# Full wwPDB EM Validation Report

Nov 20, 2022 – 07:28 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 4CR2 |
| EMDB ID | : | EMD-2594 |
| Title | : | Deep classification of a large cryo-EM dataset defines the conformational landscape of the 26S proteasome |
| Authors | : | Unverdorben, P.; Beck, F.; Sledz, P.; Schweitzer, A.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Foerster, F. |
| Deposited on | : | 2014-02-25 |
| Resolution | : | 7.70 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

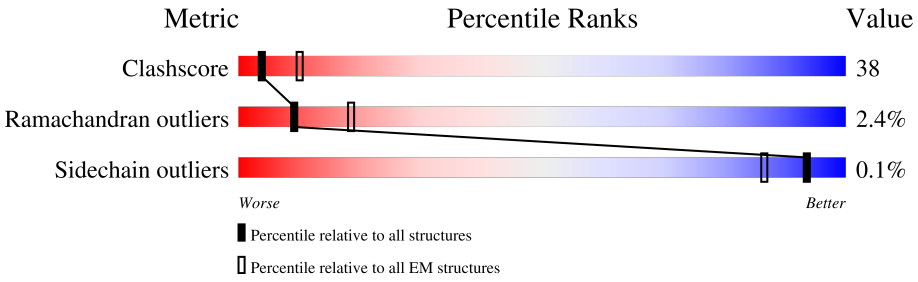
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 7.70 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1 | 215 | 35% 45% 47% · 5% |
| 2 | 2 | 261 | 28% 54% 30% · 15% |
| 3 | 3 | 205 | 37% 55% 41% · |
| 4 | 4 | 198 | 23% 56% 42% · |
| 5 | 5 | 287 | 18% 45% 27% · 26% |
| 6 | 6 | 241 | 27% 58% 33% · 8% |
| 7 | 7 | 266 | 30% 51% 35% · 12% |
| 8 | A | 252 | 35% 54% 39% · · |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | B | 250 | 38% 63% 34% |
| 10 | C | 258 | 32% 52% 41% 5% |
| 11 | D | 254 | 30% 56% 37% 5% |
| 12 | E | 260 | 33% 59% 32% 7% |
| 13 | F | 234 | 30% 50% 45% |
| 14 | G | 288 | 33% 51% 31% 15% |
| 15 | H | 467 | 34% 38% 33% 6% 23% |
| 16 | I | 437 | 31% 49% 29% 17% |
| 17 | J | 405 | 26% 48% 41% 8% |
| 18 | K | 428 | 31% 50% 37% 11% |
| 19 | L | 437 | 29% 46% 34% 17% |
| 20 | M | 434 | 32% 47% 33% 15% |
| 21 | N | 945 | 22% 50% 38% 10% |
| 22 | O | 393 | 26% 55% 41% |
| 23 | P | 445 | 12% 53% 36% 7% |
| 24 | Q | 434 | 17% 57% 40% |
| 25 | R | 429 | 24% 50% 41% 7% |
| 26 | S | 523 | 23% 40% 25% 33% |
| 27 | T | 274 | 18% 48% 47% |
| 28 | U | 338 | 18% 42% 30% 25% |
| 29 | V | 306 | 22% 47% 31% 19% |
| 30 | W | 268 | 32% 36% 34% 26% |
| 31 | X | 156 | 33% 33% 46% 19% |
| 32 | Y | 89 | 13% 8% 79% |
| 33 | Z | 993 | 30% 38% 39% 5% 18% |

# 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 80139 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 PROTEASOME COMPONENT PRE3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1576 | 996 | 261 | 312 | 7 | | |

- Molecule 2 is a protein called PROTEASOME COMPONENT PUP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 2 | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1692 | 1067 | 294 | 324 | 7 | | |

- Molecule 3 is a protein called PROTEASOME COMPONENT PUP3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 3 | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 1010 | 258 | 305 | 8 | | |

- Molecule 4 is a protein called PROTEASOME COMPONENT C11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | 4 | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | |

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 5 | 212 | Total | C | N | O | S | 0 | 0 |
| | | | 1646 | 1045 | 282 | 312 | 7 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 5 | 33 | ARG | LYS | SEE REMARK 999 | UNP P30656 |

- Molecule 6 is a protein called PROTEASOME COMPONENT C5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | 6 | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1757 | 1115 | 303 | 335 | 4 | | |

- Molecule 7 is a protein called PROTEASOME COMPONENT PRE4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 7 | 233 | Total | C | N | O | S | 0 | 0 |
| | | | 1824 | 1154 | 312 | 351 | 7 | | |

- Molecule 8 is a protein called PROTEASOME COMPONENT C7-ALPHA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | A | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | |

- Molecule 9 is a protein called PROTEASOME COMPONENT Y7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | B | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | |

- Molecule 10 is a protein called PROTEASOME COMPONENT Y13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | C | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 1913 | 1207 | 323 | 380 | 3 | | |

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | D | 242 | Total | C | N | O | S | 0 | 0 |
| | | | 1899 | 1186 | 333 | 376 | 4 | | |

- Molecule 12 is a protein called PROTEASOME COMPONENT PUP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | E | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1867 | 1165 | 315 | 380 | 7 | | |

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | F | 233 | Total | C | N | O | S | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | |

- Molecule 14 is a protein called PROTEASOME COMPONENT C1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | G | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 1900 | 1207 | 331 | 358 | 4 | | |

- Molecule 15 is a protein called 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | H | 359 | Total | C | N | O | S | 0 | 0 |
| | | | 2792 | 1755 | 499 | 523 | 15 | | |

- Molecule 16 is a protein called 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | I | 362 | Total | C | N | O | S | 0 | 0 |
| | | | 2822 | 1773 | 471 | 563 | 15 | | |

- Molecule 17 is a protein called 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | J | 373 | Total | C | N | O | S | 0 | 0 |
| | | | 2928 | 1837 | 527 | 547 | 17 | | |

- Molecule 18 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | K | 381 | Total | C | N | O | S | 0 | 0 |
| | | | 3019 | 1898 | 530 | 581 | 10 | | |

- Molecule 19 is a protein called 26S PROTEASE SUBUNIT RPT4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | L | 361 | Total | C | N | O | S | 0 | 0 |
| | | | 2853 | 1798 | 507 | 536 | 12 | | |

- Molecule 20 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | M | 367 | Total | C | N | O | S | 0 | 0 |
| | | | 2866 | 1799 | 503 | 553 | 11 | | |

- Molecule 21 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | N | 849 | Total | C | N | O | S | 0 | 0 |
| | | | 6562 | 4174 | 1099 | 1261 | 28 | | |

- Molecule 22 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | O | 387 | Total | C | N | O | S | 0 | 0 |
| | | | 3182 | 2047 | 520 | 606 | 9 | | |

- Molecule 23 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | P | 415 | Total | C | N | O | S | 0 | 0 |
| | | | 3401 | 2166 | 571 | 655 | 9 | | |

- Molecule 24 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | Q | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3471 | 2205 | 574 | 676 | 16 | | |

- Molecule 25 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | R | 400 | Total | C | N | O | S | 0 | 0 |
| | | | 3218 | 2051 | 527 | 630 | 10 | | |

- Molecule 26 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | S | 353 | Total | C | N | O | S | 0 | 0 |
| | | | 2893 | 1857 | 482 | 541 | 13 | | |

- Molecule 27 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | T | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2235 | 1432 | 355 | 441 | 7 | | |

- Molecule 28 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | U | 255 | Total | C | N | O | S | 0 | 0 |
| | | | 2061 | 1312 | 352 | 391 | 6 | | |

- Molecule 29 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | V | 247 | Total | C | N | O | S | 0 | 0 |
| | | | 1942 | 1225 | 328 | 376 | 13 | | |

- Molecule 30 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | W | 197 | Total | C | N | O | S | 0 | 0 |
| | | | 1534 | 962 | 269 | 300 | 3 | | |

- Molecule 31 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | X | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 664 | 169 | 195 | 4 | | |

- Molecule 32 is a protein called 26S PROTEASOME COMPLEX SUBUNIT SEM1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 32 | Y | 19 | Total | C | N | O | 0 | 0 |
| | | | 168 | 101 | 30 | 37 | | |

- Molecule 33 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN1.

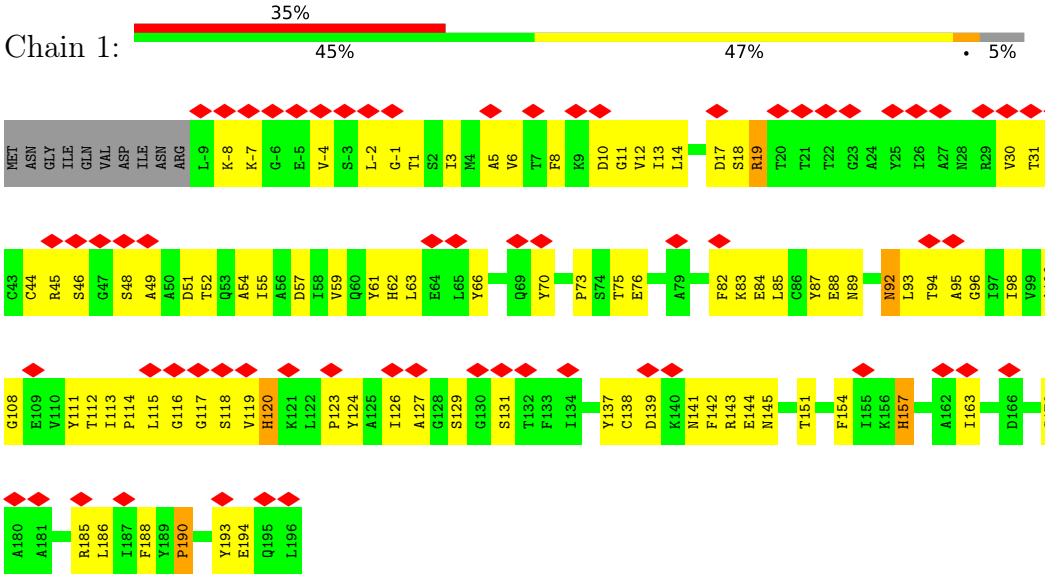
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | Z | 813 | Total | C | N | O | S | 0 | 0 |
| | | | 6289 | 3995 | 1029 | 1236 | 29 | | |

# 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.

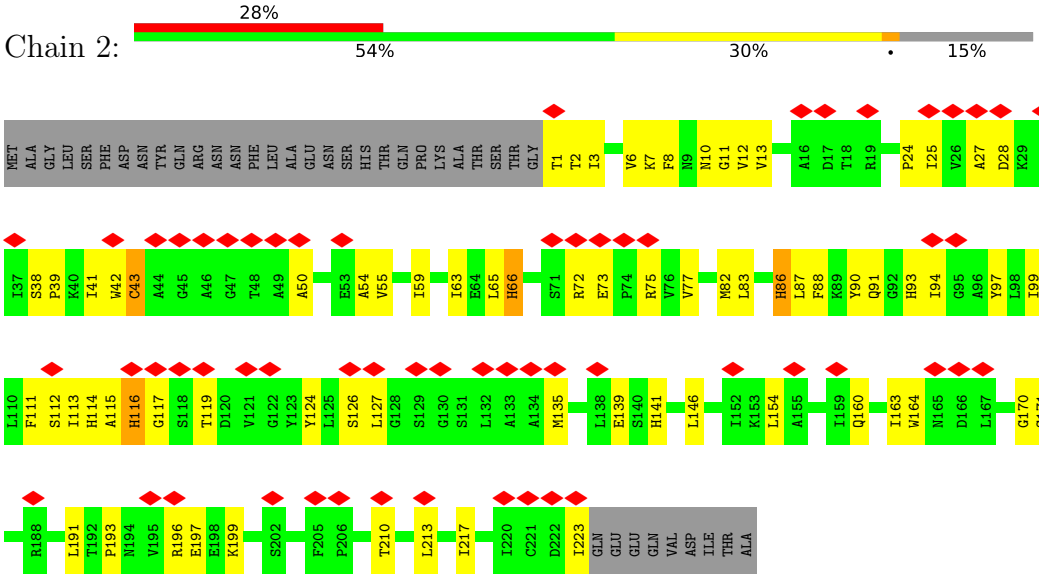
• Molecule 1: PROTEASOME COMPONENT PRE3

Chain 1:



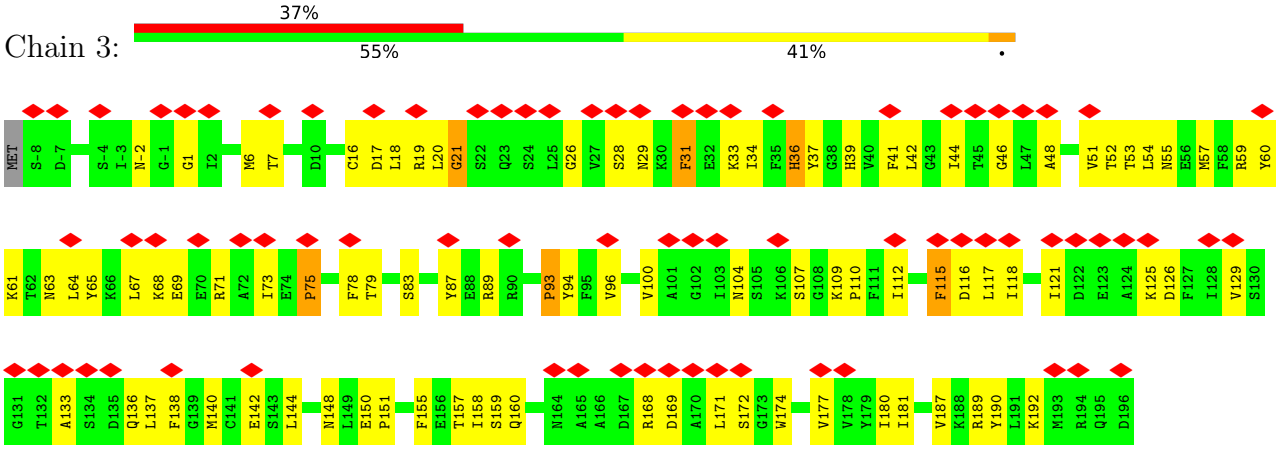

• Molecule 2: PROTEASOME COMPONENT PUP1

Chain 2:



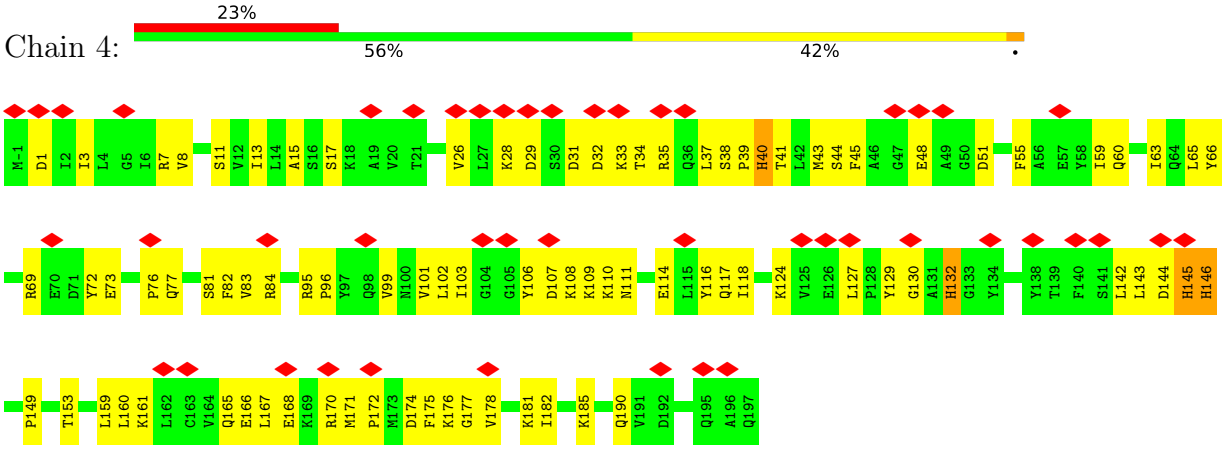

• Molecule 3: PROTEASOME COMPONENT PUP3

Chain 3:



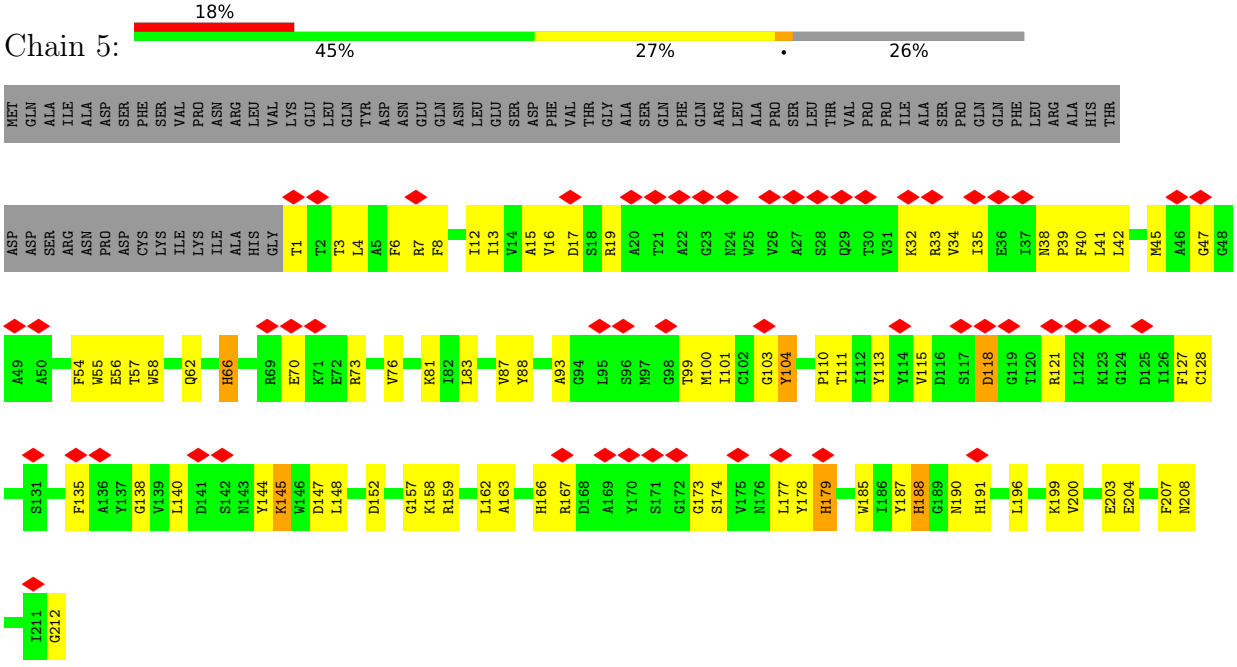

• Molecule 4: PROTEASOME COMPONENT C11

Chain 4:



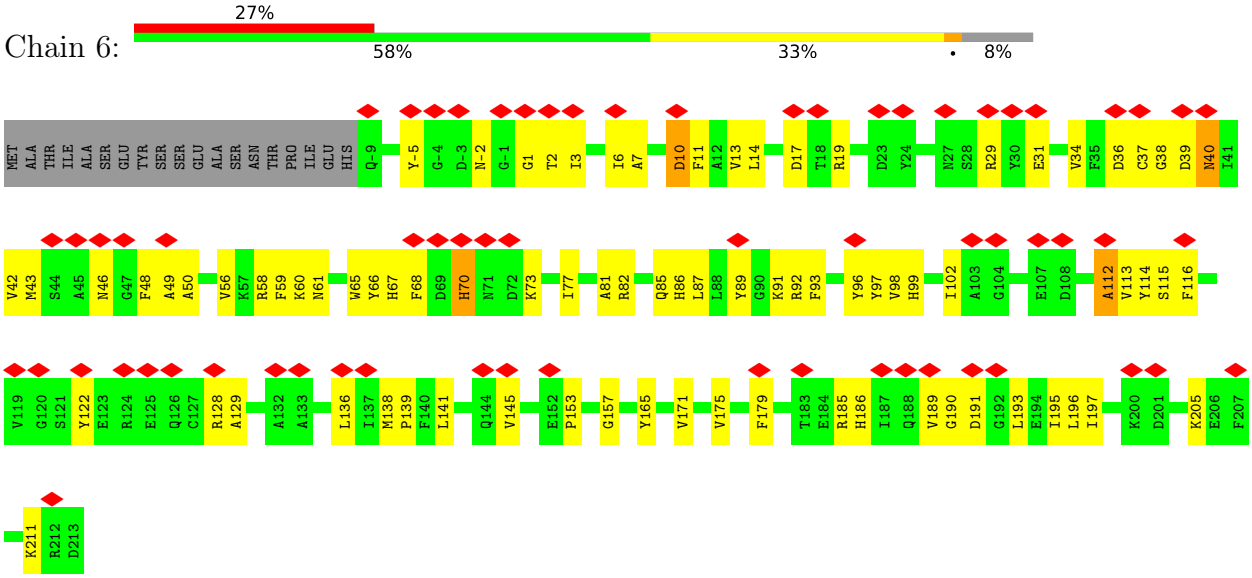

• Molecule 5: PROTEASOME COMPONENT PRE2

Chain 5:



