN:NE2 | 2.69 | 0.40 |
| 15:O:516:LEU:O | 15:O:516:LEU:CG | 2.66 | 0.40 |
| 16:P:110:ILE:O | 16:P:114:THR:HG22 | 2.22 | 0.40 |
| 18:R:505:HIS:O | 18:R:508:PHE:N | 2.50 | 0.40 |
| 20:X:7:DA:H2" | 20:X:8:DC:C5 | 2.56 | 0.40 |
| 20:X:52:DA:H8 | 20:X:52:DA:OP2 | 2.03 | 0.40 |
| 1:A:526:GLU:O | 1:A:529:ALA:N | 2.54 | 0.40 |
| 1:A:530:GLU:OE2 | 2:B:1075:ALA:HA | 2.21 | 0.40 |
| 1:A:1329:GLU:CD | 5:E:200:ARG:HH21 | 2.25 | 0.40 |
| 1:A:1350:VAL:O | 1:A:1351:ASP:HB2 | 2.22 | 0.40 |
| 2:B:249:GLU:HB3 | 2:B:250:GLU:HG2 | 2.03 | 0.40 |
| 2:B:789:ARG:O | 2:B:899:LEU:HA | 2.21 | 0.40 |
| 2:B:929:GLU:OE2 | 3:C:73:SER:OG | 2.28 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:944:MET:HE1 | 2:B:957:LYS:HE2 | 2.03 | 0.40 |
| 2:B:1005:TYR:OH | 3:C:293:ARG:NH1 | 2.54 | 0.40 |
| 2:B:1042:PRO:HB3 | 18:R:38:VAL:HG22 | 2.04 | 0.40 |
| 9:I:19:SER:O | 9:I:21:VAL:HG23 | 2.21 | 0.40 |
| 12:L:29:TYR:HB2 | 12:L:30:ILE:H | 1.75 | 0.40 |
| 13:M:158:GLN:NE2 | 14:N:308:GLN:HE21 | 2.05 | 0.40 |
| 14:N:279:GLU:O | 14:N:282:LEU:HB2 | 2.22 | 0.40 |
| 14:N:287:HIS:ND1 | 14:N:369:GLY:O | 2.50 | 0.40 |
| 15:O:127:ILE:O | 15:O:130:LEU:HB2 | 2.21 | 0.40 |
| 15:O:133:SER:O | 15:O:137:ILE:HG13 | 2.22 | 0.40 |
| 15:O:190:LEU:CD1 | 15:O:194:LEU:CD2 | 2.97 | 0.40 |
| 15:O:509:ARG:O | 15:O:512:ARG:HB3 | 2.20 | 0.40 |
| 15:O:636:ASN:O | 15:O:640:ARG:HG2 | 2.20 | 0.40 |
| 16:P:140:VAL:CG2 | 16:P:158:ASP:HB3 | 2.51 | 0.40 |
| 18:R:509:SER:HA | 18:R:521:TYR:HA | 2.02 | 0.40 |
| 19:S:415:SER:OG | 19:S:416:TYR:N | 2.53 | 0.40 |
| 20:X:11:DA:C5 | 20:X:12:DT:C4 | 3.09 | 0.40 |
| 20:X:18:DT:H73 | 20:X:19:DA:N7 | 2.36 | 0.40 |
| 1:A:496:ARG:O | 1:A:497:THR:HB | 2.21 | 0.40 |
| 1:A:498:PHE:CZ | 1:A:519:LEU:HD13 | 2.57 | 0.40 |
| 1:A:552:ALA:CB | 1:A:671:ASP:H | 2.33 | 0.40 |
| 1:A:792:LEU:HD11 | 8:H:19:ARG:NH2 | 2.37 | 0.40 |
| 1:A:1127:LYS:O | 1:A:1131:ASN:HB3 | 2.21 | 0.40 |
| 1:A:1145:LEU:HB3 | 1:A:1146:VAL:H | 1.48 | 0.40 |
| 1:A:1217:ILE:H | 1:A:1217:ILE:HD12 | 1.87 | 0.40 |
| 1:A:1318:HIS:NE2 | 1:A:1321:GLU:HB3 | 2.36 | 0.40 |
| 2:B:798:TYR:C | 18:R:99:TYR:HE1 | 2.25 | 0.40 |
| 3:C:259:ASP:HB2 | 3:C:266:TYR:CE1 | 2.57 | 0.40 |
| 7:G:2:PHE:CD2 | 7:G:79:PRO:HB3 | 2.56 | 0.40 |
| 7:G:52:LEU:HD12 | 7:G:53:THR:HG22 | 2.04 | 0.40 |
| 11:K:61:ALA:O | 11:K:104:ARG:HD2 | 2.21 | 0.40 |
| 11:K:110:GLU:CD | 11:K:111:THR:HG23 | 2.40 | 0.40 |
| 15:O:226:ILE:O | 15:O:228:ARG:N | 2.46 | 0.40 |
| 15:O:253:ILE:O | 15:O:256:PRO:HD2 | 2.21 | 0.40 |
| 15:O:465:PHE:HA | 15:O:466:PRO:HA | 1.86 | 0.40 |
| 15:O:482:LYS:C | 15:O:485:PRO:HD2 | 2.42 | 0.40 |
| 15:O:519:GLU:HG3 | 15:O:534:ARG:NH2 | 2.36 | 0.40 |
| 16:P:117:HIS:HB3 | 16:P:119:HIS:ND1 | 2.36 | 0.40 |
| 18:R:609:GLU:HG2 | 18:R:613:HIS:NE2 | 2.36 | 0.40 |
| 20:X:5:DC:H2" | 20:X:6:DA:H8 | 1.85 | 0.40 |
| 1:A:395:PRO:CB | 1:A:496:ARG:HA | 2.43 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:400:LYS:CA | 1:A:465:HIS:HD2 | 2.26 | 0.40 |
| 1:A:1164:THR:CB | 1:A:1271:VAL:HA | 2.49 | 0.40 |
| 2:B:721:ILE:HG22 | 2:B:790:LYS:HD3 | 2.04 | 0.40 |
| 2:B:1041:GLY:HA3 | 2:B:1057:ASP:OD2 | 2.22 | 0.40 |
| 3:C:31:TRP:CE3 | 11:K:82:LYS:HD2 | 2.56 | 0.40 |
| 8:H:110:ASP:O | 8:H:111:LEU:HD12 | 2.21 | 0.40 |
| 13:M:140:TRP:CG | 13:M:185:TYR:HB3 | 2.57 | 0.40 |
| 14:N:286:ASP:O | 14:N:290:ILE:HG22 | 2.22 | 0.40 |
| 15:O:358:GLY:HA2 | 15:O:361:PHE:CD2 | 2.56 | 0.40 |
| 16:P:218:THR:OG1 | 16:P:219:GLN:N | 2.54 | 0.40 |
| 18:R:269:LYS:O | 18:R:272:VAL:HG12 | 2.21 | 0.40 |
| 20:X:54:DG:H2" | 20:X:55:DA:C8 | 2.57 | 0.40 |
| 1:A:85:LYS:HD2 | 1:A:260:TYR:HE1 | 1.87 | 0.40 |
| 1:A:228:LEU:HD21 | 1:A:232:LYS:HE3 | 2.03 | 0.40 |
| 1:A:384:ASP:HA | 2:B:765:TYR:CE2 | 2.57 | 0.40 |
| 1:A:889:LEU:HD12 | 1:A:889:LEU:HA | 1.88 | 0.40 |
| 1:A:995:VAL:HG21 | 5:E:209:ALA:HB2 | 2.02 | 0.40 |
| 1:A:1122:GLY:C | 1:A:1124:PRO:HD2 | 2.42 | 0.40 |
| 2:B:244:HIS:ND1 | 2:B:332:ILE:HD12 | 2.37 | 0.40 |
| 2:B:309:VAL:HG22 | 2:B:310:LYS:N | 2.35 | 0.40 |
| 2:B:756:THR:N | 10:J:48:ARG:HH12 | 2.19 | 0.40 |
| 2:B:775:LYS:C | 2:B:777:SER:N | 2.74 | 0.40 |
| 2:B:888:VAL:HG23 | 2:B:893:GLN:O | 2.21 | 0.40 |
| 7:G:207:LEU:HB3 | 7:G:210:TRP:CE2 | 2.56 | 0.40 |
| 8:H:94:ASP:HB3 | 8:H:145:ARG:HA | 2.04 | 0.40 |
| 14:N:364:ARG:HG3 | 14:N:365:VAL:N | 2.36 | 0.40 |
| 15:O:528:MET:HG3 | 15:O:529:LYS:N | 2.37 | 0.40 |
| 15:O:537:LEU:O | 15:O:540:LEU:HB3 | 2.21 | 0.40 |
| 16:P:203:LYS:HD2 | 16:P:206:VAL:CG2 | 2.52 | 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 | A | 1422/1460 (97%) | 1135 (80%) | 265 (19%) | 22 (2%) | 10 44 |
| 2 | B | 1112/1149 (97%) | 912 (82%) | 183 (16%) | 17 (2%) | 10 44 |
| 3 | C | 333/335 (99%) | 278 (84%) | 50 (15%) | 5 (2%) | 10 44 |
| 4 | D | 113/161 (70%) | 85 (75%) | 27 (24%) | 1 (1%) | 17 54 |
| 5 | E | 213/215 (99%) | 177 (83%) | 32 (15%) | 4 (2%) | 8 39 |
| 6 | F | 81/155 (52%) | 69 (85%) | 11 (14%) | 1 (1%) | 13 48 |
| 7 | G | 178/212 (84%) | 147 (83%) | 27 (15%) | 4 (2%) | 6 37 |
| 8 | H | 136/146 (93%) | 111 (82%) | 25 (18%) | 0 | 100 100 |
| 9 | I | 40/110 (36%) | 30 (75%) | 8 (20%) | 2 (5%) | 2 22 |
| 10 | J | 65/70 (93%) | 54 (83%) | 11 (17%) | 0 | 100 100 |
| 11 | K | 99/142 (70%) | 82 (83%) | 17 (17%) | 0 | 100 100 |
| 12 | L | 44/70 (63%) | 37 (84%) | 7 (16%) | 0 | 100 100 |
| 13 | M | 160/282 (57%) | 126 (79%) | 29 (18%) | 5 (3%) | 4 31 |
| 14 | N | 106/422 (25%) | 84 (79%) | 21 (20%) | 1 (1%) | 17 54 |
| 15 | O | 533/654 (82%) | 411 (77%) | 108 (20%) | 14 (3%) | 5 34 |
| 16 | P | 271/317 (86%) | 225 (83%) | 44 (16%) | 2 (1%) | 22 60 |
| 17 | Q | 33/251 (13%) | 26 (79%) | 5 (15%) | 2 (6%) | 1 19 |
| 18 | R | 514/736 (70%) | 453 (88%) | 59 (12%) | 2 (0%) | 34 71 |
| 19 | S | 172/594 (29%) | 156 (91%) | 16 (9%) | 0 | 100 100 |
| All | All | 5625/7481 (75%) | 4598 (82%) | 945 (17%) | 82 (2%) | 14 44 |