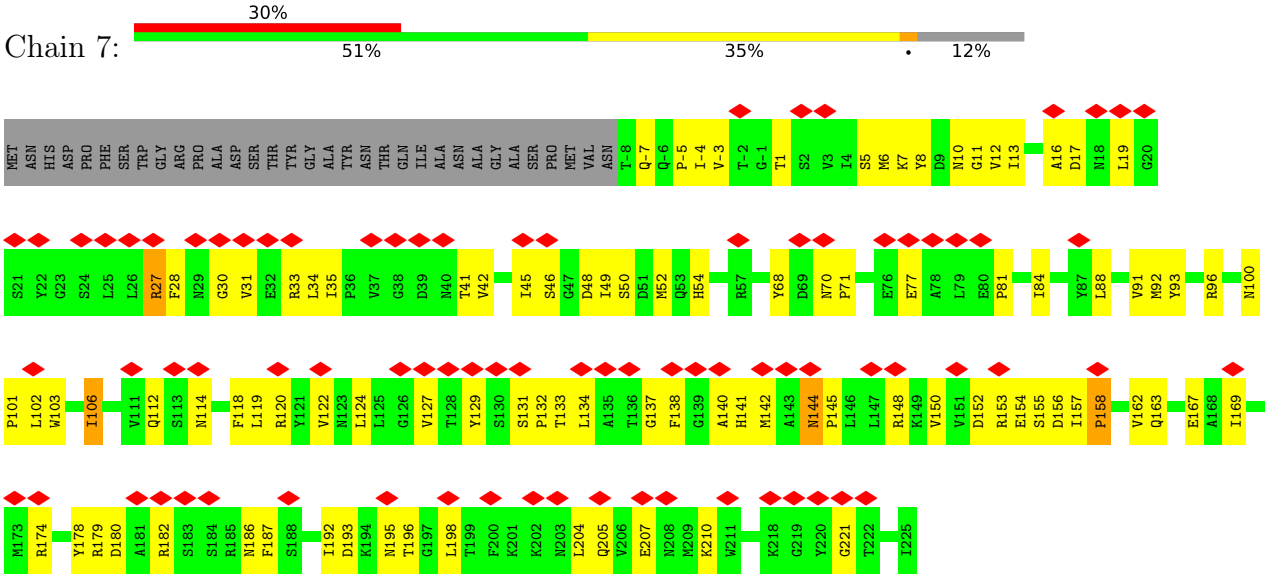

• Molecule 6: PROTEASOME COMPONENT C5

Chain 6:



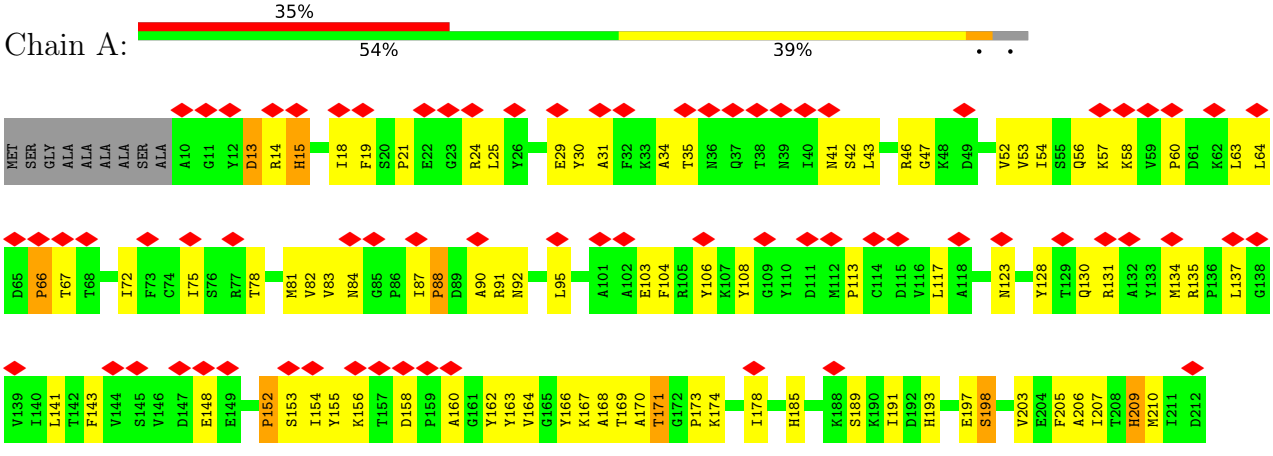

• Molecule 7: PROTEASOME COMPONENT PRE4

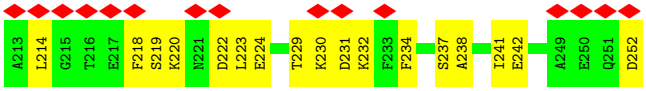
Chain 7:




• Molecule 8: PROTEASOME COMPONENT C7-ALPHA

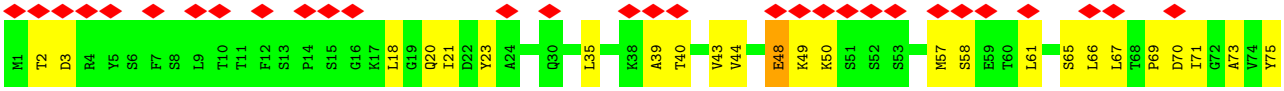
Chain A:

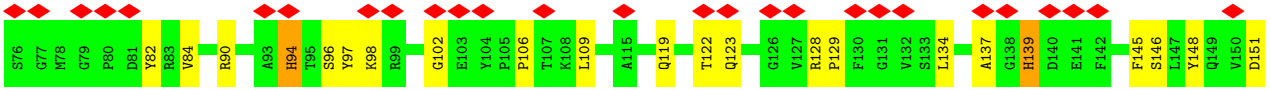


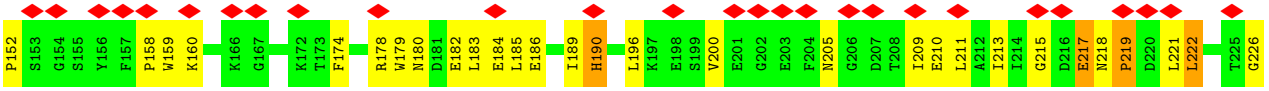


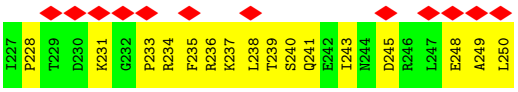

• Molecule 9: PROTEASOME COMPONENT Y7

Chain B:

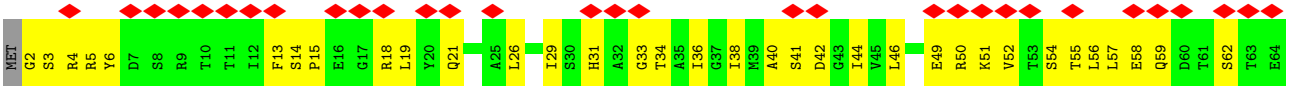



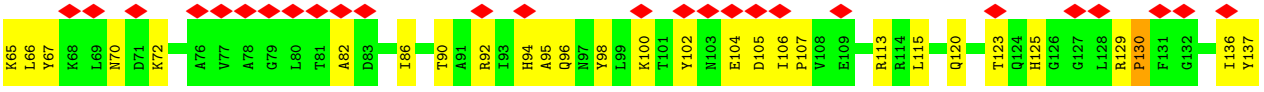



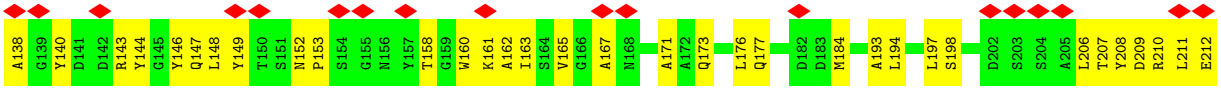



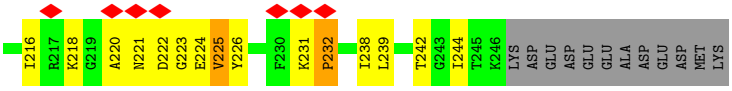

• Molecule 10: PROTEASOME COMPONENT Y13

Chain C:

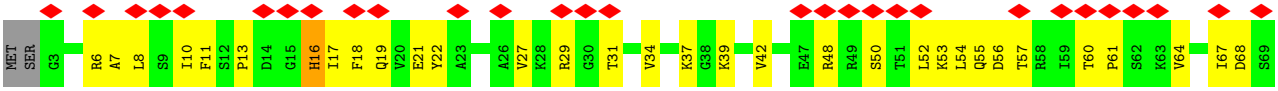



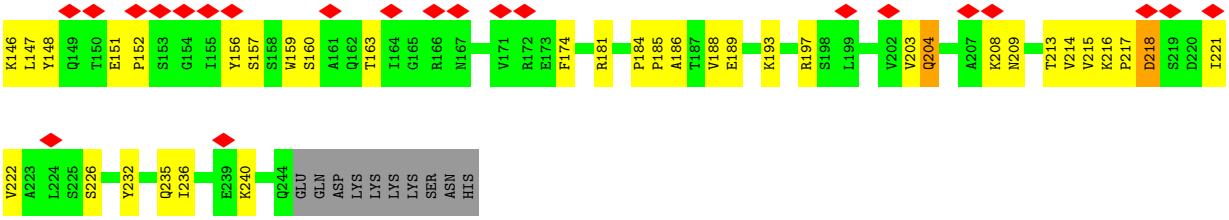



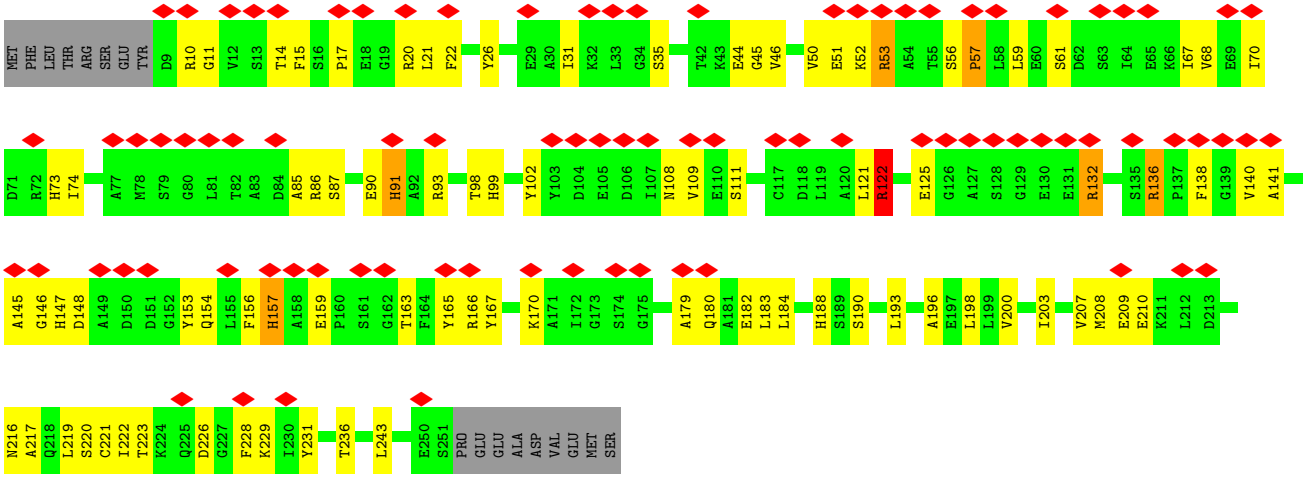

• Molecule 11: PROTEASOME COMPONENT PRE6

Chain D:

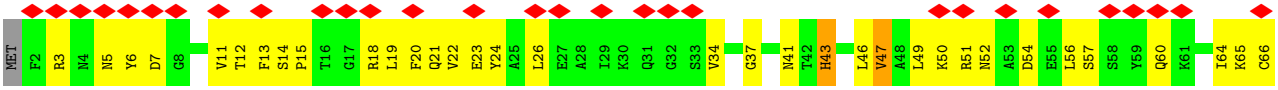



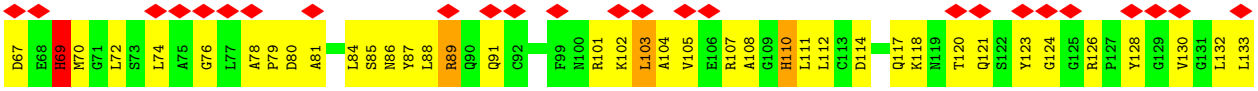



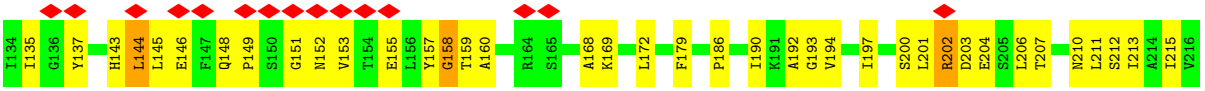

• Molecule 12: PROTEASOME COMPONENT PUP2

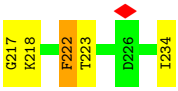




• Molecule 13: PROTEASOME COMPONENT PRE5

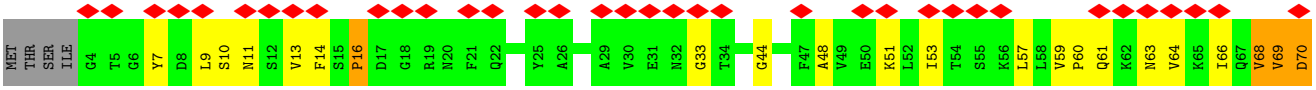



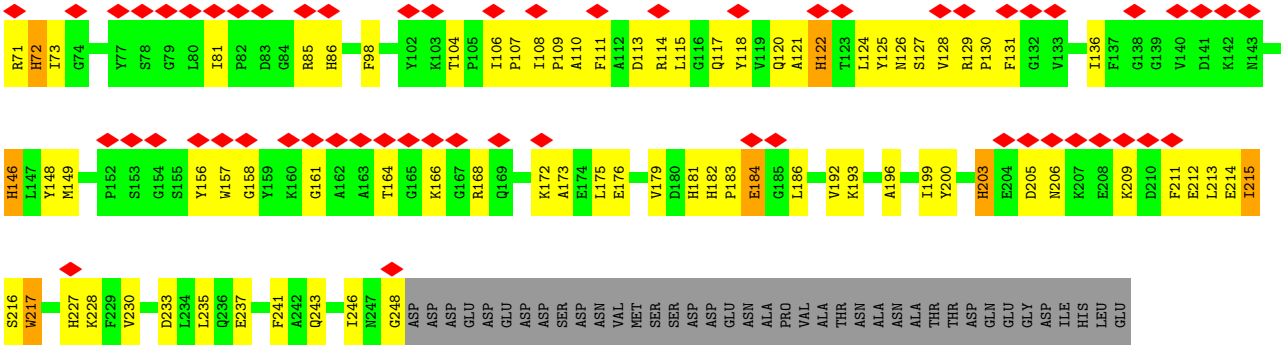



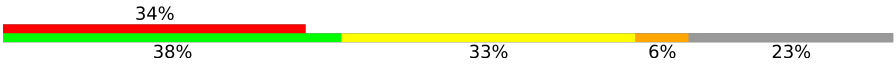

• Molecule 14: PROTEASOME COMPONENT C1

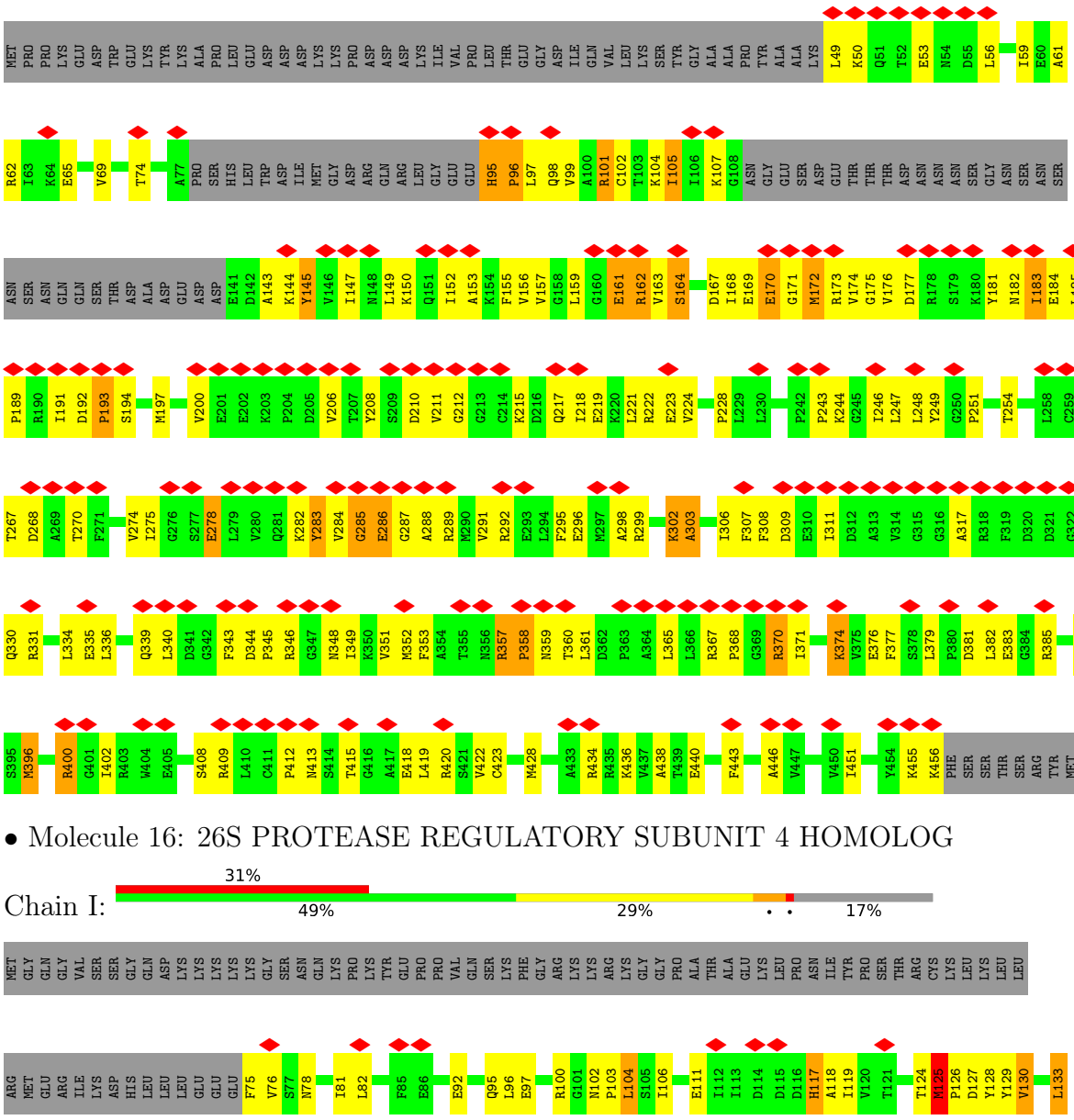





• Molecule 15: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG

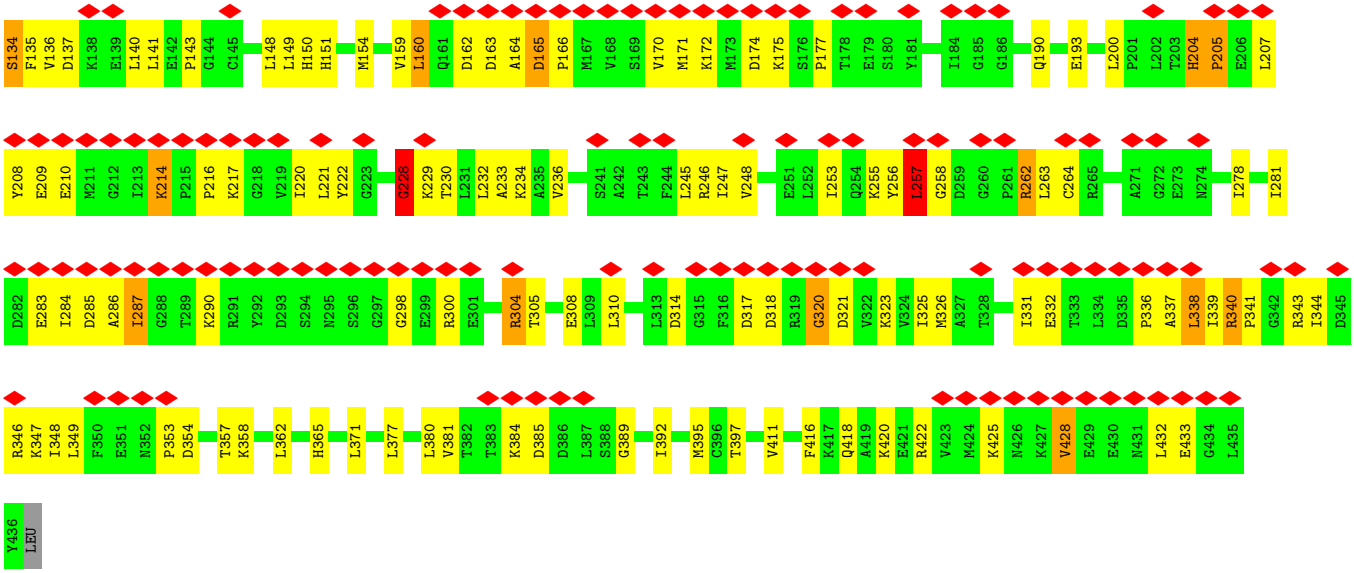
Chain H:



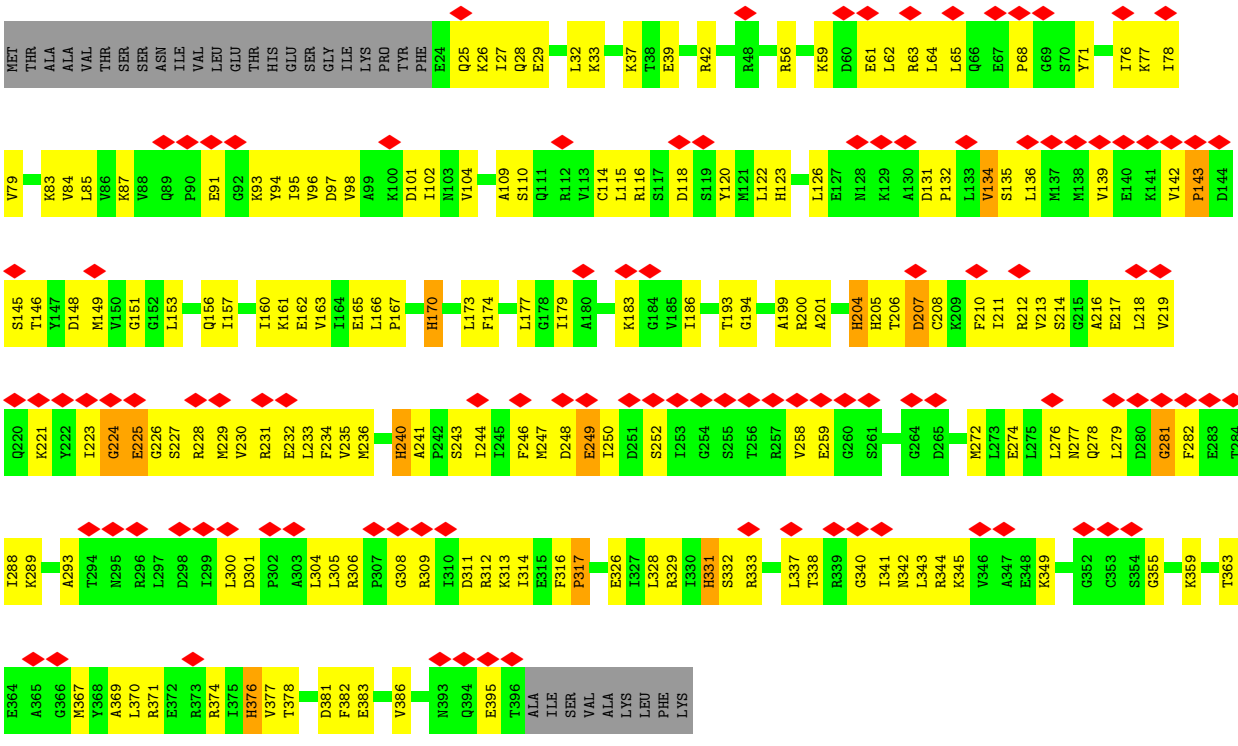
• Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