All (82) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 249 | PRO |
| 1 | A | 587 | ILE |
| 1 | A | 599 | LYS |
| 1 | A | 1371 | ILE |
| 2 | B | 1046 | LEU |
| 2 | B | 1140 | ARG |
| 3 | C | 87 | ASN |
| 5 | E | 180 | ARG |
| 5 | E | 181 | ALA |
| 9 | I | 21 | VAL |
| 13 | M | 84 | SER |
| 13 | M | 103 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | M | 107 | ILE |
| 14 | N | 391 | LEU |
| 15 | O | 146 | VAL |
| 15 | O | 188 | SER |
| 15 | O | 189 | SER |
| 15 | O | 194 | LEU |
| 17 | Q | 39 | ILE |
| 1 | A | 975 | VAL |
| 1 | A | 995 | VAL |
| 1 | A | 1372 | THR |
| 2 | B | 87 | VAL |
| 2 | B | 168 | GLU |
| 3 | C | 120 | LEU |
| 7 | G | 125 | GLU |
| 9 | I | 35 | ILE |
| 13 | M | 105 | PRO |
| 15 | O | 352 | VAL |
| 16 | P | 295 | ASN |
| 1 | A | 39 | LEU |
| 1 | A | 236 | SER |
| 1 | A | 238 | ASP |
| 1 | A | 239 | CYS |
| 1 | A | 307 | ILE |
| 1 | A | 675 | HIS |
| 1 | A | 998 | TYR |
| 2 | B | 335 | LEU |
| 2 | B | 418 | ALA |
| 2 | B | 1056 | ARG |
| 3 | C | 122 | ASP |
| 3 | C | 255 | VAL |
| 13 | M | 243 | ILE |
| 15 | O | 133 | SER |
| 15 | O | 190 | LEU |
| 18 | R | 274 | LYS |
| 1 | A | 109 | ASN |
| 1 | A | 1328 | ILE |
| 2 | B | 713 | ILE |
| 2 | B | 766 | ASP |
| 2 | B | 767 | ILE |
| 2 | B | 823 | SER |
| 2 | B | 934 | ASN |
| 2 | B | 1057 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 147 | HIS |
| 5 | E | 182 | ASP |
| 6 | F | 144 | GLU |
| 7 | G | 111 | PRO |
| 15 | O | 191 | PHE |
| 1 | A | 43 | GLU |
| 1 | A | 829 | ASP |
| 1 | A | 1145 | LEU |
| 3 | C | 223 | SER |
| 7 | G | 191 | PRO |
| 15 | O | 499 | THR |
| 1 | A | 277 | SER |
| 1 | A | 1300 | LEU |
| 2 | B | 822 | GLN |
| 2 | B | 215 | ILE |
| 15 | O | 274 | VAL |
| 1 | A | 672 | GLY |
| 4 | D | 127 | LEU |
| 15 | O | 187 | ILE |
| 15 | O | 297 | ILE |
| 2 | B | 811 | VAL |
| 2 | B | 1137 | ILE |
| 15 | O | 88 | VAL |
| 15 | O | 473 | PRO |
| 16 | P | 206 | VAL |
| 17 | Q | 40 | PRO |
| 18 | R | 516 | PHE |
| 7 | G | 158 | VAL |