Chain I:



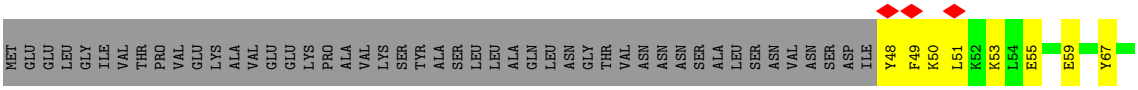
• Molecule 17: 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG

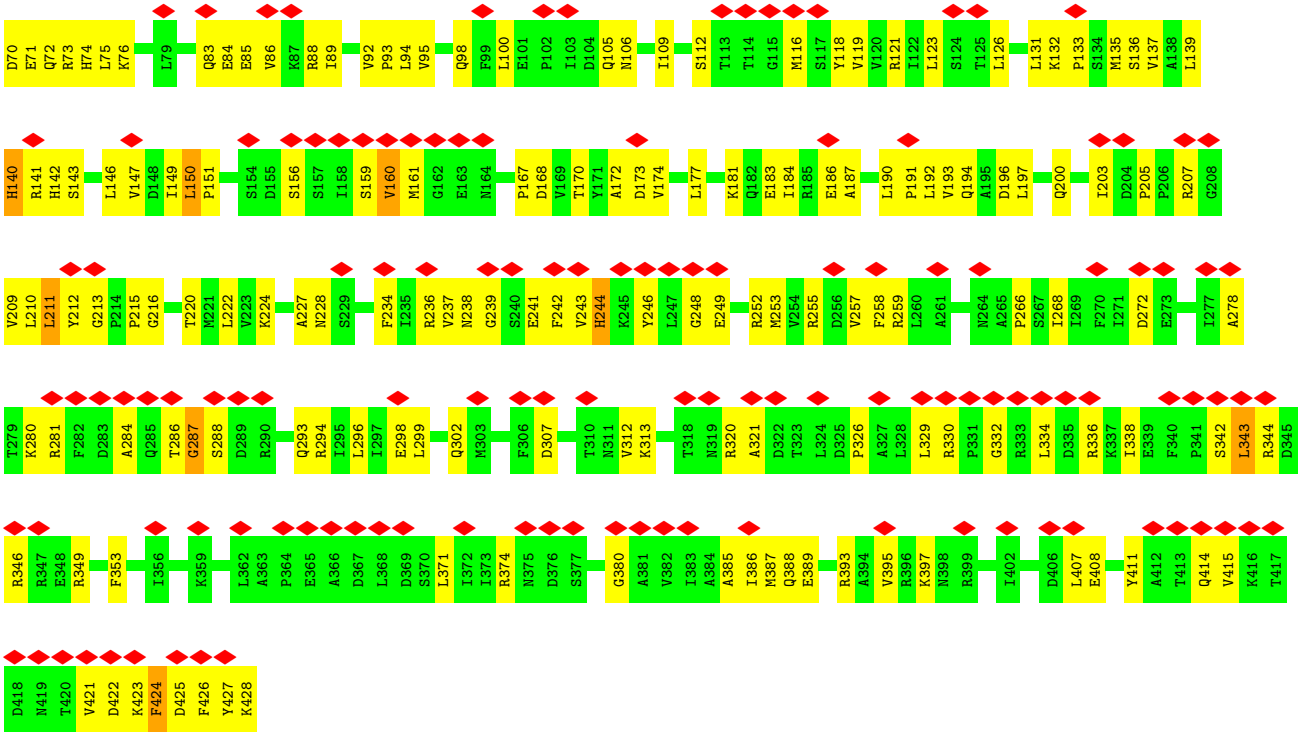
Chain J:

• Molecule 18: 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG

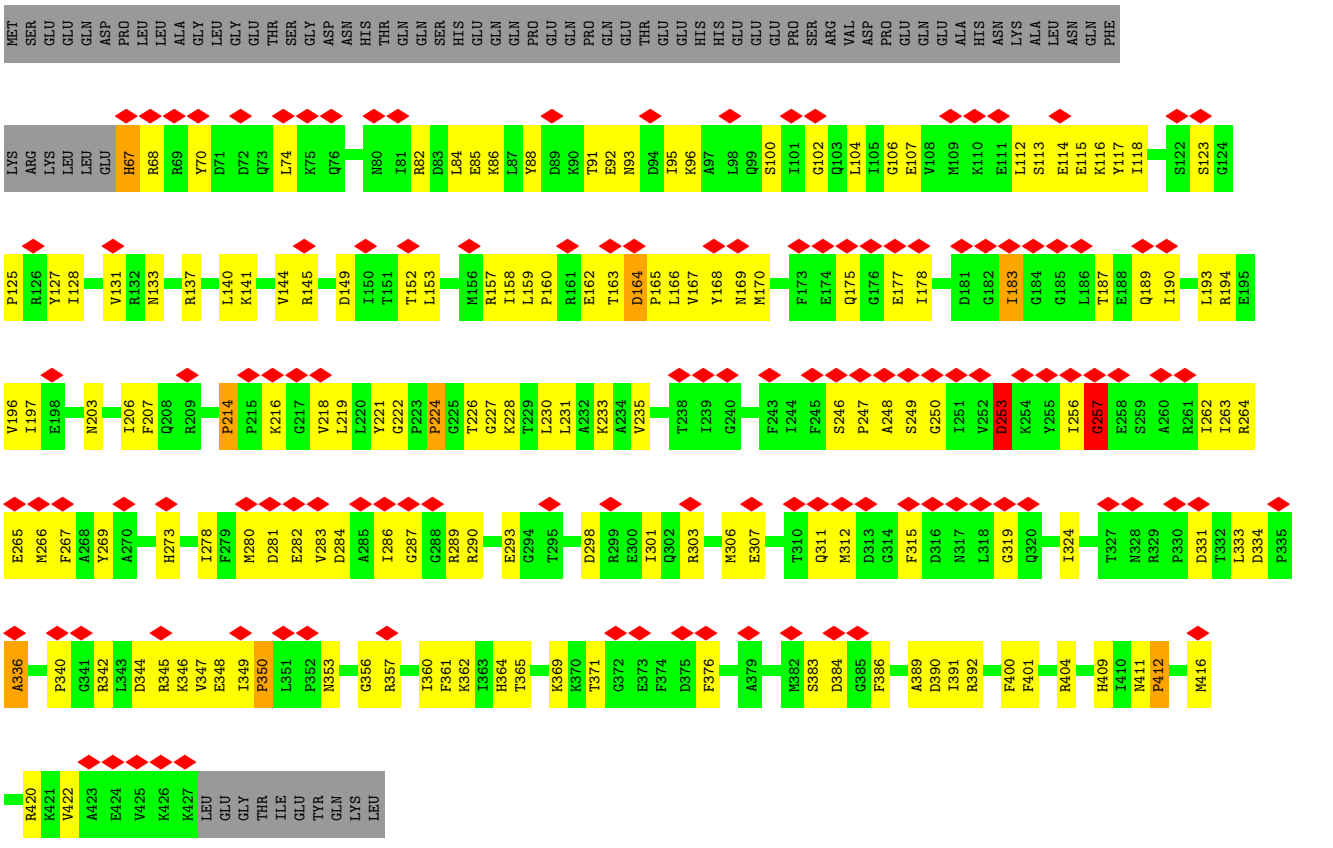
Chain K:



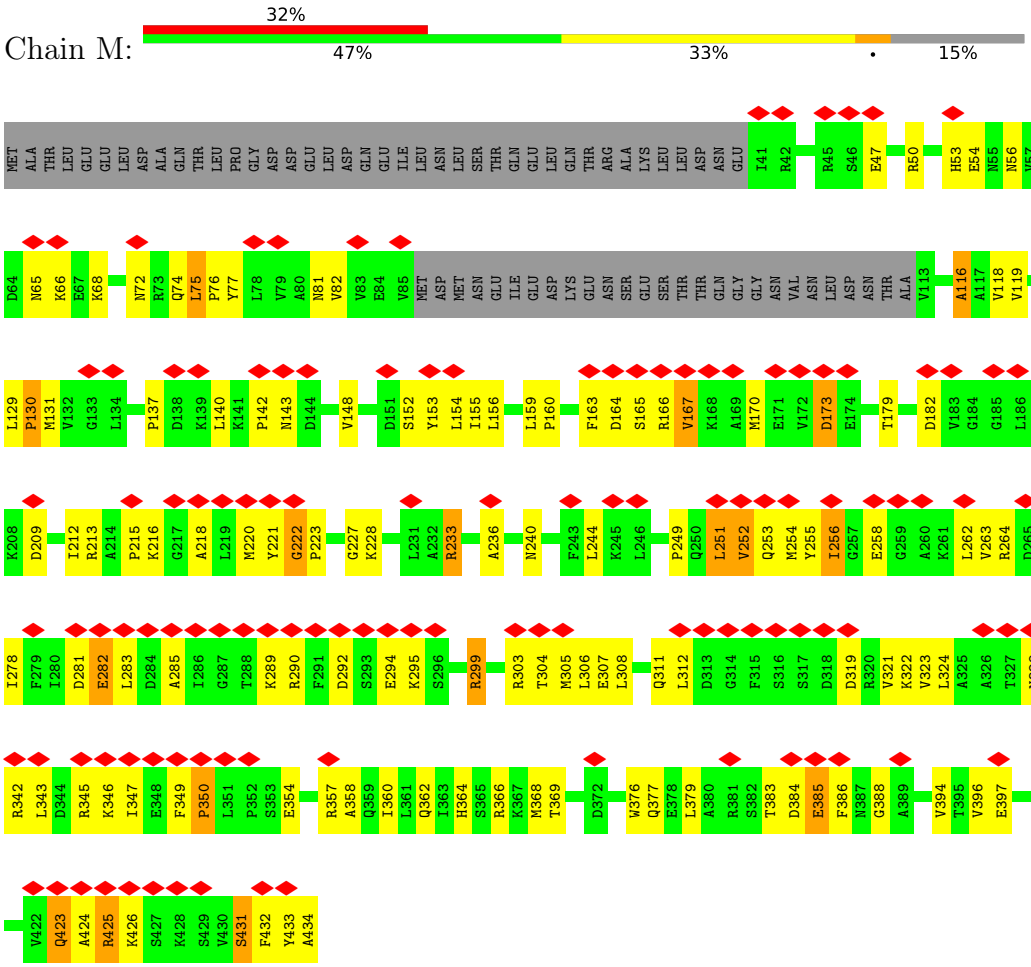
• Molecule 19: 26S PROTEASE SUBUNIT RPT4

Chain L:

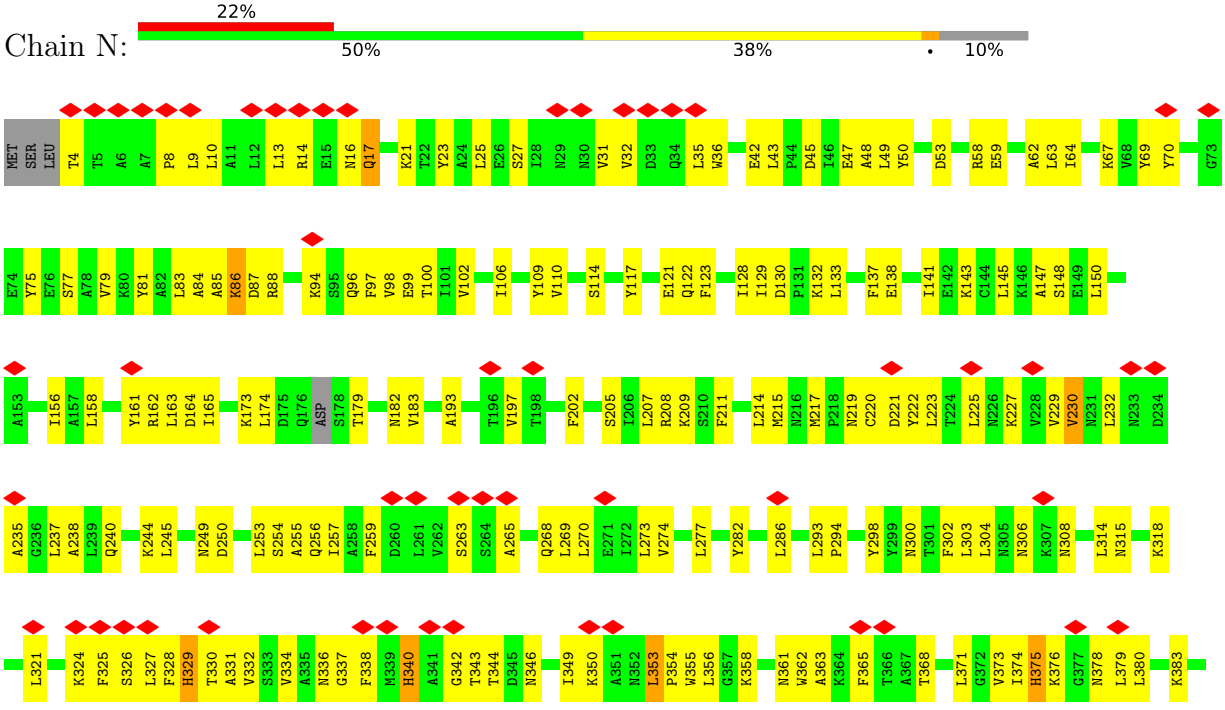
• Molecule 20: 26S PROTEASE REGULATORY SUBUNIT 6A

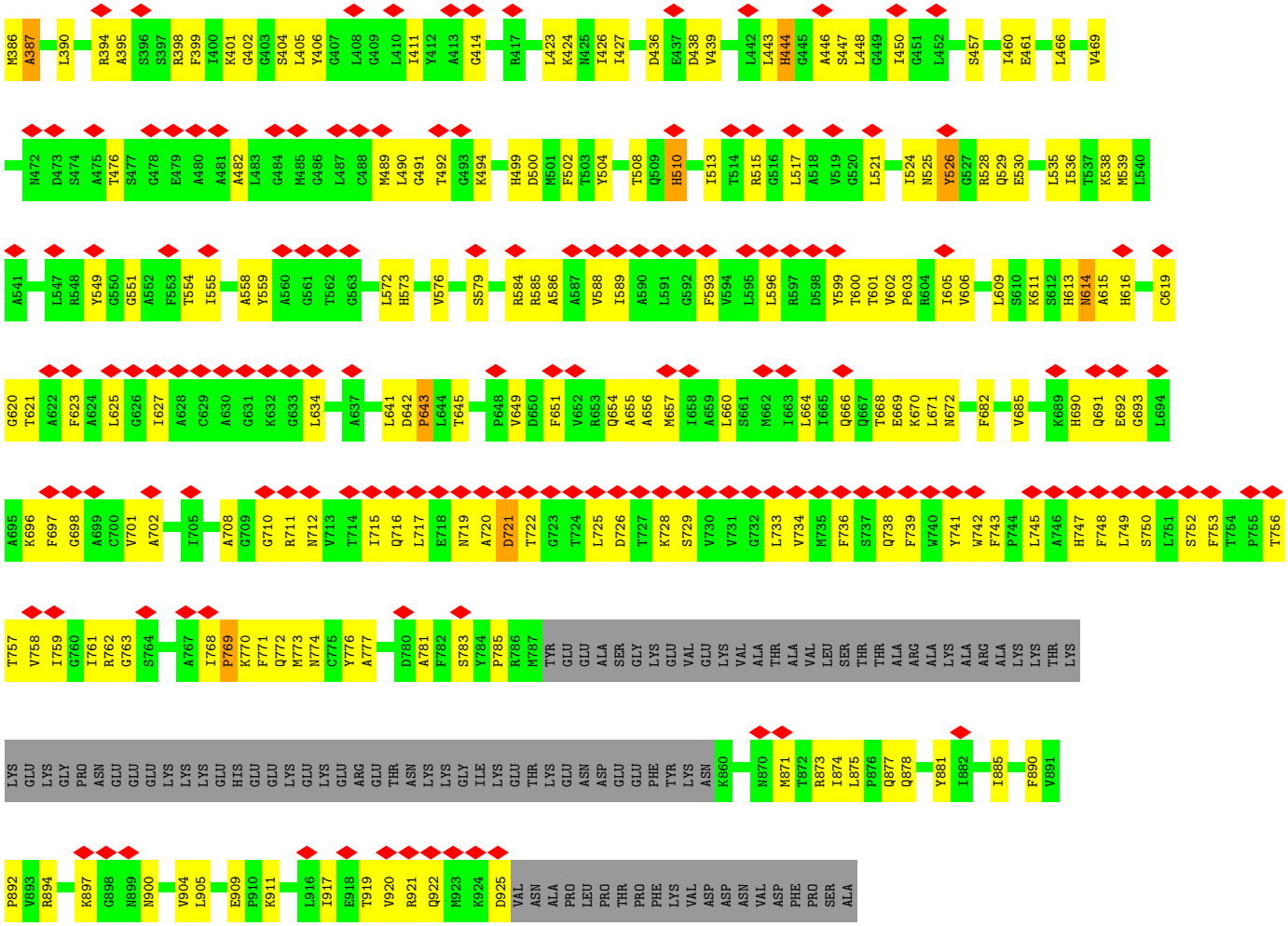
Chain M:




• Molecule 21: 26S PROTEASOME REGULATORY SUBUNIT RPN2

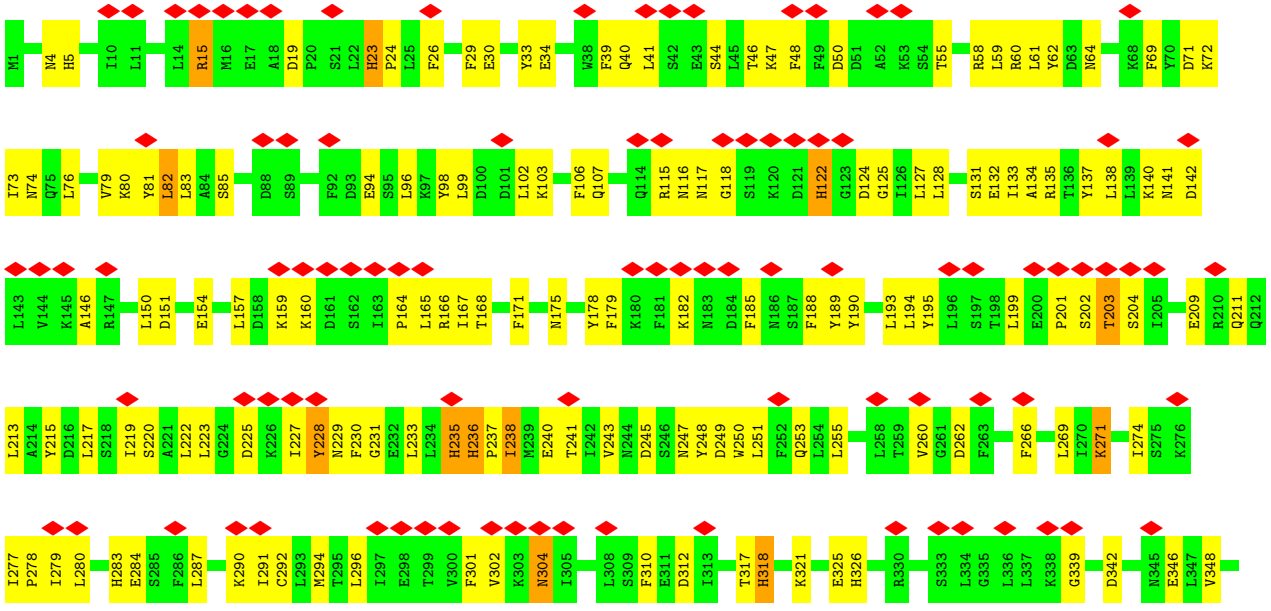
Chain N:

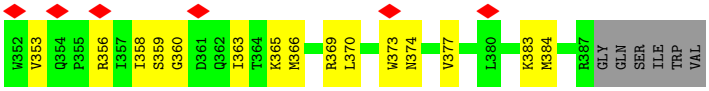




• Molecule 22: 26S PROTEASOME REGULATORY SUBUNIT RPN9

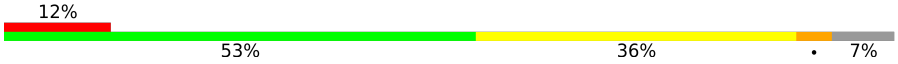
Chain O:

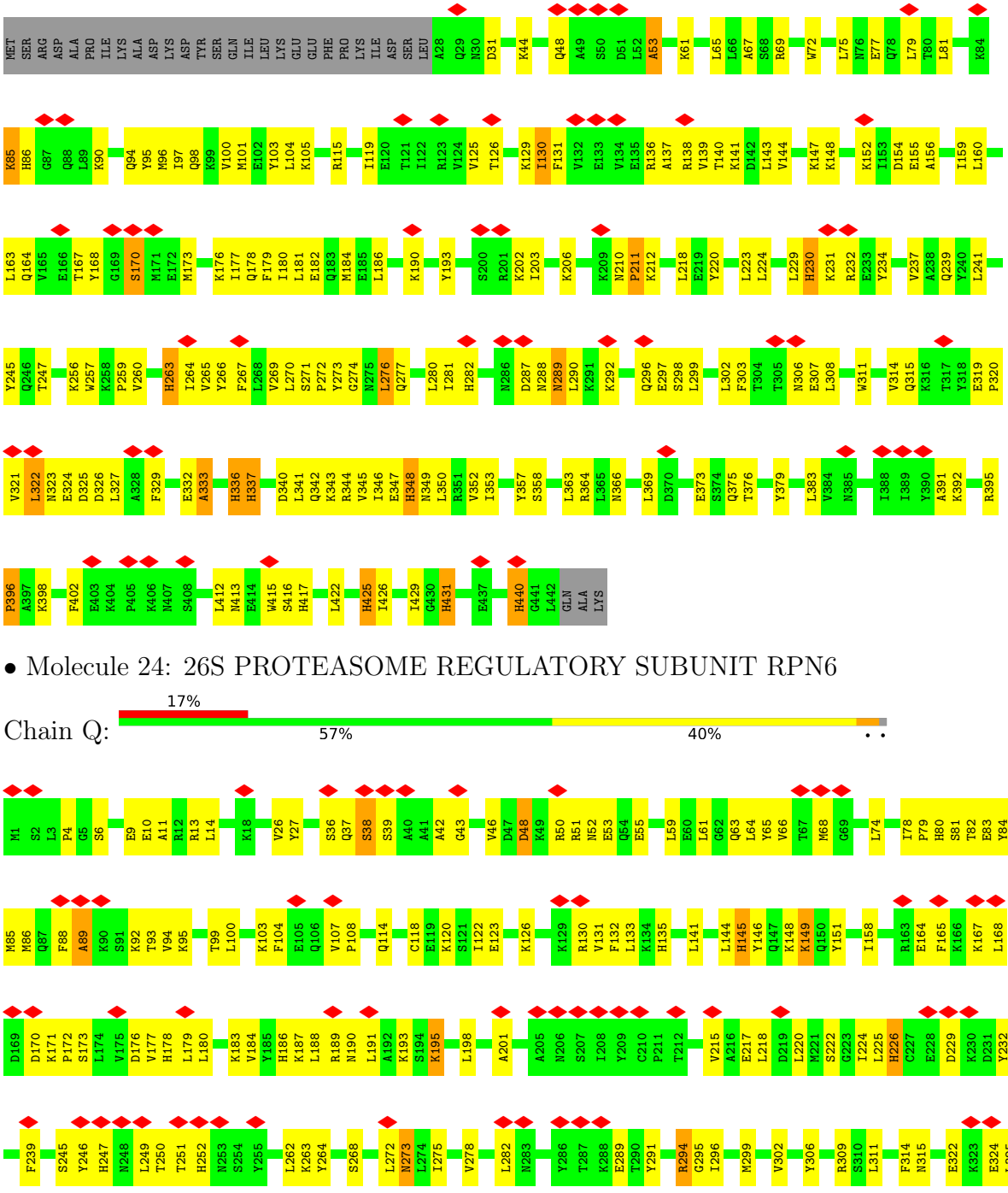





• Molecule 23: 26S PROTEASOME REGULATORY SUBUNIT RPN5

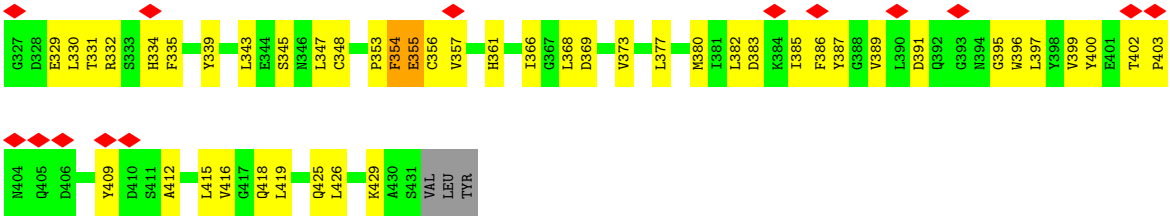
Chain P:



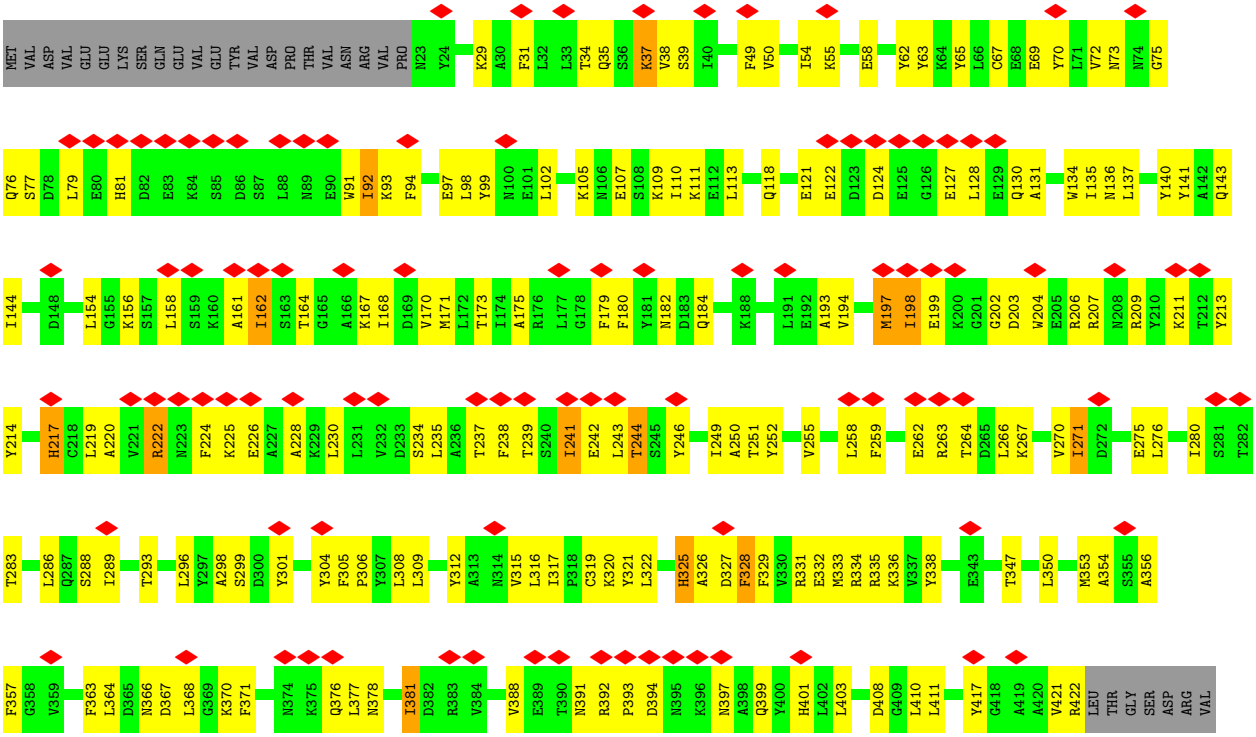
• Molecule 24: 26S PROTEASOME REGULATORY SUBUNIT RPN6

Chain Q:



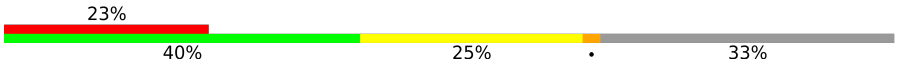
• Molecule 25: 26S PROTEASOME REGULATORY SUBUNIT RPN7

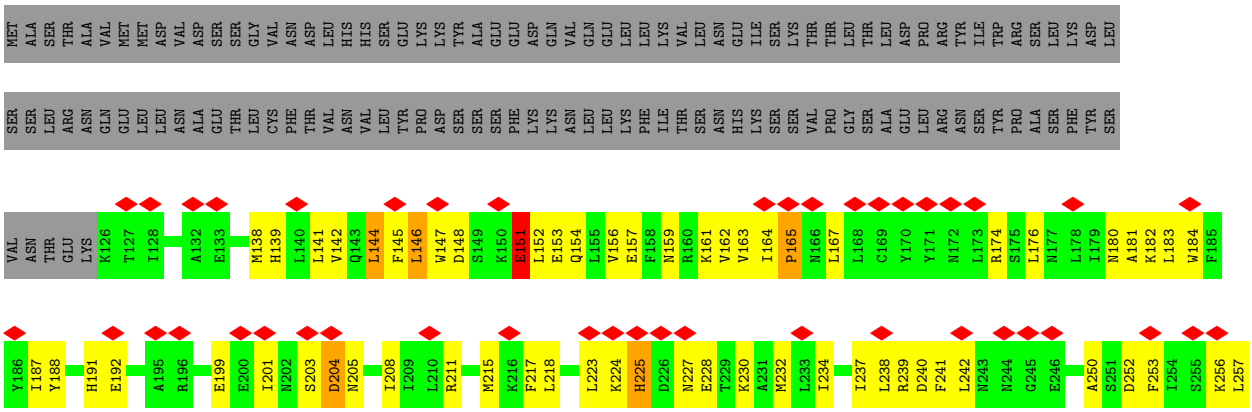
Chain R:

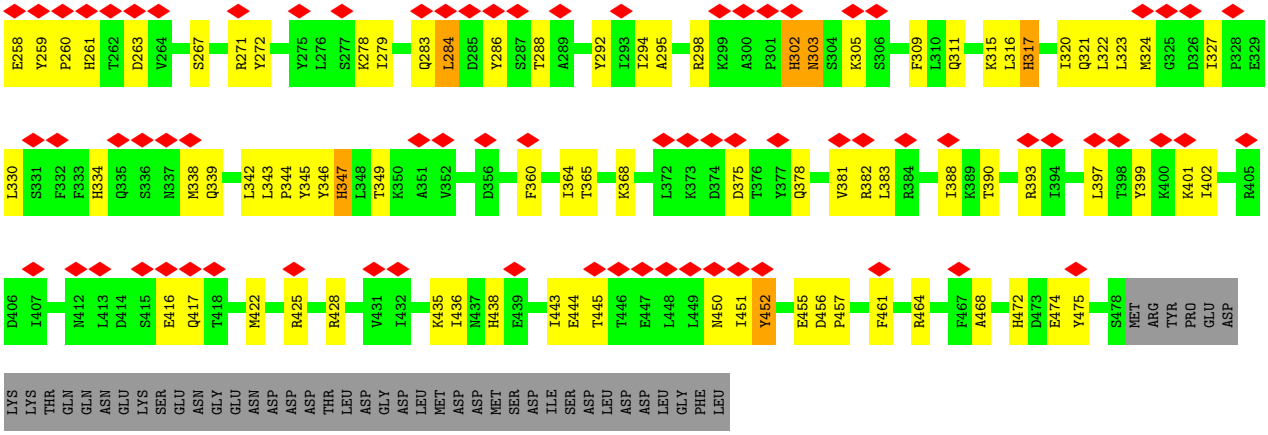



• Molecule 26: 26S PROTEASOME REGULATORY SUBUNIT RPN3

Chain S:

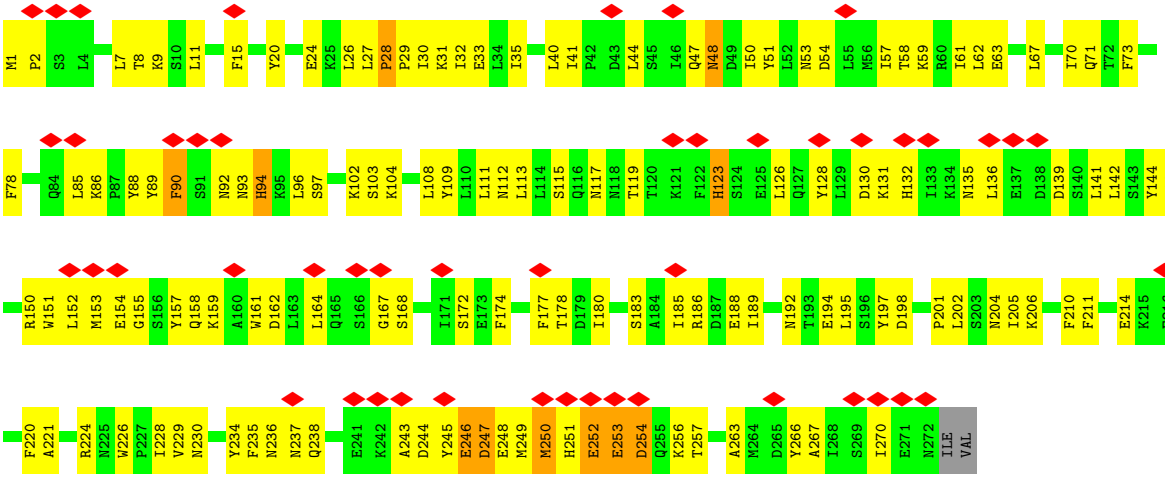




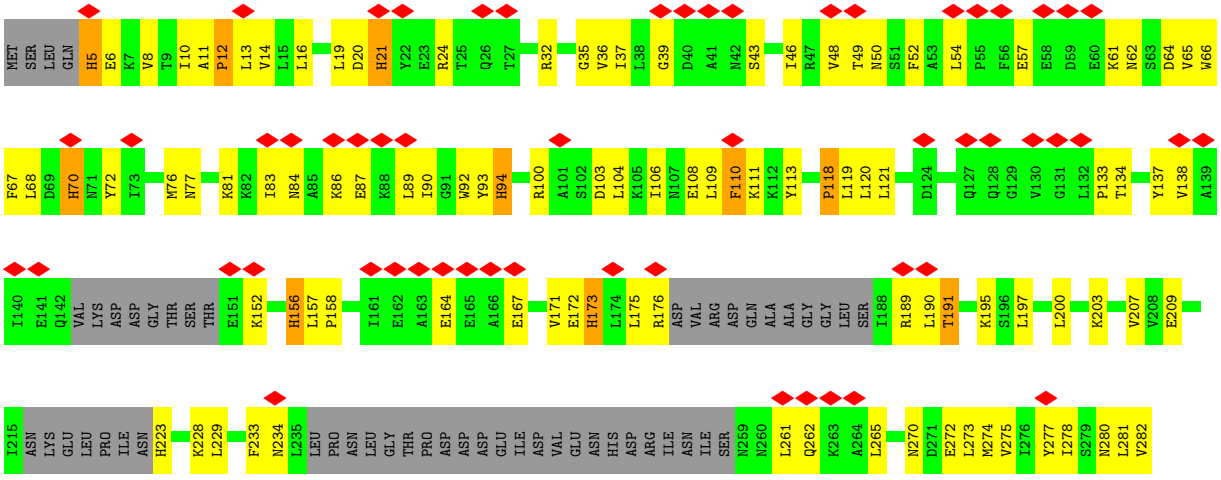
• Molecule 27: 26S PROTEASOME REGULATORY SUBUNIT RPN12

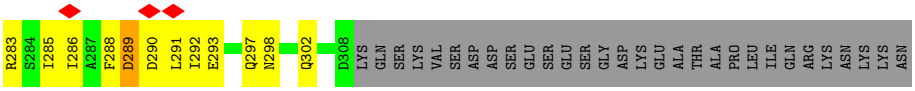
Chain T:

• Molecule 28: 26S PROTEASOME REGULATORY SUBUNIT RPN8

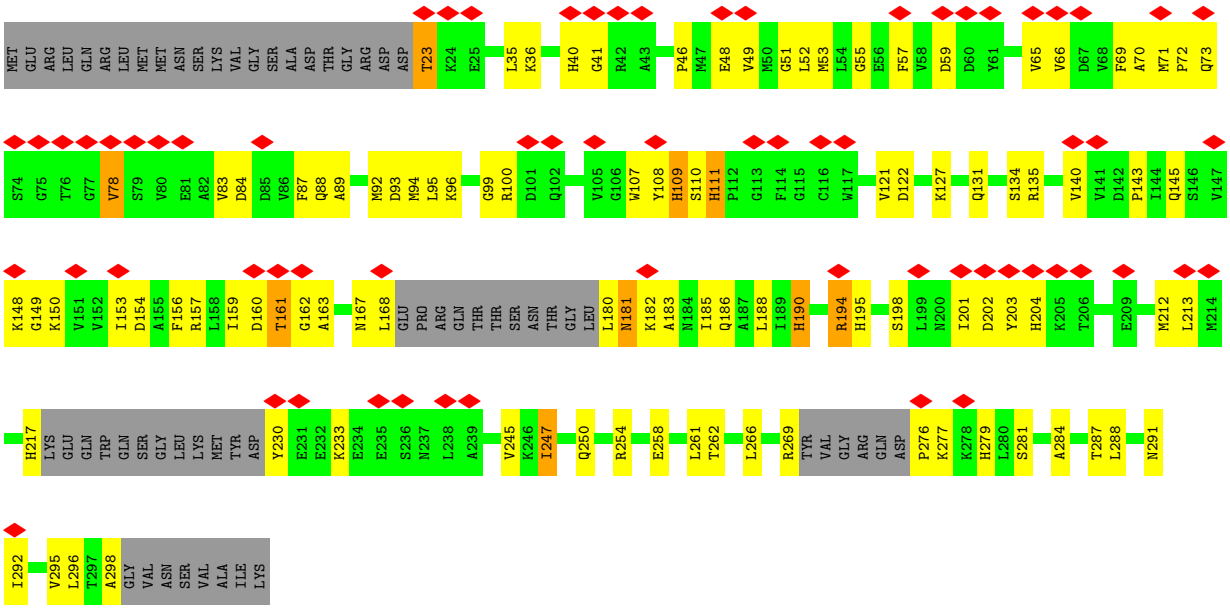
Chain U:



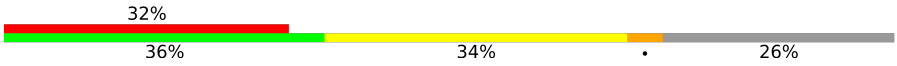

• Molecule 29: 26S PROTEASOME REGULATORY SUBUNIT RPN11

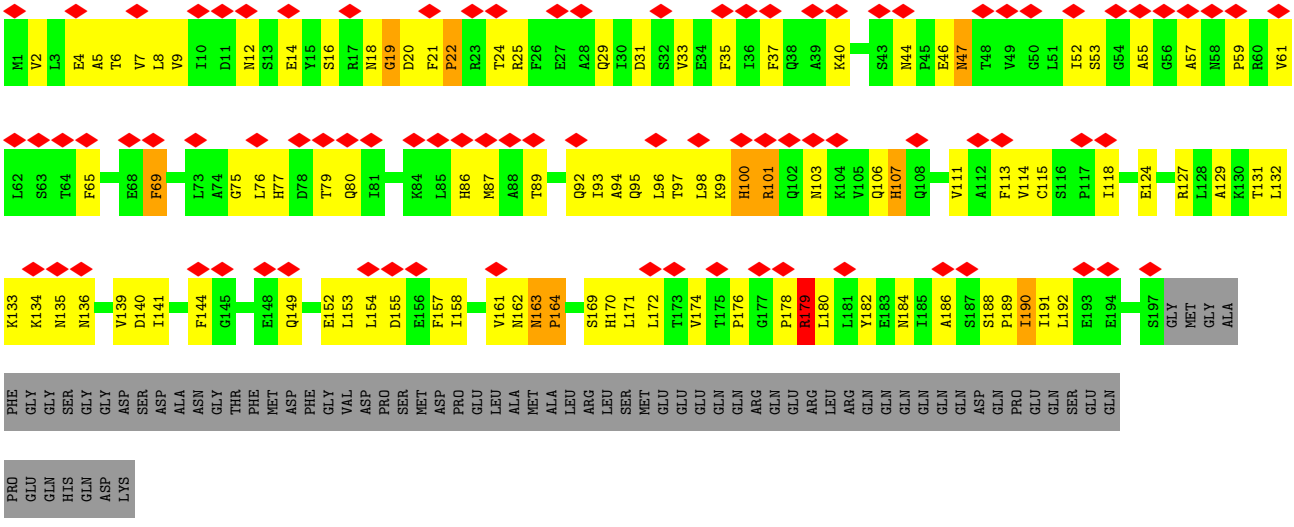
Chain V:


• Molecule 30: 26S PROTEASOME REGULATORY SUBUNIT RPN10

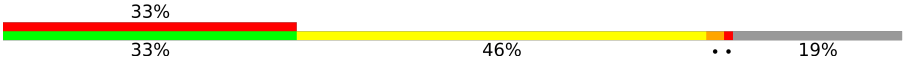
Chain W:

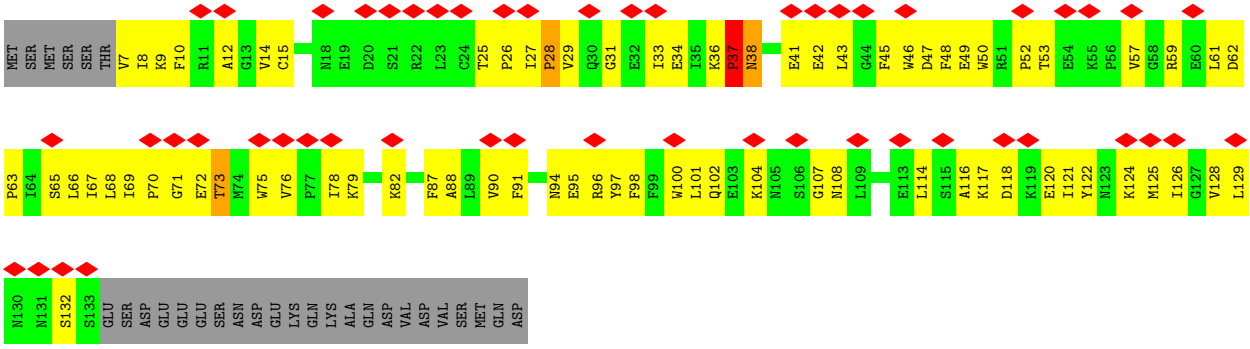



• Molecule 31: 26S PROTEASOME REGULATORY SUBUNIT RPN13

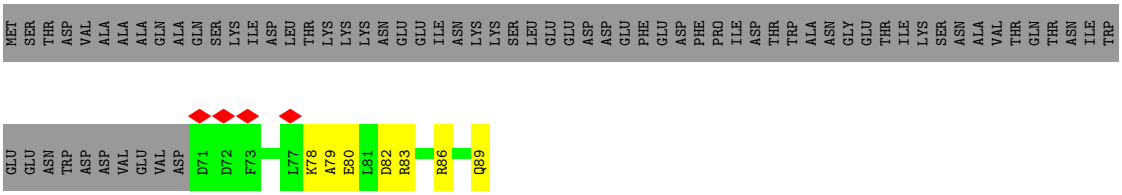
Chain X:





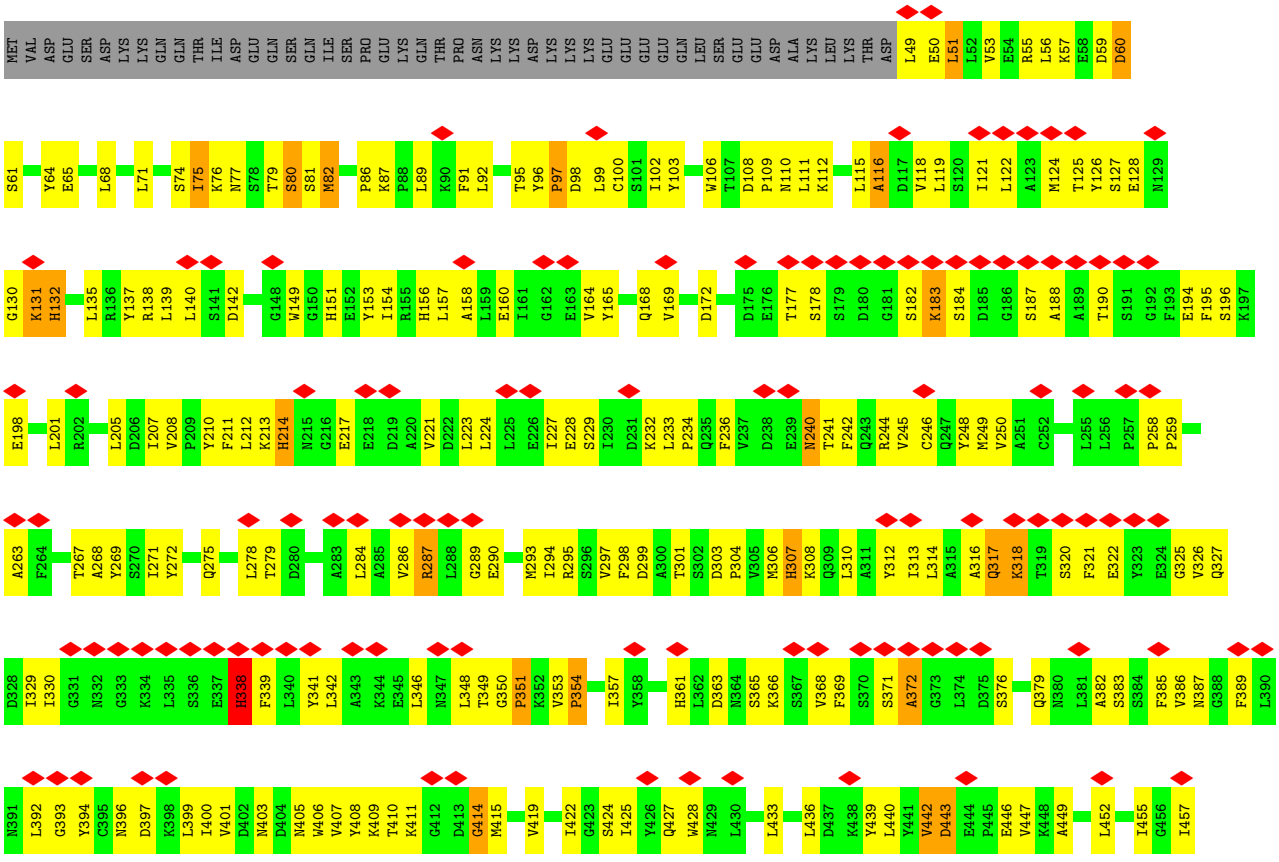
• Molecule 32: 26S PROTEASOME COMPLEX SUBUNIT SEM1

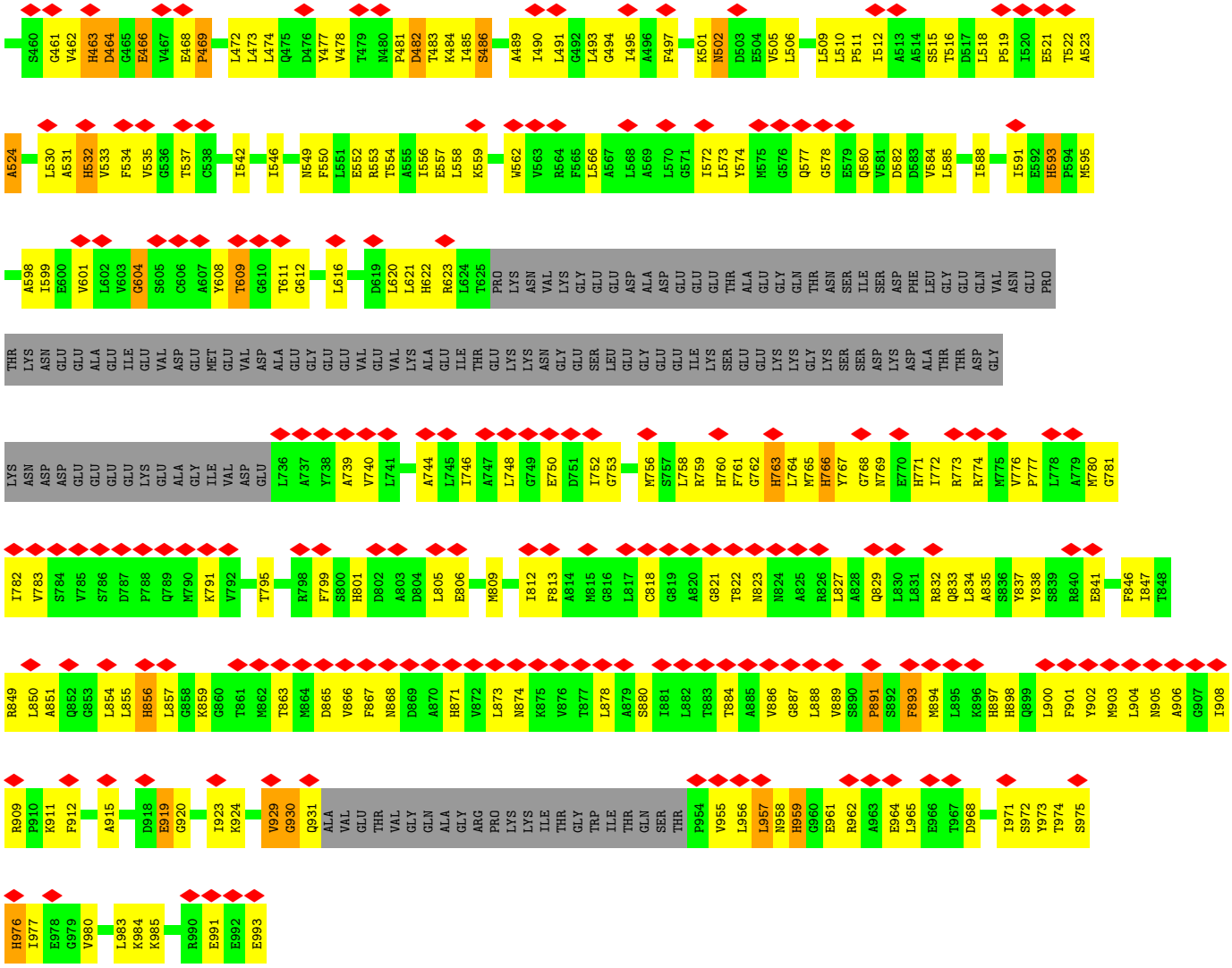
Chain Y:

• Molecule 33: 26S PROTEASOME REGULATORY SUBUNIT RPN1

Chain Z:


S460 G461 V462 H463 D464 G465 E466 V467 E468 P469 L472 L473 L474 Q475 D476 Y477 V478 T479 N480 P481 D482 T483 K484 I485 S486 A489 I490 L491 G492 L493 G494 I495 A496 F497 K501 N502 D503 E504 V505 L506 L509 L510 P511 I512 A513 A514 S515 T516 D517 L518 P519 I520 E521 T522 A523
A524 L530 A531 H532 V533 F534 V535 G536 T537 C538 I542 I546 N549 F550 L551 E552 R553 T554 A555 I556 E557 L558 K559 W562 V563 R564 F565 L566 A567 L568 A569 L570 G571 I572 L573 Y574 M575 G576 Q577 G578 E579 Q580 V581 D582 D583 V584 L585 I588 I591 E592 H593 P594 M595
A598 I599 E600 V601 L602 V603 G604 S605 C606 A607 Y608 T609 G610 T611 G612 L616 D619 L620 L621 H622 R623 L624 T625 PRO LYS ASN VAL LYS GLY GLU GLU ASP ALA ASP GLU GLU GLU THR ALA GLU GLY GLN THR ASN SER ILE SER ASP PHE LEU GLY GLU GLN VAL ASN GLU PRO
THR LYS ASN GLU GLU ALA GLU ILE GLU VAL ASP GLU MET GLU VAL ASP ALA GLU GLY GLU GLU VAL GLU VAL LYS ALA GLU ILE THR GLU LYS LYS ASN GLY GLU SER LEU GLU GLY GLU GLU ILE LYS SER GLU GLU LYS LYS GLY LYS SER SER ASP LYS ASP ALA THR THR ASP GLY
LYS ASN ASP ASP GLU GLU GLU GLU LYS GLU ALA GLY ILE VAL ASP GLU L736 A737 Y738 A739 V740 L741 A744 L745 I746 A747 L748 G749 E750 D751 I752 G753 M756 S757 L758 R759 H760 F761 G762 H763 L764 M765 H766 Y767 G768 N769 E770 H771 I772 R773 R774 M775 V776 P777 L778 A779 M780 G781
I782 V783 S784 V785 S786 D787 P788 Q789 M790 K791 V792 T795 R798 F799 S800 H801 D802 A803 D804 L805 E806 M809 I812 F813 A814 M815 G816 L817 C818 G819 A820 G821 T822 N823 N824 A825 R826 L827 A828 Q829 L830 L831 R832 Q833 L834 A835 S836 Y837 Y838 S839 R840 E841 F846 I847 T848
R849 L850 A851 Q852 G853 L854 L855 H856 L857 G858 K859 G860 T861 M862 T863 M864 D865 V866 F867 N868 D869 A870 H871 V872 L873 N874 K875 V876 T877 L878 A879 S880 I881 L882 T883 T884 A885 V886 G887 L888 V889 S890 P891 S892 F893 M894 L895 K896 H897 H898 Q899 L900 F901 Y902 M903 L904 N905 A906 G907 I908
R909 P910 K911 F912 A915 D918 E919 G920 I923 K924 V929 G930 Q931 ALA VAL GLU THR VAL GLY GLN ALA GLY ARG PRO LYS LYS ILE THR GLY TRP ILE THR GLN SER THR P954 V955 L956 L957 N958 H959 G960 E961 R962 A963 E964 L965 E966 T967 D968 I971 S972 Y973 T974 S975
H976 I977 E978 G979 V980 L983 K984 K985 R990 E991 E992 E993

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 1300000 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | MICROGRAPH | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 25 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3500 | Depositor |
| Magnification | Not provided | |
| Image detector | TVIPS TEMCAM-F816 (8k x 8k) | Depositor |
| Maximum map value | 6.242 | Depositor |
| Minimum map value | -4.111 | Depositor |
| Average map value | 0.010 | Depositor |
| Map value standard deviation | 0.157 | Depositor |
| Recommended contour level | 0.74 | Depositor |
| Map size (Å) | 557.2, 557.2, 557.2 | wwPDB |
| Map dimensions | 280, 280, 280 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.99, 1.99, 1.99 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 1 | 1.19 | 7/1605 (0.4%) | 1.18 | 2/2171 (0.1%) |
| 2 | 2 | 1.20 | 10/1723 (0.6%) | 1.23 | 3/2337 (0.1%) |
| 3 | 3 | 1.17 | 7/1611 (0.4%) | 1.16 | 0/2174 |
| 4 | 4 | 1.17 | 7/1613 (0.4%) | 1.17 | 1/2173 (0.0%) |
| 5 | 5 | 1.18 | 9/1683 (0.5%) | 1.13 | 2/2277 (0.1%) |
| 6 | 6 | 1.16 | 7/1795 (0.4%) | 1.17 | 2/2420 (0.1%) |
| 7 | 7 | 1.16 | 7/1855 (0.4%) | 1.17 | 3/2514 (0.1%) |
| 8 | A | 1.20 | 10/1959 (0.5%) | 1.16 | 1/2652 (0.0%) |
| 9 | B | 1.23 | 9/1952 (0.5%) | 1.17 | 3/2642 (0.1%) |
| 10 | C | 1.14 | 6/1943 (0.3%) | 1.20 | 0/2629 |
| 11 | D | 1.16 | 6/1928 (0.3%) | 1.21 | 2/2610 (0.1%) |
| 12 | E | 1.23 | 11/1892 (0.6%) | 1.23 | 4/2549 (0.2%) |
| 13 | F | 1.17 | 8/1823 (0.4%) | 1.21 | 4/2463 (0.2%) |
| 14 | G | 1.24 | 12/1940 (0.6%) | 1.20 | 3/2619 (0.1%) |
| 15 | H | 1.12 | 8/2831 (0.3%) | 1.23 | 13/3808 (0.3%) |
| 16 | I | 1.14 | 11/2859 (0.4%) | 1.16 | 10/3853 (0.3%) |
| 17 | J | 1.19 | 13/2963 (0.4%) | 1.17 | 4/3978 (0.1%) |
| 18 | K | 1.15 | 12/3061 (0.4%) | 1.19 | 7/4129 (0.2%) |
| 19 | L | 1.18 | 11/2896 (0.4%) | 1.27 | 9/3895 (0.2%) |
| 20 | M | 1.18 | 12/2903 (0.4%) | 1.26 | 15/3909 (0.4%) |
| 21 | N | 1.12 | 19/6670 (0.3%) | 1.13 | 12/9023 (0.1%) |
| 22 | O | 1.09 | 13/3243 (0.4%) | 1.10 | 1/4374 (0.0%) |
| 23 | P | 1.04 | 12/3452 (0.3%) | 1.11 | 1/4657 (0.0%) |
| 24 | Q | 1.09 | 14/3527 (0.4%) | 1.09 | 4/4748 (0.1%) |
| 25 | R | 1.06 | 6/3272 (0.2%) | 1.07 | 1/4412 (0.0%) |
| 26 | S | 1.08 | 13/2945 (0.4%) | 1.07 | 2/3976 (0.1%) |
| 27 | T | 1.03 | 5/2279 (0.2%) | 1.11 | 5/3077 (0.2%) |
| 28 | U | 1.16 | 11/2087 (0.5%) | 1.10 | 3/2811 (0.1%) |
| 29 | V | 1.19 | 14/1969 (0.7%) | 1.17 | 1/2652 (0.0%) |
| 30 | W | 1.19 | 9/1557 (0.6%) | 1.24 | 7/2111 (0.3%) |
| 31 | X | 1.16 | 5/1058 (0.5%) | 1.18 | 3/1432 (0.2%) |
| 32 | Y | 1.04 | 0/169 | 1.14 | 0/223 |
| 33 | Z | 1.11 | 31/6403 (0.5%) | 1.11 | 10/8686 (0.1%) |
| All | All | 1.14 | 335/81466 (0.4%) | 1.16 | 138/109984 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 7 | 7 | 0 | 1 |
| 11 | D | 0 | 1 |
| 12 | E | 0 | 3 |
| 13 | F | 0 | 1 |
| 15 | H | 0 | 8 |
| 16 | I | 0 | 4 |
| 18 | K | 0 | 2 |
| 19 | L | 0 | 4 |
| 20 | M | 0 | 2 |
| 21 | N | 0 | 1 |
| 22 | O | 0 | 4 |
| 23 | P | 0 | 2 |
| 24 | Q | 0 | 1 |
| 25 | R | 0 | 2 |
| 27 | T | 0 | 4 |
| 29 | V | 0 | 1 |
| 30 | W | 0 | 1 |
| 33 | Z | 0 | 2 |
| All | All | 0 | 44 |