### 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 | A | 1232/1257 (98%) | 1223 (99%) | 9 (1%) | 84 90 |
| 2 | B | 975/1006 (97%) | 970 (100%) | 5 (0%) | 88 93 |
| 3 | C | 296/296 (100%) | 295 (100%) | 1 (0%) | 92 95 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 4 | D | 110/145 (76%) | 109 (99%) | 1 (1%) | 78 87 |
| 5 | E | 197/197 (100%) | 196 (100%) | 1 (0%) | 88 93 |
| 6 | F | 73/137 (53%) | 73 (100%) | 0 | 100 100 |
| 7 | G | 164/190 (86%) | 163 (99%) | 1 (1%) | 86 92 |
| 8 | H | 123/128 (96%) | 123 (100%) | 0 | 100 100 |
| 9 | I | 38/98 (39%) | 38 (100%) | 0 | 100 100 |
| 10 | J | 62/65 (95%) | 61 (98%) | 1 (2%) | 62 78 |
| 11 | K | 91/130 (70%) | 91 (100%) | 0 | 100 100 |
| 12 | L | 40/57 (70%) | 40 (100%) | 0 | 100 100 |
| 13 | M | 142/249 (57%) | 140 (99%) | 2 (1%) | 67 80 |
| 14 | N | 92/360 (26%) | 91 (99%) | 1 (1%) | 73 84 |
| 15 | O | 495/593 (84%) | 493 (100%) | 2 (0%) | 91 94 |
| 16 | P | 255/285 (90%) | 255 (100%) | 0 | 100 100 |
| 17 | Q | 31/195 (16%) | 31 (100%) | 0 | 100 100 |
| 18 | R | 450/623 (72%) | 450 (100%) | 0 | 100 100 |
| 19 | S | 157/494 (32%) | 157 (100%) | 0 | 100 100 |
| All | All | 5023/6505 (77%) | 4999 (100%) | 24 (0%) | 89 93 |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 239 | CYS |
| 1 | A | 247 | THR |
| 1 | A | 248 | VAL |
| 1 | A | 364 | PHE |
| 1 | A | 669 | LEU |
| 1 | A | 950 | GLN |
| 1 | A | 1145 | LEU |
| 1 | A | 1369 | LEU |
| 1 | A | 1373 | ARG |
| 2 | B | 110 | ASP |
| 2 | B | 112 | LEU |
| 2 | B | 551 | LEU |
| 2 | B | 772 | VAL |
| 2 | B | 933 | PHE |
| 3 | C | 120 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 127 | LEU |
| 5 | E | 180 | ARG |
| 7 | G | 125 | GLU |
| 10 | J | 43 | ARG |
| 13 | M | 104 | HIS |
| 13 | M | 183 | PHE |
| 14 | N | 391 | LEU |
| 15 | O | 498 | SER |
| 15 | O | 561 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 109 | ASN |
| 1 | A | 161 | ASN |
| 1 | A | 207 | HIS |
| 1 | A | 315 | HIS |
| 1 | A | 386 | ASN |
| 1 | A | 520 | HIS |
| 1 | A | 523 | GLN |
| 1 | A | 533 | ASN |
| 1 | A | 566 | HIS |
| 1 | A | 589 | HIS |
| 1 | A | 618 | HIS |
| 1 | A | 619 | ASN |
| 1 | A | 675 | HIS |
| 1 | A | 808 | GLN |
| 1 | A | 828 | GLN |
| 1 | A | 1385 | GLN |
| 2 | B | 140 | ASN |
| 2 | B | 217 | GLN |
| 2 | B | 225 | HIS |
| 2 | B | 270 | GLN |
| 2 | B | 275 | ASN |
| 2 | B | 286 | ASN |
| 2 | B | 396 | ASN |
| 2 | B | 425 | HIS |
| 2 | B | 519 | HIS |
| 2 | B | 574 | GLN |
| 2 | B | 600 | HIS |
| 2 | B | 626 | HIS |
| 2 | B | 693 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 717 | GLN |
| 2 | B | 754 | ASN |
| 2 | B | 774 | ASN |
| 2 | B | 800 | ASN |
| 2 | B | 902 | GLN |
| 2 | B | 928 | GLN |
| 2 | B | 936 | GLN |
| 2 | B | 1029 | HIS |
| 3 | C | 93 | GLN |
| 3 | C | 99 | HIS |
| 3 | C | 130 | ASN |
| 3 | C | 161 | HIS |
| 3 | C | 175 | GLN |
| 4 | D | 31 | GLN |
| 4 | D | 64 | ASN |
| 4 | D | 69 | ASN |
| 4 | D | 126 | GLN |
| 5 | E | 54 | GLN |
| 5 | E | 104 | ASN |
| 5 | E | 114 | ASN |
| 5 | E | 174 | GLN |
| 7 | G | 32 | ASN |
| 13 | M | 86 | HIS |
| 13 | M | 178 | GLN |
| 13 | M | 190 | ASN |
| 13 | M | 254 | GLN |
| 14 | N | 288 | GLN |
| 14 | N | 308 | GLN |
| 14 | N | 377 | ASN |
| 15 | O | 43 | ASN |
| 15 | O | 56 | HIS |
| 15 | O | 128 | HIS |
| 15 | O | 147 | ASN |
| 15 | O | 222 | HIS |
| 15 | O | 310 | GLN |
| 15 | O | 332 | GLN |
| 15 | O | 337 | GLN |
| 15 | O | 549 | GLN |
| 15 | O | 580 | ASN |
| 15 | O | 587 | ASN |
| 15 | O | 626 | GLN |
| 16 | P | 117 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | P | 189 | ASN |
| 16 | P | 219 | GLN |
| 16 | P | 239 | ASN |
| 16 | P | 305 | HIS |
| 18 | R | 6 | ASN |
| 18 | R | 20 | ASN |
| 18 | R | 35 | ASN |
| 18 | R | 184 | HIS |
| 18 | R | 236 | ASN |
| 18 | R | 414 | HIS |
| 19 | S | 444 | GLN |
| 19 | S | 499 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no monosaccharides in this entry.