All (335) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | M | 251 | LEU | C-N | -21.72 | 0.84 | 1.34 |
| 17 | J | 224 | GLY | C-N | 17.02 | 1.73 | 1.34 |
| 19 | L | 257 | GLY | C-N | -8.59 | 1.14 | 1.34 |
| 25 | R | 306 | PRO | N-CD | 8.54 | 1.59 | 1.47 |
| 22 | O | 201 | PRO | N-CD | 8.22 | 1.59 | 1.47 |
| 3 | 3 | 75 | PRO | N-CD | 8.16 | 1.59 | 1.47 |
| 8 | A | 60 | PRO | N-CD | 8.14 | 1.59 | 1.47 |
| 29 | V | 143 | PRO | N-CD | 8.11 | 1.59 | 1.47 |
| 15 | H | 358 | PRO | N-CD | 7.78 | 1.58 | 1.47 |
| 13 | F | 149 | PRO | N-CD | 7.70 | 1.58 | 1.47 |
| 33 | Z | 891 | PRO | N-CD | 7.64 | 1.58 | 1.47 |
| 21 | N | 8 | PRO | N-CD | 7.63 | 1.58 | 1.47 |
| 31 | X | 37 | PRO | N-CD | 7.42 | 1.58 | 1.47 |
| 33 | Z | 354 | PRO | N-CD | 7.41 | 1.58 | 1.47 |
| 31 | X | 70 | PRO | N-CD | 7.33 | 1.58 | 1.47 |
| 20 | M | 255 | TYR | CG-CD2 | 7.30 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | 7 | -5 | PRO | N-CD | 7.24 | 1.57 | 1.47 |
| 21 | N | 643 | PRO | N-CD | 7.23 | 1.57 | 1.47 |
| 8 | A | 47 | GLY | N-CA | -7.16 | 1.35 | 1.46 |
| 29 | V | 46 | PRO | N-CD | 7.12 | 1.57 | 1.47 |
| 9 | B | 69 | PRO | N-CD | 7.06 | 1.57 | 1.47 |
| 28 | U | 133 | PRO | N-CD | 6.99 | 1.57 | 1.47 |
| 1 | 1 | 190 | PRO | N-CD | 6.94 | 1.57 | 1.47 |
| 14 | G | 44 | GLY | CA-C | -6.92 | 1.40 | 1.51 |
| 26 | S | 260 | PRO | N-CD | 6.86 | 1.57 | 1.47 |
| 14 | G | 16 | PRO | N-CD | 6.80 | 1.57 | 1.47 |
| 12 | E | 136 | ARG | CD-NE | 6.78 | 1.57 | 1.46 |
| 24 | Q | 403 | PRO | N-CD | 6.73 | 1.57 | 1.47 |
| 31 | X | 26 | PRO | N-CD | 6.68 | 1.57 | 1.47 |
| 18 | K | 252 | ARG | CD-NE | 6.65 | 1.57 | 1.46 |
| 18 | K | 215 | PRO | N-CD | 6.64 | 1.57 | 1.47 |
| 21 | N | 620 | GLY | CA-C | -6.58 | 1.41 | 1.51 |
| 20 | M | 350 | PRO | N-CD | 6.54 | 1.57 | 1.47 |
| 22 | O | 339 | GLY | CA-C | 6.53 | 1.62 | 1.51 |
| 18 | K | 287 | GLY | CA-C | -6.49 | 1.41 | 1.51 |
| 5 | 5 | 212 | GLY | N-CA | -6.48 | 1.36 | 1.46 |
| 18 | K | 93 | PRO | N-CD | 6.48 | 1.56 | 1.47 |
| 10 | C | 130 | PRO | N-CD | 6.44 | 1.56 | 1.47 |
| 17 | J | 68 | PRO | N-CD | 6.42 | 1.56 | 1.47 |
| 12 | E | 146 | GLY | N-CA | -6.33 | 1.36 | 1.46 |
| 15 | H | 324 | GLY | N-CA | -6.31 | 1.36 | 1.46 |
| 28 | U | 118 | PRO | N-CD | 6.30 | 1.56 | 1.47 |
| 4 | 4 | 76 | PRO | N-CD | 6.25 | 1.56 | 1.47 |
| 17 | J | 281 | GLY | CA-C | -6.24 | 1.41 | 1.51 |
| 10 | C | 223 | GLY | CA-C | -6.24 | 1.41 | 1.51 |
| 31 | X | 52 | PRO | N-CD | 6.20 | 1.56 | 1.47 |
| 13 | F | 151 | GLY | CA-C | -6.20 | 1.42 | 1.51 |
| 4 | 4 | 172 | PRO | N-CD | 6.18 | 1.56 | 1.47 |
| 13 | F | 76 | GLY | N-CA | -6.18 | 1.36 | 1.46 |
| 8 | A | 152 | PRO | N-CD | 6.17 | 1.56 | 1.47 |
| 18 | K | 151 | PRO | N-CD | 6.17 | 1.56 | 1.47 |
| 17 | J | 143 | PRO | N-CD | 6.17 | 1.56 | 1.47 |
| 33 | Z | 351 | PRO | N-CD | 6.13 | 1.56 | 1.47 |
| 9 | B | 233 | PRO | N-CD | 6.12 | 1.56 | 1.47 |
| 16 | I | 143 | PRO | C-N | 6.11 | 1.44 | 1.33 |
| 24 | Q | 80 | HIS | CG-CD2 | 6.11 | 1.46 | 1.35 |
| 16 | I | 117 | HIS | CG-CD2 | 6.10 | 1.46 | 1.35 |
| 19 | L | 214 | PRO | N-CD | 6.10 | 1.56 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 13 | F | 186 | PRO | N-CD | 6.09 | 1.56 | 1.47 |
| 14 | G | 146 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 16 | I | 150 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 6 | 6 | 67 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 22 | O | 236 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 28 | U | 173 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 29 | V | 109 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 14 | G | 122 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 1 | 1 | 157 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 12 | E | 73 | HIS | CG-CD2 | 6.09 | 1.46 | 1.35 |
| 24 | Q | 334 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 33 | Z | 898 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 1 | 1 | 62 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 14 | G | 72 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 20 | M | 364 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 23 | P | 282 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 27 | T | 251 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 28 | U | 21 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 11 | D | 16 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 26 | S | 334 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 12 | E | 147 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 23 | P | 417 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 9 | B | 94 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 10 | C | 125 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 23 | P | 440 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 24 | Q | 135 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 25 | R | 81 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 33 | Z | 132 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 1 | 1 | 38 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 3 | 3 | 36 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 6 | 6 | 99 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 22 | O | 5 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 24 | Q | 247 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 26 | S | 438 | HIS | CG-CD2 | 6.08 | 1.46 | 1.35 |
| 9 | B | 139 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 15 | H | 95 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 24 | Q | 186 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 33 | Z | 214 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 4 | 4 | 40 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 5 | 5 | 188 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 9 | B | 190 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 20 | M | 53 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | R | 325 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 29 | V | 190 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 29 | V | 195 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 33 | Z | 760 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 33 | Z | 871 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 33 | Z | 463 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 6 | 6 | 86 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 8 | A | 193 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 12 | E | 99 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 14 | G | 182 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 23 | P | 336 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 33 | Z | 771 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 33 | Z | 856 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 33 | Z | 976 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 5 | 5 | 179 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 14 | G | 227 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 17 | J | 123 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 17 | J | 376 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 21 | N | 573 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 27 | T | 123 | HIS | CG-CD2 | 6.07 | 1.46 | 1.35 |
| 13 | F | 110 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 21 | N | 616 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 26 | S | 261 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 26 | S | 472 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 13 | F | 69 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 14 | G | 86 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 23 | P | 425 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 26 | S | 317 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 5 | 5 | 66 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 7 | 7 | 141 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 22 | O | 235 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 30 | W | 86 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 14 | G | 203 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 17 | J | 331 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 18 | K | 142 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 19 | L | 364 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 21 | N | 690 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 29 | V | 204 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 30 | W | 170 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 7 | 7 | 54 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 24 | Q | 178 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 26 | S | 191 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 28 | U | 70 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 33 | Z | 361 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 8 | A | 15 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 12 | E | 157 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 21 | N | 340 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 33 | Z | 593 | HIS | CG-CD2 | 6.06 | 1.46 | 1.35 |
| 13 | F | 43 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 16 | I | 204 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 21 | N | 375 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 22 | O | 122 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 33 | Z | 801 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 2 | 2 | 109 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 16 | I | 151 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 18 | K | 140 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 22 | O | 23 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 18 | K | 244 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 26 | S | 347 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 27 | T | 132 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 28 | U | 5 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 28 | U | 94 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 29 | V | 111 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 33 | Z | 151 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 33 | Z | 959 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 11 | D | 96 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 14 | G | 181 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 16 | I | 365 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 23 | P | 263 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 29 | V | 40 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 33 | Z | 338 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 2 | 2 | 66 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 24 | Q | 108 | PRO | N-CD | 6.04 | 1.56 | 1.47 |
| 25 | R | 401 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 33 | Z | 307 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 5 | 5 | 166 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 6 | 6 | 70 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 19 | L | 409 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 26 | S | 302 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 2 | 2 | 35 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 2 | 2 | 116 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 2 | 2 | 141 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 18 | K | 74 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 19 | L | 106 | GLY | CA-C | -6.04 | 1.42 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | N | 329 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 22 | O | 326 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 24 | Q | 226 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 28 | U | 223 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 33 | Z | 532 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 8 | A | 209 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 30 | W | 77 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 30 | W | 100 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 11 | D | 70 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 12 | E | 91 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 17 | J | 170 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 17 | J | 205 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 29 | V | 217 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 29 | V | 279 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 22 | O | 283 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 1 | 1 | 120 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 2 | 2 | 93 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 21 | N | 444 | HIS | CG-CD2 | 6.04 | 1.46 | 1.35 |
| 2 | 2 | 114 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 12 | E | 188 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 24 | Q | 145 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 4 | 4 | 132 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 4 | 4 | 145 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 10 | C | 31 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 15 | H | 392 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 19 | L | 67 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 23 | P | 431 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 21 | N | 613 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 5 | 5 | 191 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 8 | A | 185 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 13 | F | 143 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 21 | N | 510 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 26 | S | 139 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 27 | T | 94 | HIS | CG-CD2 | 6.03 | 1.46 | 1.35 |
| 2 | 2 | 86 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 20 | M | 130 | PRO | N-CD | 6.02 | 1.56 | 1.47 |
| 21 | N | 747 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 33 | Z | 766 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 6 | 6 | 186 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 26 | S | 225 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 33 | Z | 763 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 19 | L | 273 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | 4 | 146 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 23 | P | 230 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 24 | Q | 361 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 33 | Z | 622 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 6 | 6 | 153 | PRO | N-CD | 6.02 | 1.56 | 1.47 |
| 30 | W | 107 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 33 | Z | 156 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 33 | Z | 897 | HIS | CG-CD2 | 6.02 | 1.46 | 1.35 |
| 10 | C | 94 | HIS | CG-CD2 | 6.01 | 1.46 | 1.35 |
| 17 | J | 240 | HIS | CG-CD2 | 6.01 | 1.46 | 1.35 |
| 20 | M | 412 | HIS | CG-CD2 | 6.01 | 1.46 | 1.35 |
| 21 | N | 499 | HIS | CG-CD2 | 6.01 | 1.46 | 1.35 |
| 28 | U | 156 | HIS | CG-CD2 | 6.01 | 1.46 | 1.35 |
| 23 | P | 348 | HIS | CG-CD2 | 6.01 | 1.46 | 1.35 |
| 25 | R | 217 | HIS | CG-CD2 | 6.01 | 1.46 | 1.35 |
| 22 | O | 318 | HIS | CG-CD2 | 6.00 | 1.46 | 1.35 |
| 24 | Q | 252 | HIS | CG-CD2 | 6.00 | 1.46 | 1.35 |
| 23 | P | 337 | HIS | CG-CD2 | 6.00 | 1.46 | 1.35 |
| 18 | K | 298 | GLU | CG-CD | 6.00 | 1.60 | 1.51 |
| 3 | 3 | 39 | HIS | CG-CD2 | 6.00 | 1.46 | 1.35 |
| 17 | J | 204 | HIS | CG-CD2 | 6.00 | 1.46 | 1.35 |
| 4 | 4 | 96 | PRO | N-CD | 5.99 | 1.56 | 1.47 |
| 2 | 2 | 24 | PRO | N-CD | 5.98 | 1.56 | 1.47 |
| 27 | T | 28 | PRO | N-CD | 5.97 | 1.56 | 1.47 |
| 20 | M | 220 | MET | N-CA | -5.96 | 1.34 | 1.46 |
| 21 | N | 294 | PRO | N-CD | 5.93 | 1.56 | 1.47 |
| 33 | Z | 289 | GLY | CA-C | -5.92 | 1.42 | 1.51 |
| 21 | N | 785 | PRO | CA-C | -5.91 | 1.41 | 1.52 |
| 21 | N | 600 | THR | N-CA | -5.90 | 1.34 | 1.46 |
| 20 | M | 275 | PRO | N-CD | 5.86 | 1.56 | 1.47 |
| 15 | H | 278 | GLU | CG-CD | 5.86 | 1.60 | 1.51 |
| 28 | U | 12 | PRO | N-CD | 5.85 | 1.56 | 1.47 |
| 30 | W | 176 | PRO | N-CD | 5.85 | 1.56 | 1.47 |
| 26 | S | 165 | PRO | N-CD | 5.84 | 1.56 | 1.47 |
| 33 | Z | 604 | GLY | CA-C | 5.84 | 1.61 | 1.51 |
| 10 | C | 232 | PRO | N-CD | 5.84 | 1.56 | 1.47 |
| 9 | B | 219 | PRO | N-CD | 5.81 | 1.55 | 1.47 |
| 11 | D | 185 | PRO | N-CD | 5.70 | 1.55 | 1.47 |
| 9 | B | 222 | LEU | C-N | 5.66 | 1.43 | 1.33 |
| 21 | N | 763 | GLY | CA-C | -5.66 | 1.42 | 1.51 |
| 33 | Z | 494 | GLY | CA-C | -5.66 | 1.42 | 1.51 |
| 5 | 5 | 47 | GLY | CA-C | -5.64 | 1.42 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | I | 216 | PRO | N-CD | 5.59 | 1.55 | 1.47 |
| 33 | Z | 97 | PRO | N-CD | 5.59 | 1.55 | 1.47 |
| 22 | O | 230 | PHE | C-N | 5.58 | 1.43 | 1.33 |
| 3 | 3 | 46 | GLY | CA-C | -5.57 | 1.43 | 1.51 |
| 18 | K | 332 | GLY | CA-C | -5.57 | 1.43 | 1.51 |
| 19 | L | 350 | PRO | N-CD | 5.57 | 1.55 | 1.47 |
| 8 | A | 66 | PRO | N-CD | 5.57 | 1.55 | 1.47 |
| 21 | N | 250 | ASP | N-CA | -5.57 | 1.35 | 1.46 |
| 5 | 5 | 138 | GLY | CA-C | 5.54 | 1.60 | 1.51 |
| 29 | V | 276 | PRO | N-CD | 5.53 | 1.55 | 1.47 |
| 23 | P | 276 | LEU | N-CA | -5.53 | 1.35 | 1.46 |
| 26 | S | 468 | ALA | C-N | 5.52 | 1.46 | 1.34 |
| 30 | W | 75 | GLY | N-CA | -5.49 | 1.37 | 1.46 |
| 6 | 6 | 112 | ALA | N-CA | -5.48 | 1.35 | 1.46 |
| 14 | G | 216 | SER | N-CA | -5.48 | 1.35 | 1.46 |
| 23 | P | 396 | PRO | N-CD | 5.47 | 1.55 | 1.47 |
| 20 | M | 222 | GLY | CA-C | -5.46 | 1.43 | 1.51 |
| 12 | E | 44 | GLU | C-N | 5.41 | 1.42 | 1.33 |
| 18 | K | 294 | ARG | CA-CB | 5.39 | 1.65 | 1.53 |
| 7 | 7 | 158 | PRO | CA-C | -5.36 | 1.42 | 1.52 |
| 19 | L | 412 | PRO | N-CD | 5.35 | 1.55 | 1.47 |
| 25 | R | 143 | GLN | N-CA | -5.35 | 1.35 | 1.46 |
| 31 | X | 71 | GLY | CA-C | -5.35 | 1.43 | 1.51 |
| 3 | 3 | 21 | GLY | N-CA | -5.34 | 1.38 | 1.46 |
| 15 | H | 96 | PRO | N-CD | 5.34 | 1.55 | 1.47 |
| 15 | H | 368 | PRO | N-CD | 5.34 | 1.55 | 1.47 |
| 14 | G | 68 | VAL | N-CA | -5.33 | 1.35 | 1.46 |
| 17 | J | 306 | ARG | C-N | -5.33 | 1.24 | 1.34 |
| 1 | 1 | 108 | GLY | CA-C | -5.31 | 1.43 | 1.51 |
| 16 | I | 287 | ILE | C-N | 5.29 | 1.42 | 1.33 |
| 19 | L | 224 | PRO | C-N | 5.29 | 1.42 | 1.33 |
| 33 | Z | 116 | ALA | N-CA | -5.29 | 1.35 | 1.46 |
| 9 | B | 226 | GLY | N-CA | -5.28 | 1.38 | 1.46 |
| 17 | J | 131 | ASP | C-N | 5.26 | 1.44 | 1.34 |
| 8 | A | 171 | THR | C-N | 5.24 | 1.42 | 1.33 |
| 3 | 3 | 115 | PHE | N-CA | -5.23 | 1.35 | 1.46 |
| 20 | M | 388 | GLY | CA-C | 5.23 | 1.60 | 1.51 |
| 8 | A | 88 | PRO | N-CD | 5.22 | 1.55 | 1.47 |
| 22 | O | 122 | HIS | N-CA | -5.19 | 1.35 | 1.46 |
| 12 | E | 148 | ASP | CA-C | -5.18 | 1.39 | 1.52 |
| 22 | O | 278 | PRO | CA-C | -5.18 | 1.42 | 1.52 |
| 7 | 7 | 144 | ASN | N-CA | -5.18 | 1.35 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 33 | Z | 414 | GLY | CA-C | 5.16 | 1.60 | 1.51 |
| 16 | I | 353 | PRO | N-CD | 5.16 | 1.55 | 1.47 |
| 29 | V | 99 | GLY | CA-C | -5.15 | 1.43 | 1.51 |
| 15 | H | 212 | GLY | N-CA | -5.14 | 1.38 | 1.46 |
| 9 | B | 228 | PRO | N-CA | -5.13 | 1.38 | 1.47 |
| 16 | I | 133 | LEU | N-CA | -5.13 | 1.36 | 1.46 |
| 11 | D | 77 | GLY | CA-C | -5.13 | 1.43 | 1.51 |
| 11 | D | 184 | PRO | N-CD | 5.12 | 1.55 | 1.47 |
| 16 | I | 166 | PRO | N-CD | 5.12 | 1.55 | 1.47 |
| 1 | 1 | 171 | GLY | CA-C | -5.10 | 1.43 | 1.51 |
| 30 | W | 53 | SER | C-N | 5.10 | 1.42 | 1.33 |
| 5 | 5 | 157 | GLY | N-CA | -5.09 | 1.38 | 1.46 |
| 24 | Q | 195 | LYS | C-N | 5.08 | 1.45 | 1.34 |
| 29 | V | 55 | GLY | N-CA | -5.08 | 1.38 | 1.46 |
| 19 | L | 319 | GLY | N-CA | -5.08 | 1.38 | 1.46 |
| 7 | 7 | 162 | VAL | N-CA | 5.08 | 1.56 | 1.46 |
| 24 | Q | 43 | GLY | N-CA | -5.07 | 1.38 | 1.46 |
| 30 | W | 69 | PHE | C-N | 5.06 | 1.42 | 1.33 |
| 7 | 7 | 81 | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 20 | M | 360 | ILE | N-CA | -5.05 | 1.36 | 1.46 |
| 12 | E | 57 | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 3 | 3 | 93 | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 2 | 2 | 181 | GLY | CA-C | -5.02 | 1.43 | 1.51 |
| 28 | U | 191 | THR | N-CA | 5.01 | 1.56 | 1.46 |
| 29 | V | 23 | THR | N-CA | 5.01 | 1.56 | 1.46 |

All (138) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | L | 257 | GLY | O-C-N | -21.29 | 88.64 | 122.70 |
| 20 | M | 299 | ARG | NE-CZ-NH1 | 14.99 | 127.79 | 120.30 |
| 19 | L | 257 | GLY | CA-C-N | 13.23 | 146.30 | 117.20 |
| 19 | L | 257 | GLY | C-N-CA | 12.51 | 152.97 | 121.70 |
| 18 | K | 252 | ARG | NE-CZ-NH2 | -11.18 | 114.71 | 120.30 |
| 20 | M | 251 | LEU | O-C-N | -11.13 | 104.89 | 122.70 |
| 18 | K | 294 | ARG | NE-CZ-NH2 | -9.74 | 115.43 | 120.30 |
| 16 | I | 262 | ARG | NE-CZ-NH1 | 9.70 | 125.15 | 120.30 |
| 20 | M | 251 | LEU | CA-C-N | 9.57 | 138.25 | 117.20 |
| 18 | K | 294 | ARG | NE-CZ-NH1 | 9.06 | 124.83 | 120.30 |
| 20 | M | 251 | LEU | C-N-CA | 9.03 | 144.27 | 121.70 |
| 20 | M | 255 | TYR | CB-CG-CD2 | 8.36 | 126.02 | 121.00 |
| 12 | E | 132 | ARG | NE-CZ-NH1 | 8.16 | 124.38 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | I | 257 | LEU | CB-CG-CD1 | 7.98 | 124.57 | 111.00 |
| 15 | H | 162 | ARG | NE-CZ-NH1 | 7.59 | 124.09 | 120.30 |
| 19 | L | 248 | ALA | N-CA-CB | -7.14 | 100.10 | 110.10 |
| 16 | I | 304 | ARG | NE-CZ-NH2 | -7.12 | 116.74 | 120.30 |
| 20 | M | 255 | TYR | CB-CG-CD1 | -7.10 | 116.74 | 121.00 |
| 17 | J | 224 | GLY | C-N-CA | -7.01 | 104.17 | 121.70 |
| 11 | D | 50 | SER | N-CA-C | -6.80 | 92.65 | 111.00 |
| 18 | K | 249 | GLU | OE1-CD-OE2 | -6.79 | 115.16 | 123.30 |
| 28 | U | 164 | GLU | N-CA-C | -6.63 | 93.11 | 111.00 |
| 9 | B | 217 | GLU | N-CA-C | -6.60 | 93.17 | 111.00 |
| 23 | P | 322 | LEU | C-N-CA | 6.51 | 137.97 | 121.70 |
| 2 | 2 | 41 | ILE | N-CA-C | -6.36 | 93.83 | 111.00 |
| 14 | G | 209 | LYS | N-CA-C | -6.28 | 94.03 | 111.00 |
| 33 | Z | 486 | SER | C-N-CA | 6.28 | 137.40 | 121.70 |
| 31 | X | 28 | PRO | O-C-N | 6.21 | 132.63 | 122.70 |
| 33 | Z | 77 | ASN | N-CA-C | -6.21 | 94.24 | 111.00 |
| 19 | L | 84 | LEU | O-C-N | 6.19 | 132.60 | 122.70 |
| 20 | M | 256 | ILE | CA-CB-CG2 | -6.18 | 98.54 | 110.90 |
| 12 | E | 222 | ILE | N-CA-C | -6.17 | 94.35 | 111.00 |
| 20 | M | 299 | ARG | NH1-CZ-NH2 | -6.11 | 112.68 | 119.40 |
| 7 | 7 | 35 | ILE | N-CA-C | -6.09 | 94.56 | 111.00 |
| 20 | M | 233 | ARG | O-C-N | -6.03 | 113.05 | 122.70 |
| 21 | N | 249 | ASN | O-C-N | 6.00 | 132.31 | 122.70 |
| 8 | A | 224 | GLU | N-CA-C | -5.98 | 94.84 | 111.00 |
| 16 | I | 160 | LEU | N-CA-C | -5.95 | 94.94 | 111.00 |
| 30 | W | 24 | THR | N-CA-C | -5.95 | 94.94 | 111.00 |
| 20 | M | 277 | ILE | N-CA-C | -5.93 | 94.98 | 111.00 |
| 33 | Z | 240 | ASN | O-C-N | -5.92 | 113.22 | 122.70 |
| 20 | M | 426 | LYS | N-CA-C | -5.92 | 95.03 | 111.00 |
| 15 | H | 193 | PRO | C-N-CA | 5.90 | 136.45 | 121.70 |
| 21 | N | 250 | ASP | O-C-N | -5.90 | 113.26 | 122.70 |
| 15 | H | 145 | TYR | CG-CD2-CE2 | -5.89 | 116.59 | 121.30 |
| 19 | L | 250 | GLY | O-C-N | -5.85 | 113.34 | 122.70 |
| 30 | W | 163 | ASN | N-CA-C | -5.83 | 95.27 | 111.00 |
| 21 | N | 387 | ALA | CA-C-N | 5.82 | 133.38 | 117.10 |
| 27 | T | 168 | SER | C-N-CA | 5.80 | 136.19 | 121.70 |
| 33 | Z | 599 | ILE | O-C-N | -5.79 | 113.43 | 122.70 |
| 18 | K | 211 | LEU | N-CA-C | -5.73 | 95.52 | 111.00 |
| 27 | T | 97 | SER | C-N-CA | 5.72 | 136.00 | 121.70 |
| 18 | K | 213 | GLY | N-CA-C | -5.72 | 98.81 | 113.10 |
| 30 | W | 162 | ASN | C-N-CA | 5.68 | 135.91 | 121.70 |
| 19 | L | 336 | ALA | O-C-N | -5.67 | 113.62 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | W | 19 | GLY | O-C-N | 5.67 | 131.77 | 122.70 |
| 20 | M | 240 | ASN | C-N-CA | 5.66 | 135.85 | 121.70 |
| 33 | Z | 131 | LYS | N-CA-C | -5.62 | 95.83 | 111.00 |
| 33 | Z | 611 | THR | CA-CB-CG2 | -5.61 | 104.55 | 112.40 |
| 33 | Z | 258 | PRO | CA-C-N | 5.60 | 132.79 | 117.10 |
| 16 | I | 130 | VAL | N-CA-C | 5.59 | 126.09 | 111.00 |
| 24 | Q | 226 | HIS | O-C-N | -5.59 | 113.75 | 122.70 |
| 13 | F | 144 | LEU | N-CA-C | -5.55 | 96.01 | 111.00 |
| 21 | N | 526 | TYR | N-CA-C | -5.55 | 96.02 | 111.00 |
| 12 | E | 122 | ARG | NE-CZ-NH1 | -5.54 | 117.53 | 120.30 |
| 16 | I | 338 | LEU | C-N-CA | 5.51 | 135.47 | 121.70 |
| 15 | H | 383 | GLU | O-C-N | -5.50 | 113.84 | 123.20 |
| 21 | N | 708 | ALA | C-N-CA | 5.50 | 133.85 | 122.30 |
| 30 | W | 5 | ALA | N-CA-C | -5.47 | 96.22 | 111.00 |
| 21 | N | 716 | GLN | N-CA-C | -5.46 | 96.26 | 111.00 |
| 16 | I | 130 | VAL | CB-CA-C | -5.46 | 101.04 | 111.40 |
| 15 | H | 163 | VAL | CA-CB-CG2 | -5.45 | 102.72 | 110.90 |
| 12 | E | 61 | SER | C-N-CA | 5.45 | 135.32 | 121.70 |
| 13 | F | 158 | GLY | N-CA-C | -5.44 | 99.50 | 113.10 |
| 6 | 6 | 129 | ALA | N-CA-C | -5.44 | 96.32 | 111.00 |
| 17 | J | 224 | GLY | CA-C-N | -5.43 | 105.25 | 117.20 |
| 20 | M | 173 | ASP | O-C-N | -5.43 | 114.01 | 122.70 |
| 15 | H | 286 | GLU | CA-C-N | -5.42 | 105.35 | 116.20 |
| 1 | 1 | 35 | THR | N-CA-C | -5.39 | 96.43 | 111.00 |
| 31 | X | 114 | LEU | C-N-CA | 5.37 | 135.13 | 121.70 |
| 21 | N | 378 | ASN | N-CA-C | -5.37 | 96.50 | 111.00 |
| 26 | S | 151 | GLU | N-CA-C | -5.34 | 96.57 | 111.00 |
| 24 | Q | 355 | GLU | C-N-CA | 5.34 | 135.05 | 121.70 |
| 27 | T | 93 | ASN | C-N-CA | 5.33 | 135.03 | 121.70 |
| 19 | L | 187 | THR | N-CA-C | 5.32 | 125.37 | 111.00 |
| 28 | U | 289 | ASP | O-C-N | -5.32 | 114.19 | 122.70 |
| 21 | N | 128 | ILE | O-C-N | 5.32 | 131.21 | 122.70 |
| 18 | K | 252 | ARG | NH1-CZ-NH2 | 5.31 | 125.24 | 119.40 |
| 5 | 5 | 152 | ASP | O-C-N | 5.30 | 131.19 | 122.70 |
| 17 | J | 395 | GLU | C-N-CA | 5.30 | 134.95 | 121.70 |
| 6 | 6 | 98 | VAL | O-C-N | 5.29 | 131.17 | 122.70 |
| 4 | 4 | 1 | ASP | N-CA-C | -5.28 | 96.74 | 111.00 |
| 24 | Q | 294 | ARG | C-N-CA | 5.28 | 133.38 | 122.30 |
| 11 | D | 134 | LEU | N-CA-C | -5.27 | 96.78 | 111.00 |
| 21 | N | 715 | ILE | N-CA-C | -5.27 | 96.78 | 111.00 |
| 28 | U | 110 | PHE | C-N-CA | 5.25 | 134.81 | 121.70 |
| 15 | H | 278 | GLU | N-CA-CB | 5.24 | 120.04 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | N | 230 | VAL | O-C-N | 5.24 | 131.09 | 122.70 |
| 15 | H | 197 | MET | O-C-N | 5.24 | 131.08 | 122.70 |
| 21 | N | 885 | ILE | O-C-N | -5.23 | 114.33 | 122.70 |
| 30 | W | 22 | PRO | C-N-CA | 5.20 | 134.71 | 121.70 |
| 20 | M | 233 | ARG | CA-C-O | 5.18 | 130.99 | 120.10 |
| 15 | H | 303 | ALA | N-CA-C | -5.17 | 97.03 | 111.00 |
| 14 | G | 215 | ILE | N-CA-C | -5.17 | 97.05 | 111.00 |
| 7 | 7 | 27 | ARG | O-C-N | 5.16 | 130.95 | 122.70 |
| 33 | Z | 51 | LEU | N-CA-C | -5.15 | 97.11 | 111.00 |
| 33 | Z | 178 | SER | O-C-N | -5.13 | 114.49 | 122.70 |
| 2 | 2 | 2 | THR | N-CA-C | -5.13 | 97.15 | 111.00 |
| 33 | Z | 502 | ASN | C-N-CA | 5.13 | 134.52 | 121.70 |
| 29 | V | 111 | HIS | CA-C-N | 5.13 | 131.46 | 117.10 |
| 17 | J | 131 | ASP | CA-C-O | -5.12 | 109.34 | 120.10 |
| 16 | I | 104 | LEU | N-CA-C | -5.12 | 97.18 | 111.00 |
| 15 | H | 374 | LYS | O-C-N | -5.11 | 114.52 | 122.70 |
| 19 | L | 100 | SER | C-N-CA | 5.10 | 134.46 | 121.70 |
| 13 | F | 89 | ARG | O-C-N | -5.10 | 114.54 | 122.70 |
| 14 | G | 69 | VAL | N-CA-C | -5.10 | 97.23 | 111.00 |
| 27 | T | 28 | PRO | CA-C-N | 5.10 | 131.38 | 117.10 |
| 15 | H | 162 | ARG | NH1-CZ-NH2 | -5.09 | 113.80 | 119.40 |
| 15 | H | 283 | TYR | CG-CD1-CE1 | -5.09 | 117.22 | 121.30 |
| 2 | 2 | 43 | CYS | N-CA-C | -5.09 | 97.25 | 111.00 |
| 5 | 5 | 99 | THR | O-C-N | 5.09 | 130.84 | 122.70 |
| 27 | T | 28 | PRO | CA-C-O | -5.08 | 108.00 | 120.20 |
| 9 | B | 48 | GLU | O-C-N | 5.08 | 130.82 | 122.70 |
| 16 | I | 228 | GLY | N-CA-C | -5.07 | 100.42 | 113.10 |
| 30 | W | 179 | ARG | N-CA-C | -5.07 | 97.31 | 111.00 |
| 16 | I | 134 | SER | C-N-CA | 5.07 | 134.37 | 121.70 |
| 31 | X | 73 | THR | N-CA-C | -5.06 | 97.34 | 111.00 |
| 7 | 7 | 106 | ILE | O-C-N | 5.06 | 130.79 | 122.70 |
| 13 | F | 133 | LEU | N-CA-C | -5.06 | 97.34 | 111.00 |
| 24 | Q | 118 | CYS | O-C-N | -5.05 | 114.62 | 122.70 |
| 15 | H | 302 | LYS | C-N-CA | 5.05 | 134.32 | 121.70 |
| 21 | N | 257 | ILE | O-C-N | -5.04 | 114.63 | 122.70 |
| 20 | M | 116 | ALA | N-CA-C | -5.03 | 97.42 | 111.00 |
| 22 | O | 271 | LYS | N-CA-C | -5.03 | 97.42 | 111.00 |
| 9 | B | 94 | HIS | O-C-N | -5.03 | 114.66 | 122.70 |
| 1 | 1 | 76 | GLU | O-C-N | -5.02 | 114.67 | 122.70 |
| 25 | R | 328 | PHE | C-N-CA | 5.01 | 134.22 | 121.70 |
| 26 | S | 144 | LEU | O-C-N | -5.00 | 114.70 | 122.70 |