### 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 19 | S | 1 |
| 17 | Q | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | S | 319:UNK | C | 360:THR | N | 37.73 |
| 1 | Q | 70:PHE | C | 1070:UNK | N | 12.87 |

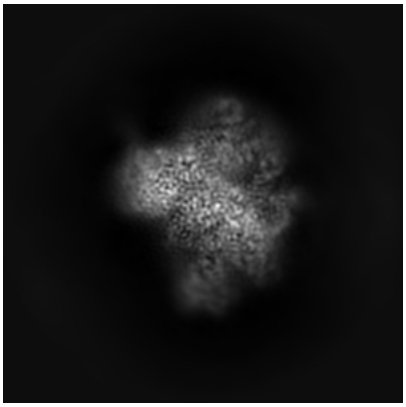
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7531. These allow visual inspection of the internal detail of the map and identification of artifacts.

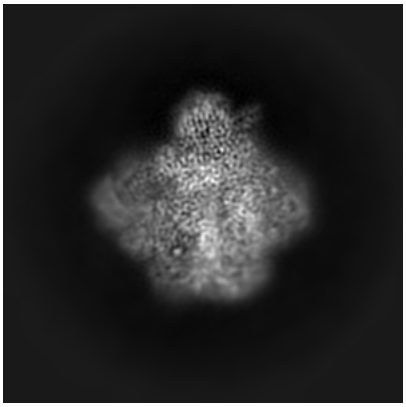
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

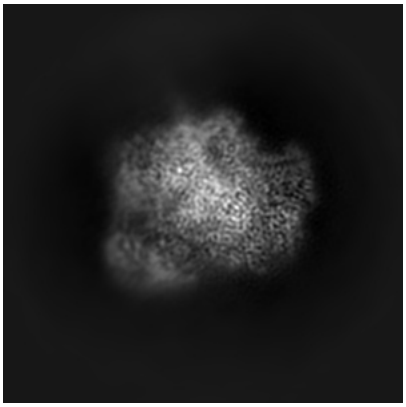
### 6.1.1 Primary map



X



Y

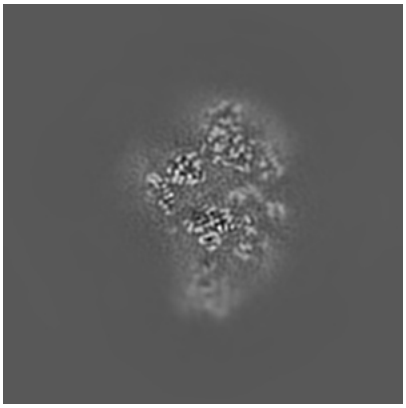


Z

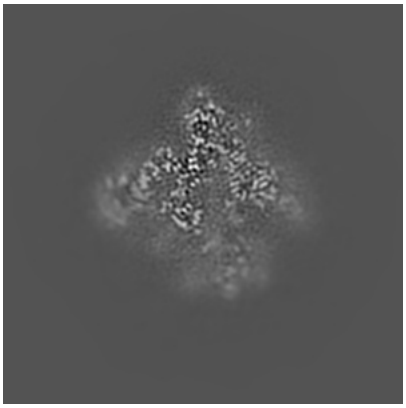
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

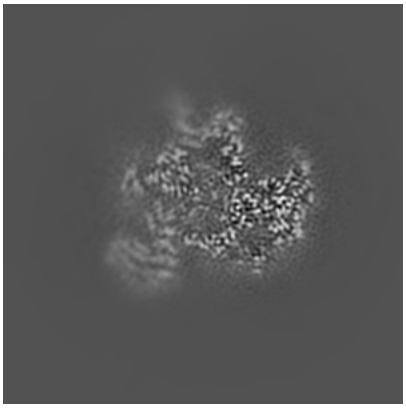
### 6.2.1 Primary map



X Index: 144



Y Index: 144

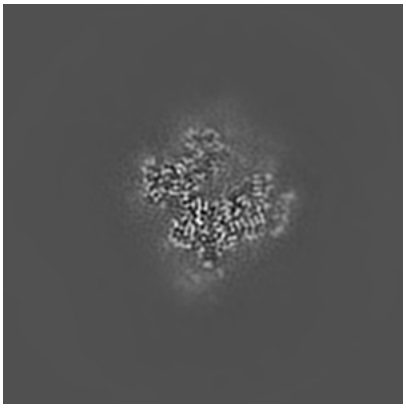


Z Index: 144

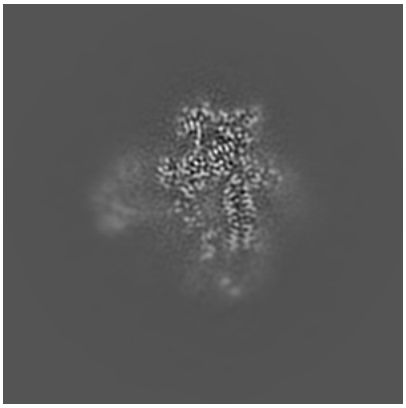
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

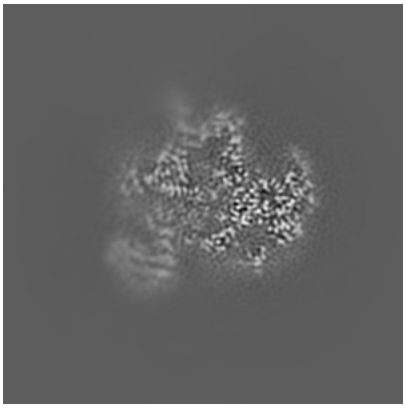
### 6.3.1 Primary map



X Index: 168



Y Index: 133

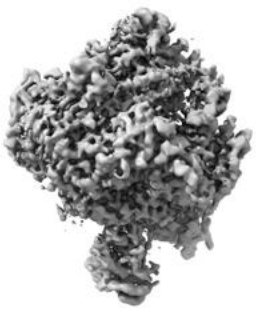


Z Index: 143

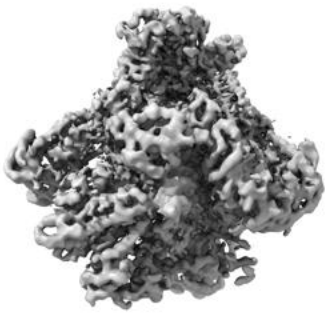
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