There are no chirality outliers.

All (44) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | 7 | 100 | ASN | Peptide |
| 11 | D | 104 | VAL | Peptide |
| 12 | E | 122 | ARG | Sidechain |
| 12 | E | 132 | ARG | Sidechain |
| 12 | E | 136 | ARG | Sidechain |
| 13 | F | 47 | VAL | Mainchain |
| 15 | H | 101 | ARG | Peptide |
| 15 | H | 145 | TYR | Sidechain |
| 15 | H | 162 | ARG | Peptide |
| 15 | H | 170 | GLU | Peptide |
| 15 | H | 283 | TYR | Sidechain |
| 15 | H | 285 | GLY | Mainchain |
| 15 | H | 400 | ARG | Peptide |
| 15 | H | 95 | HIS | Peptide |
| 16 | I | 125 | MET | Peptide |
| 16 | I | 214 | LYS | Peptide |
| 16 | I | 256 | TYR | Sidechain |
| 16 | I | 340 | ARG | Peptide |
| 18 | K | 150 | LEU | Peptide |
| 18 | K | 255 | ARG | Sidechain |
| 19 | L | 203 | ASN | Peptide |
| 19 | L | 249 | SER | Peptide |
| 19 | L | 253 | ASP | Peptide |
| 19 | L | 257 | GLY | Mainchain |
| 20 | M | 299 | ARG | Sidechain |
| 20 | M | 75 | LEU | Peptide |
| 21 | N | 774 | ASN | Peptide |
| 22 | O | 125 | GLY | Peptide |
| 22 | O | 140 | LYS | Peptide |
| 22 | O | 19 | ASP | Peptide |
| 22 | O | 240 | GLU | Peptide |
| 23 | P | 53 | ALA | Peptide |
| 23 | P | 69 | ARG | Sidechain |
| 24 | Q | 402 | THR | Peptide |
| 25 | R | 184 | GLN | Peptide |
| 25 | R | 381 | ILE | Peptide |
| 27 | T | 237 | ASN | Peptide |
| 27 | T | 247 | ASP | Peptide |
| 27 | T | 252 | GLU | Peptide |
| 27 | T | 253 | GLU | Peptide |
| 29 | V | 110 | SER | Peptide |
| 30 | W | 164 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 33 | Z | 317 | GLN | Peptide |
| 33 | Z | 350 | GLY | Peptide |

## 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 | 1 | 1576 | 0 | 1555 | 171 | 0 |
| 2 | 2 | 1692 | 0 | 1699 | 108 | 0 |
| 3 | 3 | 1581 | 0 | 1574 | 135 | 0 |
| 4 | 4 | 1585 | 0 | 1590 | 109 | 0 |
| 5 | 5 | 1646 | 0 | 1595 | 95 | 0 |
| 6 | 6 | 1757 | 0 | 1708 | 104 | 0 |
| 7 | 7 | 1824 | 0 | 1832 | 109 | 0 |
| 8 | A | 1921 | 0 | 1910 | 162 | 0 |
| 9 | B | 1915 | 0 | 1929 | 115 | 0 |
| 10 | C | 1913 | 0 | 1914 | 145 | 0 |
| 11 | D | 1899 | 0 | 1908 | 141 | 0 |
| 12 | E | 1867 | 0 | 1840 | 134 | 0 |
| 13 | F | 1795 | 0 | 1797 | 190 | 0 |
| 14 | G | 1900 | 0 | 1888 | 161 | 0 |
| 15 | H | 2792 | 0 | 2879 | 337 | 0 |
| 16 | I | 2822 | 0 | 2868 | 285 | 0 |
| 17 | J | 2928 | 0 | 3054 | 250 | 0 |
| 18 | K | 3019 | 0 | 3082 | 222 | 0 |
| 19 | L | 2853 | 0 | 2925 | 248 | 0 |
| 20 | M | 2866 | 0 | 2936 | 262 | 0 |
| 21 | N | 6562 | 0 | 6625 | 493 | 0 |
| 22 | O | 3182 | 0 | 3207 | 254 | 0 |
| 23 | P | 3401 | 0 | 3482 | 280 | 0 |
| 24 | Q | 3471 | 0 | 3494 | 277 | 0 |
| 25 | R | 3218 | 0 | 3216 | 296 | 0 |
| 26 | S | 2893 | 0 | 2937 | 218 | 0 |
| 27 | T | 2235 | 0 | 2207 | 174 | 0 |
| 28 | U | 2061 | 0 | 2115 | 247 | 0 |
| 29 | V | 1942 | 0 | 1954 | 186 | 0 |
| 30 | W | 1534 | 0 | 1542 | 145 | 0 |
| 31 | X | 1032 | 0 | 1017 | 103 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 32 | Y | 168 | 0 | 153 | 12 | 0 |
| 33 | Z | 6289 | 0 | 6235 | 798 | 0 |
| All | All | 80139 | 0 | 80667 | 6086 | 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 38.