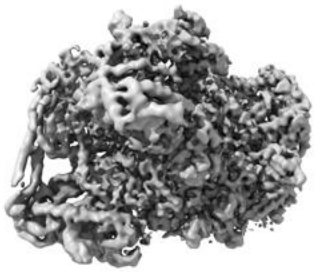
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

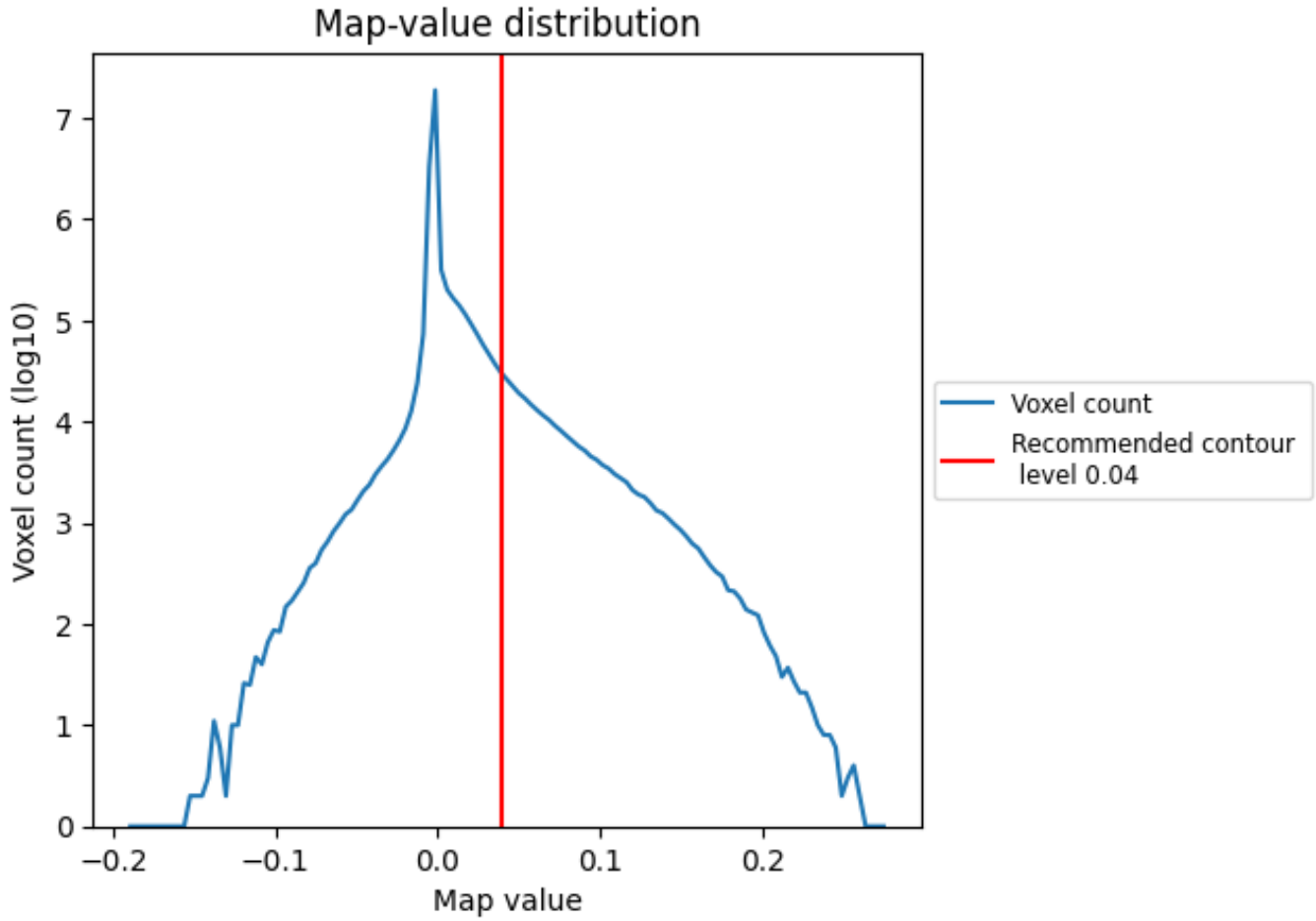
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

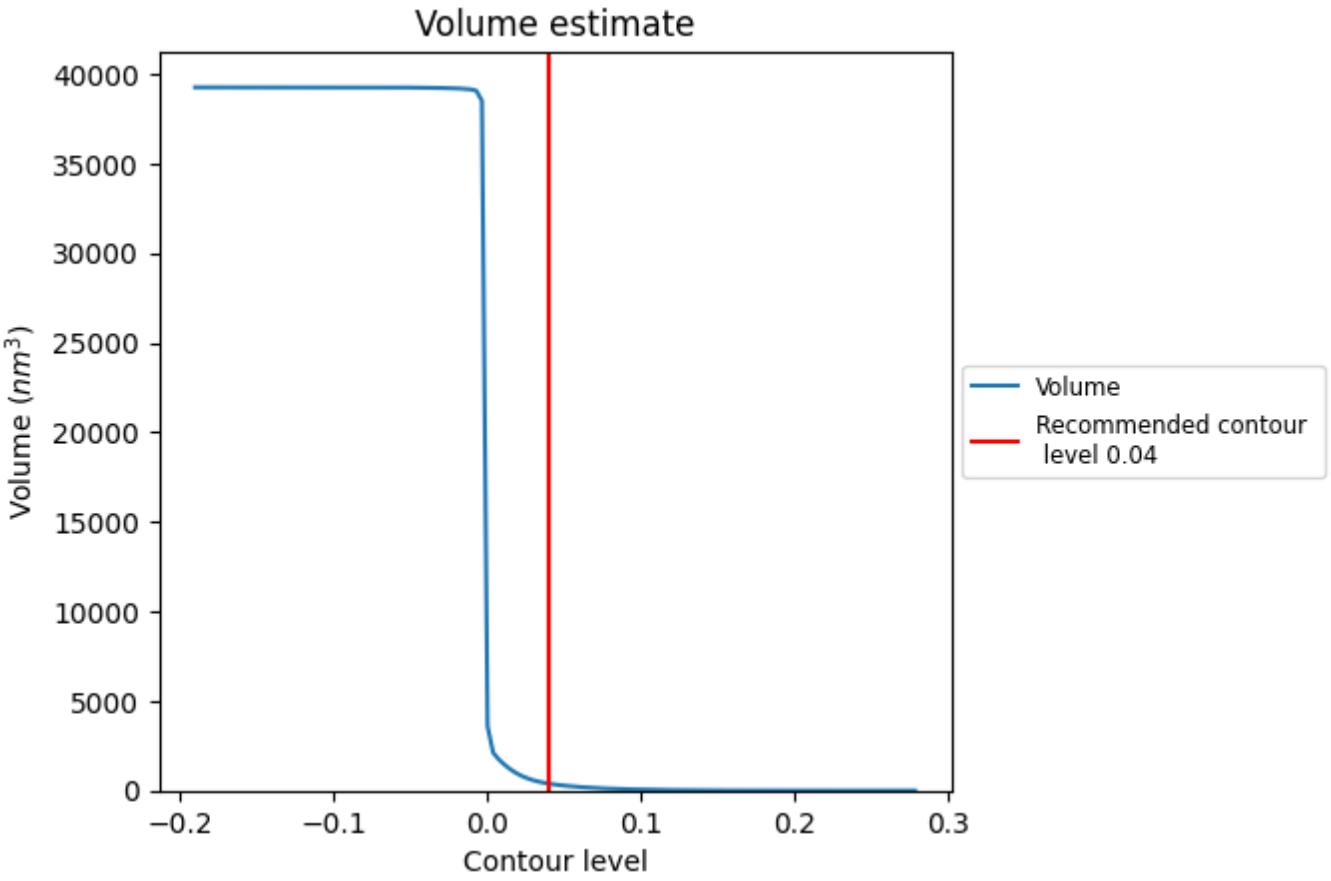
This section contains the results of statistical analysis of the map.

## 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.

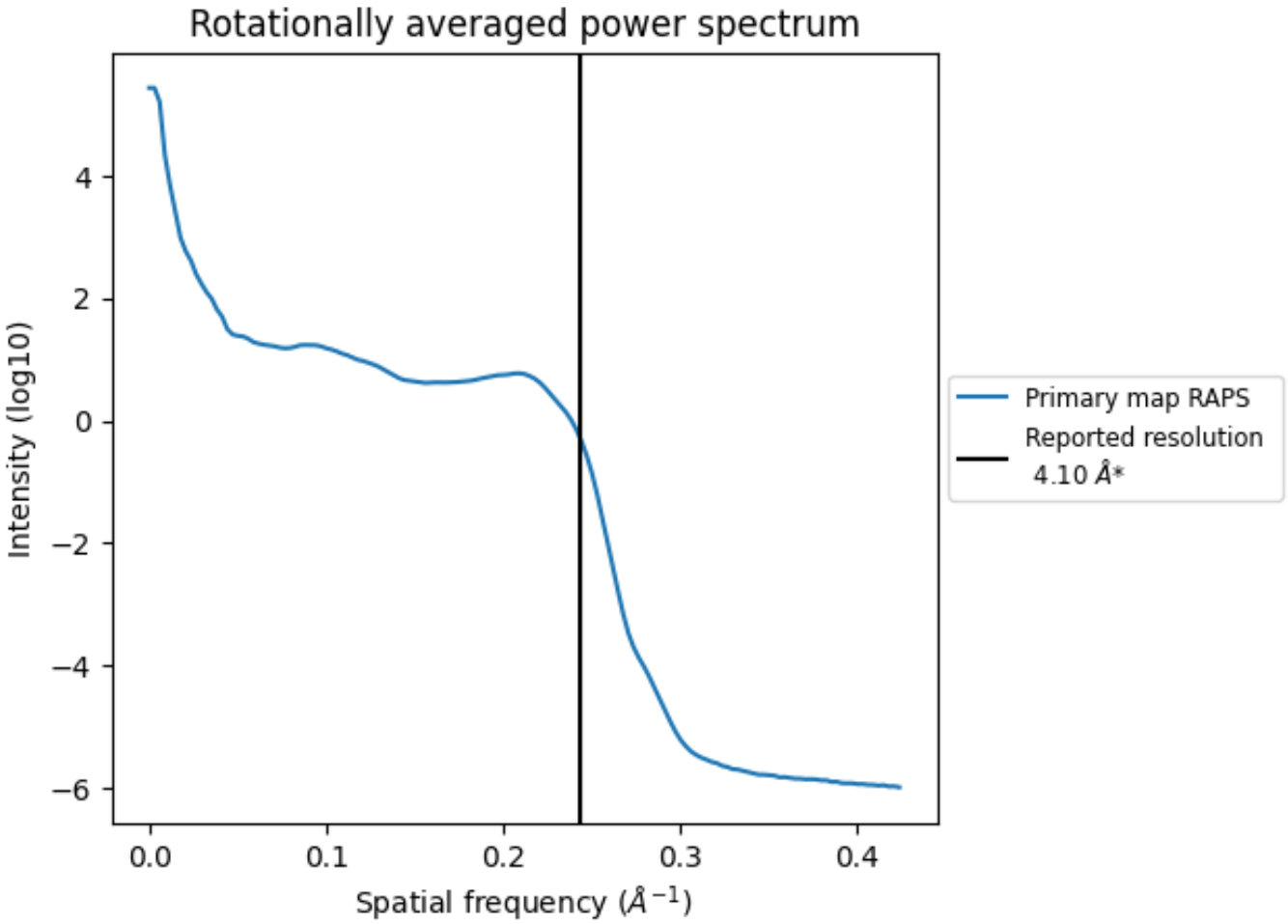
## 7.2 Volume estimate




The volume at the recommended contour level is 395 $nm^3$; this corresponds to an approximate mass of 357 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)

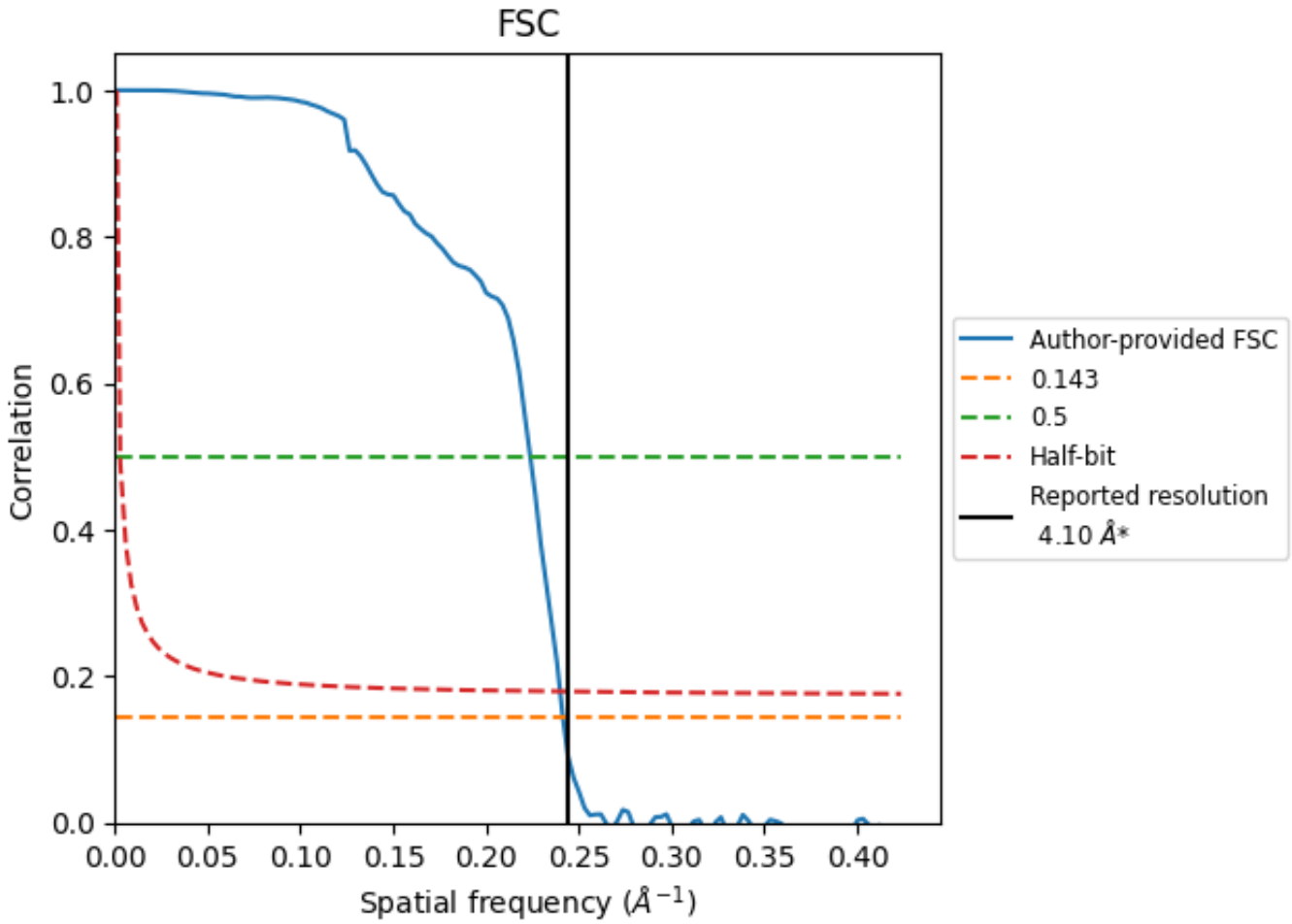



*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.244 Å$^{-1}$

## 8.2 Resolution estimates (i)

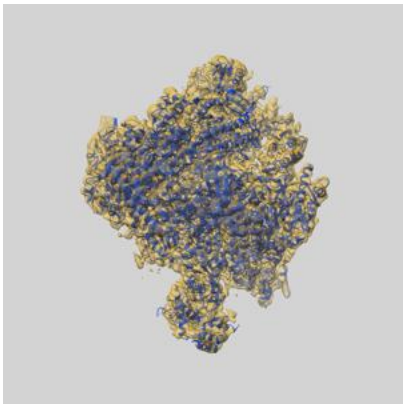
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.10 | - | - |
| Author-provided FSC curve | 4.14 | 4.47 | 4.17 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

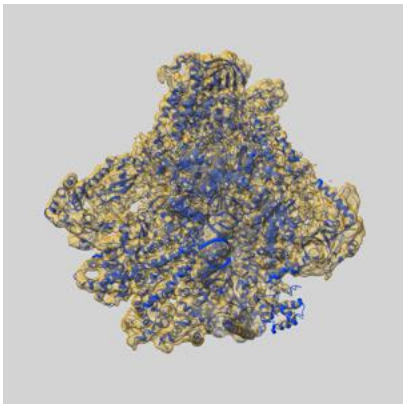
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7531 and PDB model 6CNC. Per-residue inclusion information can be found in section 3 on page 9.

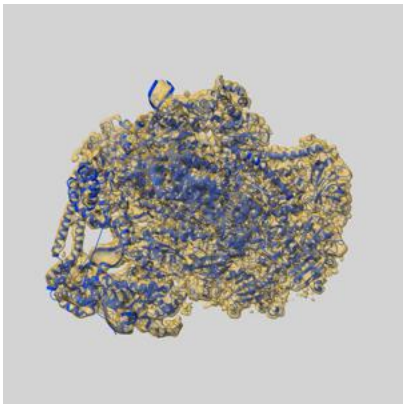
## 9.1 Map-model overlay



X



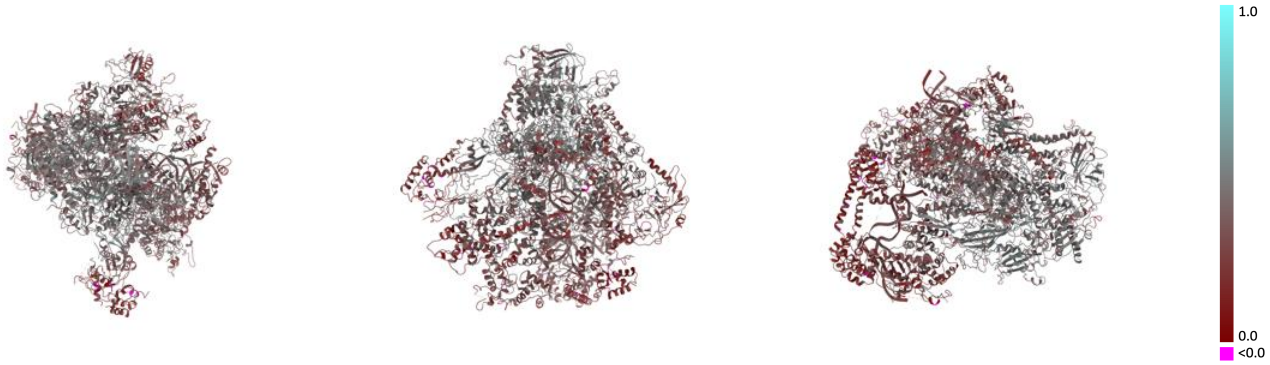
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

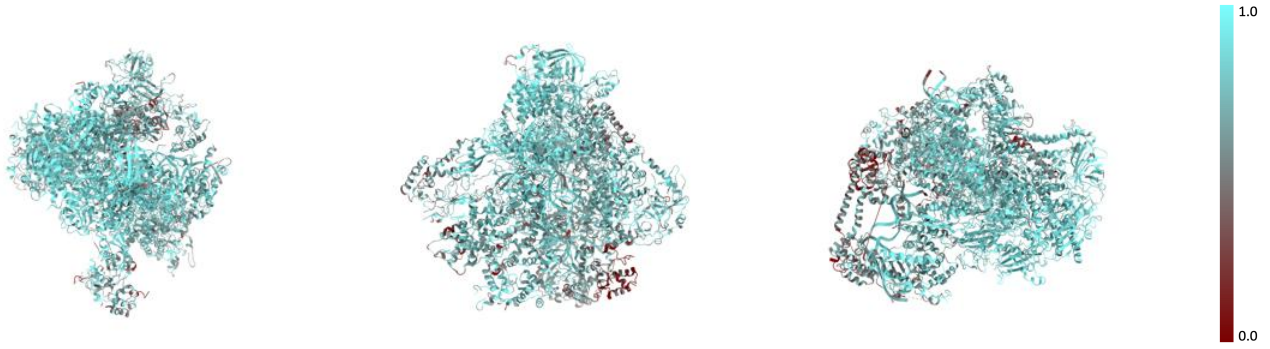
## 9.2 Q-score mapped to coordinate model (i)




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.

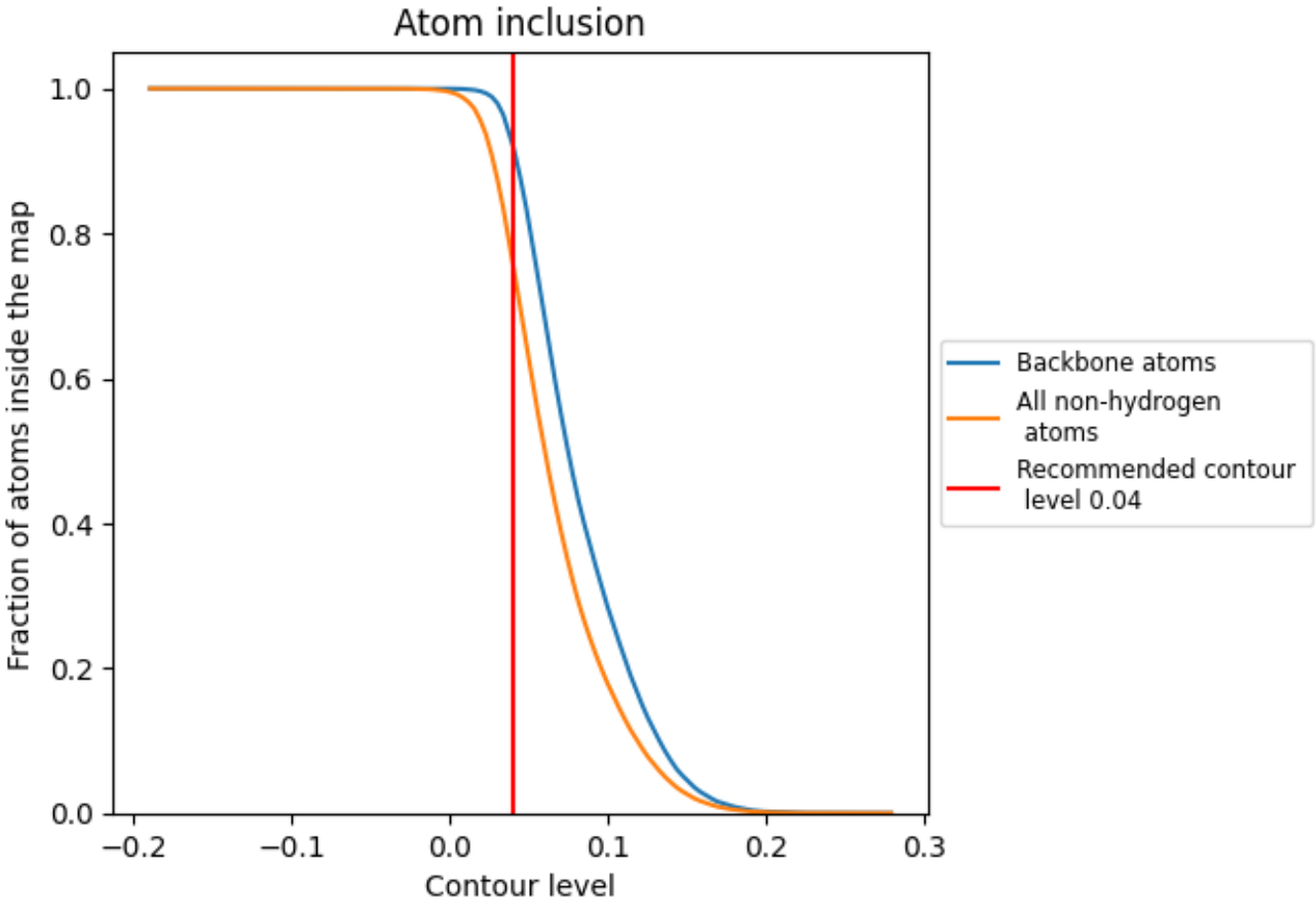
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.04).

## 9.4 Atom inclusion (i)




At the recommended contour level, 92% of all backbone atoms, 75% 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 (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7533 | 0.3610 |
| A | 0.7812 | 0.3990 |
| B | 0.8028 | 0.4160 |
| C | 0.8750 | 0.4350 |
| D | 0.6046 | 0.2130 |
| E | 0.7826 | 0.3590 |
| F | 0.8821 | 0.4480 |
| G | 0.7224 | 0.3000 |
| H | 0.8315 | 0.4340 |
| I | 0.7445 | 0.3340 |
| J | 0.8801 | 0.4440 |
| K | 0.8633 | 0.4420 |
| L | 0.8262 | 0.4250 |
| M | 0.6798 | 0.2940 |
| N | 0.6975 | 0.3070 |
| O | 0.6895 | 0.3110 |
| P | 0.5813 | 0.2640 |
| Q | 0.8603 | 0.3920 |
| R | 0.6507 | 0.2820 |
| S | 0.5480 | 0.2580 |
| X | 0.8846 | 0.3190 |
| Y | 0.8431 | 0.3360 |