All (6086) 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) |
|---|---|---|---|
| 33:Z:574:TYR:CE2 | 33:Z:584:VAL:HG11 | 1.29 | 1.68 |
| 23:P:131:PHE:CZ | 23:P:167:THR:HG22 | 1.24 | 1.65 |
| 15:H:172:MET:HB2 | 16:I:129:TYR:CD2 | 1.26 | 1.62 |
| 15:H:396:MET:CE | 15:H:438:ALA:CB | 1.78 | 1.57 |
| 15:H:172:MET:CB | 16:I:129:TYR:CE2 | 1.82 | 1.57 |
| 33:Z:64:TYR:HD2 | 33:Z:111:LEU:CD1 | 0.97 | 1.56 |
| 15:H:172:MET:CB | 16:I:129:TYR:CD2 | 1.75 | 1.55 |
| 33:Z:89:LEU:CD2 | 33:Z:125:THR:HG21 | 1.08 | 1.52 |
| 12:E:15:PHE:CE1 | 12:E:21:LEU:HD11 | 1.46 | 1.51 |
| 28:U:277:TYR:CE1 | 29:V:295:VAL:HG11 | 1.45 | 1.51 |
| 31:X:79:LYS:HE2 | 31:X:98:PHE:CE2 | 1.44 | 1.51 |
| 23:P:267:PHE:CE1 | 23:P:329:PHE:HE2 | 1.25 | 1.51 |
| 30:W:21:PHE:CE1 | 30:W:25:ARG:NH1 | 1.79 | 1.49 |
| 23:P:308:LEU:HD11 | 23:P:349:ASN:CB | 1.37 | 1.49 |
| 31:X:75:TRP:CZ2 | 31:X:125:MET:HG3 | 0.99 | 1.49 |
| 1:1:14:LEU:HD21 | 1:1:100:ALA:CB | 1.43 | 1.48 |
| 15:H:324:GLY:CA | 20:M:290:ARG:NH2 | 1.76 | 1.48 |
| 30:W:21:PHE:HE1 | 30:W:25:ARG:NH1 | 1.03 | 1.48 |
| 31:X:75:TRP:CZ3 | 31:X:125:MET:CE | 1.91 | 1.47 |
| 18:K:272:ASP:CB | 19:L:306:MET:HE1 | 1.45 | 1.47 |
| 16:I:204:HIS:CD2 | 16:I:207:LEU:CD1 | 1.98 | 1.46 |
| 26:S:184:TRP:CZ2 | 26:S:217:PHE:HE2 | 1.28 | 1.46 |
| 33:Z:64:TYR:CD2 | 33:Z:111:LEU:HD13 | 0.94 | 1.46 |
| 21:N:329:HIS:CB | 29:V:182:LYS:HZ1 | 1.28 | 1.45 |
| 30:W:186:ALA:HA | 30:W:191:ILE:CG2 | 1.43 | 1.44 |
| 33:Z:188:ALA:H | 33:Z:201:LEU:CD1 | 1.29 | 1.44 |
| 31:X:75:TRP:CZ2 | 31:X:125:MET:CG | 1.95 | 1.44 |
| 23:P:267:PHE:CE1 | 23:P:329:PHE:CE2 | 2.06 | 1.44 |
| 23:P:308:LEU:HD13 | 23:P:349:ASN:CG | 1.20 | 1.43 |
| 1:1:14:LEU:CD2 | 1:1:100:ALA:HB3 | 1.48 | 1.43 |
| 3:3:129:VAL:HG22 | 3:3:138:PHE:CE1 | 1.54 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:252:ASP:CG | 23:P:85:LYS:NZ | 1.73 | 1.42 |
| 23:P:308:LEU:CD1 | 23:P:349:ASN:CG | 1.87 | 1.42 |
| 18:K:272:ASP:CB | 19:L:306:MET:CE | 1.98 | 1.42 |
| 30:W:25:ARG:NH1 | 30:W:144:PHE:HE2 | 1.13 | 1.42 |
| 17:J:224:GLY:C | 17:J:225:GLU:N | 1.73 | 1.41 |
| 8:A:252:ASP:OD1 | 23:P:85:LYS:CE | 1.68 | 1.40 |
| 18:K:272:ASP:HB3 | 19:L:306:MET:CE | 1.48 | 1.40 |
| 16:I:126:PRO:HB3 | 16:I:128:TYR:CE2 | 1.54 | 1.40 |
| 1:1:83:LYS:NZ | 1:1:118:SER:HA | 1.34 | 1.40 |
| 15:H:324:GLY:N | 20:M:290:ARG:HH21 | 1.07 | 1.40 |
| 24:Q:309:ARG:HH21 | 24:Q:345:SER:CB | 1.35 | 1.40 |
| 33:Z:53:VAL:HG13 | 33:Z:95:THR:CG2 | 1.51 | 1.40 |
| 15:H:173:ARG:CA | 16:I:129:TYR:OH | 1.67 | 1.40 |
| 26:S:461:PHE:CZ | 28:U:274:MET:O | 1.75 | 1.39 |
| 1:1:19:ARG:NH2 | 1:1:171:GLY:N | 1.68 | 1.39 |
| 15:H:396:MET:HE3 | 15:H:438:ALA:CB | 1.42 | 1.39 |
| 33:Z:474:LEU:CD2 | 33:Z:493:LEU:HD22 | 1.51 | 1.39 |
| 33:Z:493:LEU:HD11 | 33:Z:497:PHE:CZ | 1.54 | 1.37 |
| 24:Q:309:ARG:HH21 | 24:Q:345:SER:CA | 1.36 | 1.37 |
| 26:S:461:PHE:CE2 | 28:U:274:MET:O | 1.77 | 1.37 |
| 15:H:172:MET:HB2 | 16:I:129:TYR:CE2 | 1.47 | 1.36 |
| 33:Z:89:LEU:CD2 | 33:Z:125:THR:CG2 | 2.03 | 1.36 |
| 29:V:135:ARG:NE | 29:V:157:ARG:HH12 | 1.23 | 1.35 |
| 17:J:337:LEU:HD22 | 17:J:382:PHE:CZ | 1.58 | 1.35 |
| 22:O:69:PHE:HE2 | 22:O:74:ASN:O | 1.06 | 1.35 |
| 1:1:19:ARG:HH21 | 1:1:171:GLY:N | 1.20 | 1.35 |
| 16:I:126:PRO:CB | 16:I:128:TYR:HE2 | 1.40 | 1.35 |
| 30:W:21:PHE:HE1 | 30:W:25:ARG:CZ | 1.36 | 1.35 |
| 31:X:75:TRP:CZ3 | 31:X:125:MET:HE2 | 1.56 | 1.34 |
| 25:R:209:ARG:NH2 | 25:R:243:LEU:HD11 | 1.35 | 1.34 |
| 16:I:204:HIS:HD2 | 16:I:207:LEU:CD1 | 1.33 | 1.34 |
| 30:W:186:ALA:CA | 30:W:191:ILE:HG22 | 1.56 | 1.34 |
| 20:M:47:GLU:OE2 | 20:M:50:ARG:NH2 | 1.61 | 1.34 |
| 30:W:186:ALA:CA | 30:W:191:ILE:CG2 | 2.06 | 1.34 |
| 8:A:252:ASP:CG | 23:P:85:LYS:HZ1 | 1.25 | 1.33 |
| 29:V:135:ARG:HE | 29:V:157:ARG:NH1 | 1.27 | 1.33 |
| 28:U:203:LYS:CE | 28:U:229:LEU:HD21 | 1.59 | 1.33 |
| 26:S:184:TRP:HZ2 | 26:S:217:PHE:CE2 | 1.46 | 1.32 |
| 23:P:308:LEU:CD1 | 23:P:349:ASN:CB | 2.05 | 1.32 |
| 31:X:75:TRP:CE3 | 31:X:125:MET:HE3 | 1.62 | 1.32 |
| 30:W:25:ARG:NH1 | 30:W:144:PHE:CE2 | 1.96 | 1.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:284:VAL:HB | 20:M:254:MET:CA | 1.60 | 1.31 |
| 26:S:184:TRP:CZ2 | 26:S:217:PHE:CE2 | 2.15 | 1.31 |
| 21:N:424:LYS:NZ | 21:N:461:GLU:HB3 | 1.43 | 1.31 |
| 33:Z:474:LEU:HD23 | 33:Z:493:LEU:CD2 | 1.60 | 1.31 |
| 16:I:204:HIS:CD2 | 16:I:207:LEU:HD13 | 1.60 | 1.31 |
| 23:P:308:LEU:CD1 | 23:P:349:ASN:HB2 | 1.61 | 1.30 |
| 1:1:19:ARG:NH2 | 1:1:171:GLY:H | 1.18 | 1.30 |
| 15:H:156:VAL:HG22 | 15:H:181:TYR:OH | 1.13 | 1.30 |
| 21:N:329:HIS:CB | 29:V:182:LYS:NZ | 1.94 | 1.30 |
| 28:U:277:TYR:CE1 | 29:V:295:VAL:CG1 | 2.14 | 1.30 |
| 3:3:52:THR:OG1 | 4:4:84:ARG:NH2 | 1.63 | 1.30 |
| 29:V:135:ARG:HD2 | 29:V:157:ARG:NH2 | 1.47 | 1.29 |
| 24:Q:418:GLN:HB3 | 29:V:262:THR:CG2 | 1.60 | 1.29 |
| 33:Z:562:TRP:CE2 | 33:Z:566:LEU:HD11 | 1.67 | 1.29 |
| 27:T:86:LYS:CE | 27:T:128:TYR:HE2 | 1.43 | 1.29 |
| 14:G:122:HIS:CD2 | 14:G:128:VAL:HG11 | 1.68 | 1.29 |
| 15:H:173:ARG:N | 16:I:129:TYR:OH | 1.66 | 1.28 |
| 20:M:251:LEU:O | 20:M:252:VAL:N | 1.66 | 1.28 |
| 33:Z:443:ASP:OD2 | 33:Z:447:VAL:HG11 | 1.26 | 1.28 |
| 8:A:205:PHE:CZ | 8:A:209:HIS:CE1 | 2.22 | 1.27 |
| 15:H:284:VAL:HG11 | 20:M:253:GLN:C | 1.54 | 1.27 |
| 22:O:15:ARG:CZ | 22:O:73:ILE:HD11 | 1.63 | 1.27 |
| 18:K:212:TYR:CE1 | 18:K:320:ARG:HA | 1.67 | 1.27 |
| 8:A:220:LYS:CD | 8:A:242:GLU:HB2 | 1.64 | 1.27 |
| 16:I:175:LYS:O | 17:J:282:PHE:CE1 | 1.88 | 1.26 |
| 33:Z:865:ASP:CG | 33:Z:909:ARG:HH21 | 1.34 | 1.26 |
| 24:Q:146:TYR:CE1 | 24:Q:184:VAL:HA | 1.70 | 1.26 |
| 30:W:186:ALA:CB | 30:W:191:ILE:HG21 | 1.64 | 1.26 |
| 21:N:406:TYR:OH | 21:N:748:PHE:CE1 | 1.89 | 1.26 |
| 21:N:596:LEU:HD22 | 21:N:717:LEU:CD1 | 1.66 | 1.25 |
| 22:O:250:TRP:O | 22:O:269:LEU:HD11 | 1.19 | 1.25 |
| 15:H:172:MET:HB3 | 16:I:129:TYR:CE2 | 1.57 | 1.25 |
| 15:H:284:VAL:HB | 20:M:254:MET:CB | 1.66 | 1.25 |
| 23:P:203:ILE:HG12 | 23:P:220:TYR:OH | 1.27 | 1.25 |
| 26:S:315:LYS:HD3 | 26:S:345:TYR:CE1 | 1.69 | 1.25 |
| 22:O:342:ASP:OD1 | 23:P:358:SER:HB2 | 1.11 | 1.25 |
| 33:Z:486:SER:O | 33:Z:490:ILE:HG12 | 1.29 | 1.25 |
| 8:A:252:ASP:CG | 23:P:85:LYS:CE | 2.01 | 1.25 |
| 24:Q:309:ARG:NH2 | 24:Q:345:SER:CB | 1.99 | 1.25 |
| 6:6:91:LYS:HD3 | 6:6:96:TYR:OH | 1.30 | 1.24 |
| 13:F:3:ARG:HH21 | 15:H:359:ASN:ND2 | 1.33 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:336:ALA:HB1 | 19:L:342:ARG:NH1 | 1.53 | 1.24 |
| 23:P:131:PHE:CZ | 23:P:167:THR:CG2 | 2.19 | 1.24 |
| 24:Q:309:ARG:CZ | 24:Q:345:SER:HB3 | 1.68 | 1.24 |
| 27:T:2:PRO:O | 27:T:9:LYS:HD2 | 1.32 | 1.24 |
| 33:Z:442:VAL:HG12 | 33:Z:443:ASP:N | 1.41 | 1.23 |
| 13:F:120:THR:CB | 14:G:129:ARG:HH11 | 1.50 | 1.23 |
| 29:V:107:TRP:CZ3 | 29:V:109:HIS:CD2 | 2.26 | 1.23 |
| 17:J:167:PRO:HB3 | 17:J:174:PHE:CE2 | 1.73 | 1.23 |
| 25:R:301:TYR:CE1 | 25:R:305:PHE:CZ | 2.27 | 1.23 |
| 15:H:396:MET:CE | 15:H:438:ALA:HB1 | 1.48 | 1.22 |
| 31:X:75:TRP:CE2 | 31:X:125:MET:HG3 | 1.74 | 1.22 |
| 33:Z:428:TRP:CZ3 | 33:Z:461:GLY:HA3 | 1.74 | 1.22 |
| 33:Z:442:VAL:CG1 | 33:Z:443:ASP:H | 1.45 | 1.22 |
| 14:G:173:ALA:CB | 19:L:420:ARG:HH21 | 1.52 | 1.22 |
| 15:H:389:PHE:CZ | 15:H:419:LEU:HD22 | 1.73 | 1.22 |
| 17:J:337:LEU:HB2 | 25:R:204:TRP:CZ2 | 1.74 | 1.22 |
| 18:K:212:TYR:HE1 | 18:K:320:ARG:CA | 1.52 | 1.22 |
| 27:T:86:LYS:CE | 27:T:128:TYR:CE2 | 2.23 | 1.22 |
| 33:Z:865:ASP:OD2 | 33:Z:909:ARG:NH2 | 1.71 | 1.22 |
| 15:H:324:GLY:HA3 | 20:M:290:ARG:NH2 | 1.34 | 1.22 |
| 33:Z:64:TYR:OH | 33:Z:115:LEU:HD21 | 1.39 | 1.22 |
| 13:F:84:LEU:HD23 | 13:F:132:LEU:CD1 | 1.70 | 1.21 |
| 27:T:86:LYS:HE3 | 27:T:128:TYR:CE2 | 1.76 | 1.21 |
| 33:Z:246:CYS:SG | 33:Z:271:ILE:HG21 | 1.80 | 1.21 |
| 16:I:384:LYS:HZ3 | 16:I:420:LYS:NZ | 1.39 | 1.20 |
| 33:Z:89:LEU:HD21 | 33:Z:125:THR:CG2 | 1.66 | 1.20 |
| 33:Z:75:ILE:CG2 | 33:Z:121:ILE:HG21 | 1.71 | 1.20 |
| 33:Z:138:ARG:CZ | 33:Z:157:LEU:HG | 1.70 | 1.20 |
| 33:Z:392:LEU:CD1 | 33:Z:424:SER:O | 1.90 | 1.20 |
| 8:A:220:LYS:HD3 | 8:A:242:GLU:CB | 1.70 | 1.20 |
| 13:F:159:THR:HA | 13:F:169:LYS:NZ | 1.57 | 1.20 |
| 16:I:207:LEU:HD13 | 33:Z:930:GLY:HA2 | 1.20 | 1.20 |
| 33:Z:443:ASP:OD2 | 33:Z:447:VAL:CG1 | 1.88 | 1.20 |
| 33:Z:443:ASP:CG | 33:Z:447:VAL:HG11 | 1.62 | 1.20 |
| 31:X:75:TRP:CH2 | 31:X:125:MET:HG3 | 1.76 | 1.19 |
| 14:G:146:HIS:HB3 | 14:G:148:TYR:CE1 | 1.75 | 1.19 |
| 33:Z:419:VAL:O | 33:Z:422:ILE:HG12 | 1.40 | 1.19 |
| 33:Z:574:TYR:CE2 | 33:Z:584:VAL:CG1 | 2.24 | 1.19 |
| 13:F:101:ARG:NH1 | 13:F:103:LEU:HA | 1.55 | 1.19 |
| 13:F:105:VAL:HG22 | 13:F:145:LEU:CD1 | 1.71 | 1.19 |
| 25:R:408:ASP:HB2 | 26:S:464:ARG:NH2 | 1.55 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:S:315:LYS:HD3 | 26:S:345:TYR:CZ | 1.78 | 1.19 |
| 33:Z:823:ASN:HB3 | 33:Z:856:HIS:CE1 | 1.78 | 1.19 |
| 24:Q:309:ARG:NE | 24:Q:345:SER:HB3 | 1.57 | 1.18 |
| 12:E:221:CYS:SG | 12:E:231:TYR:CE2 | 2.34 | 1.18 |
| 17:J:337:LEU:CD2 | 17:J:382:PHE:HZ | 1.56 | 1.18 |
| 17:J:216:ALA:O | 17:J:219:VAL:N | 1.74 | 1.18 |
| 13:F:84:LEU:HD23 | 13:F:132:LEU:HD11 | 1.26 | 1.18 |
| 15:H:59:ILE:HG21 | 16:I:92:GLU:OE2 | 1.41 | 1.18 |
| 25:R:301:TYR:HE1 | 25:R:305:PHE:CZ | 1.60 | 1.18 |
| 33:Z:574:TYR:CZ | 33:Z:584:VAL:HG11 | 1.78 | 1.18 |
| 2:2:50:ALA:CB | 3:3:118:ILE:HG22 | 1.73 | 1.17 |
| 21:N:53:ASP:HA | 21:N:58:ARG:HH21 | 1.08 | 1.17 |
| 24:Q:418:GLN:CB | 29:V:262:THR:HG21 | 1.74 | 1.17 |
| 33:Z:474:LEU:CD2 | 33:Z:493:LEU:CD2 | 2.17 | 1.17 |
| 24:Q:309:ARG:NH2 | 24:Q:345:SER:HB3 | 1.55 | 1.17 |
| 33:Z:217:GLU:CD | 33:Z:244:ARG:HH21 | 1.47 | 1.17 |
| 33:Z:321:PHE:HE2 | 33:Z:351:PRO:HG3 | 1.02 | 1.17 |
| 33:Z:550:PHE:CZ | 33:Z:566:LEU:HB3 | 1.77 | 1.17 |
| 10:C:161:LYS:HD2 | 11:D:56:ASP:HB2 | 1.21 | 1.17 |
| 33:Z:53:VAL:CG1 | 33:Z:95:THR:CG2 | 2.22 | 1.17 |
| 33:Z:138:ARG:NE | 33:Z:157:LEU:HG | 1.56 | 1.17 |
| 15:H:324:GLY:N | 20:M:290:ARG:NH2 | 1.84 | 1.16 |
| 18:K:272:ASP:HB2 | 19:L:306:MET:CE | 1.75 | 1.16 |
| 16:I:395:MET:HE2 | 16:I:420:LYS:NZ | 1.61 | 1.16 |
| 33:Z:823:ASN:HB3 | 33:Z:856:HIS:HE1 | 1.04 | 1.16 |
| 15:H:396:MET:HE2 | 15:H:438:ALA:CB | 1.55 | 1.16 |
| 30:W:186:ALA:CB | 30:W:191:ILE:CG2 | 2.24 | 1.16 |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:CA | 1.75 | 1.16 |
| 33:Z:385:PHE:CE2 | 33:Z:389:PHE:CE2 | 2.33 | 1.15 |
| 8:A:153:SER:HB3 | 8:A:155:TYR:HE1 | 1.05 | 1.15 |
| 28:U:32:ARG:CB | 28:U:94:HIS:HE1 | 1.60 | 1.15 |
| 30:W:9:VAL:HG22 | 30:W:52:ILE:CD1 | 1.76 | 1.15 |
| 31:X:75:TRP:CZ3 | 31:X:125:MET:HE3 | 1.61 | 1.15 |
| 33:Z:863:THR:HG21 | 33:Z:911:LYS:HZ3 | 1.01 | 1.15 |
| 22:O:69:PHE:CE2 | 22:O:74:ASN:O | 1.99 | 1.15 |
| 33:Z:89:LEU:HD22 | 33:Z:125:THR:CG2 | 1.69 | 1.15 |
| 33:Z:385:PHE:CZ | 33:Z:389:PHE:CE2 | 2.33 | 1.15 |
| 23:P:303:PHE:CE1 | 23:P:345:VAL:HG22 | 1.82 | 1.15 |
| 15:H:173:ARG:CB | 16:I:129:TYR:OH | 1.93 | 1.15 |
| 17:J:134:VAL:HG12 | 17:J:135:SER:N | 1.57 | 1.15 |
| 23:P:131:PHE:CE2 | 23:P:167:THR:HG22 | 1.80 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:R:266:LEU:HA | 25:R:270:VAL:HG22 | 1.28 | 1.15 |
| 27:T:157:TYR:OH | 27:T:188:GLU:HG2 | 1.46 | 1.15 |
| 33:Z:205:LEU:HG | 33:Z:236:PHE:CE1 | 1.80 | 1.15 |
| 14:G:7:TYR:CE1 | 14:G:13:VAL:HG21 | 1.80 | 1.14 |
| 11:D:68:ASP:OD2 | 11:D:97:ARG:NH2 | 1.80 | 1.14 |
| 23:P:303:PHE:HE1 | 23:P:345:VAL:HG22 | 1.06 | 1.14 |
| 28:U:277:TYR:CZ | 29:V:295:VAL:HG13 | 1.83 | 1.14 |
| 21:N:282:TYR:CZ | 21:N:286:LEU:HD13 | 1.81 | 1.14 |
| 21:N:329:HIS:HB2 | 29:V:182:LYS:CE | 1.77 | 1.14 |
| 23:P:167:THR:OG1 | 23:P:168:TYR:HD1 | 1.27 | 1.14 |
| 28:U:189:ARG:NH1 | 29:V:296:LEU:HD13 | 1.60 | 1.14 |
| 14:G:111:PHE:HD1 | 14:G:114:ARG:NH2 | 1.44 | 1.14 |
| 23:P:267:PHE:CZ | 23:P:329:PHE:CE2 | 2.35 | 1.14 |
| 1:1:137:TYR:CZ | 1:1:157:HIS:HD2 | 1.65 | 1.14 |
| 30:W:20:ASP:HB3 | 30:W:25:ARG:NH2 | 1.62 | 1.14 |
| 21:N:515:ARG:NH2 | 21:N:738:GLN:OE1 | 1.80 | 1.13 |
| 22:O:250:TRP:HB3 | 22:O:269:LEU:HD21 | 1.25 | 1.13 |
| 26:S:401:LYS:HE2 | 26:S:444:GLU:OE2 | 1.46 | 1.13 |
| 30:W:124:GLU:OE1 | 30:W:127:ARG:NH2 | 1.80 | 1.13 |
| 33:Z:64:TYR:CE2 | 33:Z:111:LEU:HD13 | 1.82 | 1.13 |
| 23:P:308:LEU:HD22 | 23:P:369:LEU:HD23 | 1.30 | 1.13 |
| 29:V:131:GLN:NE2 | 29:V:194:ARG:HH21 | 1.47 | 1.13 |
| 21:N:327:LEU:HD21 | 21:N:743:PHE:HE1 | 1.12 | 1.13 |
| 16:I:384:LYS:NZ | 16:I:420:LYS:HZ2 | 1.44 | 1.13 |
| 28:U:32:ARG:HB3 | 28:U:94:HIS:HE1 | 1.04 | 1.13 |
| 33:Z:154:ILE:HG22 | 33:Z:211:PHE:CZ | 1.84 | 1.13 |
| 33:Z:224:LEU:HD13 | 33:Z:233:LEU:HD23 | 1.22 | 1.13 |
| 12:E:15:PHE:CD1 | 12:E:21:LEU:HD11 | 1.83 | 1.12 |
| 13:F:179:PHE:CZ | 13:F:192:ALA:HB1 | 1.84 | 1.13 |
| 25:R:107:GLU:HG2 | 25:R:111:LYS:HE2 | 1.30 | 1.12 |
| 26:S:401:LYS:HG2 | 26:S:444:GLU:HG2 | 1.28 | 1.13 |
| 13:F:120:THR:HB | 14:G:129:ARG:HH11 | 1.01 | 1.12 |
| 30:W:21:PHE:HZ | 30:W:144:PHE:CD2 | 1.66 | 1.12 |
| 33:Z:75:ILE:HG21 | 33:Z:121:ILE:CG2 | 1.78 | 1.12 |
| 33:Z:278:LEU:HD22 | 33:Z:297:VAL:CG1 | 1.79 | 1.12 |
| 24:Q:299:MET:HE3 | 24:Q:335:PHE:HZ | 1.12 | 1.12 |
| 33:Z:188:ALA:H | 33:Z:201:LEU:HD12 | 1.04 | 1.12 |
| 5:5:8:PHE:CE1 | 5:5:13:ILE:HG12 | 1.85 | 1.12 |
| 25:R:209:ARG:HG3 | 25:R:213:TYR:HE2 | 1.11 | 1.12 |
| 33:Z:138:ARG:NH2 | 33:Z:157:LEU:HD12 | 1.64 | 1.12 |
| 7:7:129:TYR:HE1 | 7:7:134:LEU:HD22 | 1.02 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:F:12:THR:HG23 | 13:F:19:LEU:CD1 | 1.78 | 1.12 |
| 21:N:329:HIS:HB2 | 29:V:182:LYS:HE3 | 1.23 | 1.12 |
| 31:X:79:LYS:CE | 31:X:98:PHE:CE2 | 2.31 | 1.12 |
| 23:P:131:PHE:HA | 23:P:136:ARG:NH1 | 1.64 | 1.11 |
| 30:W:101:ARG:NH1 | 30:W:106:GLN:O | 1.83 | 1.11 |
| 1:1:174:ARG:NH1 | 1:1:185:ARG:HH21 | 1.48 | 1.11 |
| 5:5:135:PHE:HE2 | 5:5:163:ALA:HB1 | 1.08 | 1.11 |
| 33:Z:188:ALA:N | 33:Z:201:LEU:CD1 | 2.12 | 1.11 |
| 33:Z:278:LEU:HD22 | 33:Z:297:VAL:HG13 | 1.12 | 1.11 |
| 17:J:212:ARG:NH1 | 17:J:246:PHE:CE2 | 2.19 | 1.11 |
| 4:4:3:ILE:HG22 | 4:4:102:LEU:HD12 | 1.19 | 1.11 |
| 33:Z:776:VAL:CG1 | 33:Z:777:PRO:HD3 | 1.80 | 1.11 |
| 33:Z:776:VAL:HG12 | 33:Z:777:PRO:HD3 | 1.32 | 1.11 |
| 15:H:102:CYS:CB | 15:H:105:ILE:HD11 | 1.79 | 1.11 |
| 17:J:305:LEU:HD22 | 17:J:313:LYS:HE3 | 1.17 | 1.11 |
| 21:N:492:THR:O | 21:N:528:ARG:NH1 | 1.84 | 1.11 |
| 22:O:233:LEU:HD22 | 22:O:238:ILE:HD11 | 1.30 | 1.11 |
| 24:Q:429:LYS:HB2 | 29:V:269:ARG:NH2 | 1.63 | 1.11 |
| 30:W:9:VAL:CG2 | 30:W:52:ILE:HD11 | 1.79 | 1.11 |
| 33:Z:574:TYR:CZ | 33:Z:584:VAL:HG21 | 1.84 | 1.11 |
| 20:M:251:LEU:C | 20:M:252:VAL:CA | 2.18 | 1.10 |
| 13:F:105:VAL:HG21 | 13:F:145:LEU:HB2 | 1.32 | 1.10 |
| 15:H:436:LYS:HE2 | 33:Z:365:SER:HB2 | 1.20 | 1.10 |
| 33:Z:217:GLU:OE2 | 33:Z:244:ARG:NH2 | 1.85 | 1.10 |
| 33:Z:748:LEU:CD2 | 33:Z:783:VAL:HG13 | 1.80 | 1.10 |
| 15:H:284:VAL:CG1 | 20:M:253:GLN:C | 2.20 | 1.10 |
| 24:Q:275:ILE:HD11 | 24:Q:306:TYR:CD2 | 1.87 | 1.10 |
| 28:U:32:ARG:HB3 | 28:U:94:HIS:CE1 | 1.86 | 1.10 |
| 32:Y:80:GLU:OE2 | 32:Y:83:ARG:NH2 | 1.85 | 1.10 |
| 13:F:12:THR:HG23 | 13:F:19:LEU:HD13 | 1.14 | 1.10 |
| 15:H:284:VAL:HG11 | 20:M:253:GLN:O | 1.50 | 1.10 |
| 24:Q:249:LEU:O | 24:Q:250:THR:HG22 | 1.48 | 1.10 |
| 11:D:159:TRP:CH2 | 12:E:59:LEU:HD13 | 1.86 | 1.09 |
| 19:L:177:GLU:OE1 | 19:L:233:LYS:NZ | 1.84 | 1.09 |
| 23:P:332:GLU:HB3 | 23:P:337:HIS:CE1 | 1.86 | 1.09 |
| 24:Q:61:LEU:HD21 | 24:Q:65:TYR:OH | 1.51 | 1.09 |
| 30:W:21:PHE:CE1 | 30:W:25:ARG:CZ | 2.24 | 1.09 |
| 33:Z:50:GLU:OE2 | 33:Z:55:ARG:NH2 | 1.83 | 1.09 |
| 33:Z:835:ALA:O | 33:Z:838:TYR:HD2 | 1.32 | 1.09 |
| 16:I:214:LYS:HZ2 | 16:I:318:ASP:C | 1.54 | 1.09 |
| 22:O:15:ARG:HH12 | 22:O:73:ILE:CG1 | 1.63 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:418:GLN:HB3 | 29:V:262:THR:HG22 | 1.25 | 1.09 |
| 25:R:363:PHE:HE1 | 32:Y:78:LYS:HD3 | 1.00 | 1.09 |
| 33:Z:68:LEU:CD1 | 33:Z:111:LEU:HD22 | 1.83 | 1.09 |
| 33:Z:748:LEU:HD23 | 33:Z:783:VAL:HG13 | 1.33 | 1.09 |
| 33:Z:763:HIS:CG | 33:Z:766:HIS:HE1 | 1.70 | 1.09 |
| 1:1:83:LYS:CD | 1:1:119:VAL:HG23 | 1.80 | 1.09 |
| 25:R:335:ARG:HD2 | 25:R:376:GLN:HB3 | 1.25 | 1.09 |
| 24:Q:409:TYR:HA | 25:R:403:LEU:HD21 | 1.11 | 1.09 |
| 29:V:135:ARG:CD | 29:V:157:ARG:HH22 | 1.64 | 1.09 |
| 9:B:210:GLU:HG3 | 9:B:237:LYS:HE3 | 1.27 | 1.09 |
| 13:F:7:ASP:HA | 13:F:21:GLN:HE21 | 1.11 | 1.09 |
| 17:J:134:VAL:CG1 | 17:J:135:SER:H | 1.65 | 1.09 |
| 17:J:167:PRO:CA | 17:J:174:PHE:CZ | 2.35 | 1.09 |
| 21:N:398:ARG:HD2 | 21:N:438:ASP:HB3 | 1.17 | 1.09 |
| 23:P:72:TRP:CH2 | 23:P:103:TYR:HB3 | 1.88 | 1.09 |
| 27:T:89:TYR:CD1 | 27:T:102:LYS:HD3 | 1.87 | 1.09 |
| 3:3:129:VAL:CG2 | 3:3:138:PHE:CE1 | 2.36 | 1.08 |
| 28:U:277:TYR:CZ | 29:V:295:VAL:CG1 | 2.34 | 1.08 |
| 20:M:74:GLN:O | 20:M:77:TYR:CE1 | 2.06 | 1.08 |
| 23:P:72:TRP:HH2 | 23:P:103:TYR:HB3 | 1.16 | 1.08 |
| 33:Z:304:PRO:HB3 | 33:Z:342:LEU:HD11 | 1.30 | 1.08 |
| 33:Z:821:GLY:HA2 | 33:Z:863:THR:HG22 | 1.33 | 1.08 |
| 21:N:221:ASP:CA | 21:N:894:ARG:HH22 | 1.67 | 1.08 |
| 21:N:588:VAL:HG11 | 21:N:621:THR:CG2 | 1.83 | 1.08 |
| 33:Z:71:LEU:O | 33:Z:75:ILE:HG13 | 1.53 | 1.08 |
| 33:Z:863:THR:HG21 | 33:Z:911:LYS:NZ | 1.66 | 1.08 |
| 14:G:193:LYS:HE2 | 14:G:241:PHE:HB3 | 1.32 | 1.08 |
| 21:N:327:LEU:CD2 | 21:N:743:PHE:CE1 | 2.37 | 1.08 |
| 13:F:120:THR:HB | 14:G:129:ARG:NH1 | 1.68 | 1.08 |
| 19:L:88:TYR:HD1 | 20:M:62:ILE:HD13 | 1.17 | 1.08 |
| 28:U:32:ARG:HE | 28:U:94:HIS:CE1 | 1.71 | 1.08 |
| 28:U:275:VAL:O | 28:U:278:ILE:HG22 | 1.49 | 1.08 |
| 16:I:248:VAL:HG22 | 17:J:274:GLU:OE1 | 1.54 | 1.07 |
| 25:R:408:ASP:CB | 26:S:464:ARG:HH22 | 1.66 | 1.07 |
| 33:Z:562:TRP:NE1 | 33:Z:566:LEU:HD21 | 1.68 | 1.07 |
| 16:I:204:HIS:HB3 | 16:I:207:LEU:HB2 | 1.36 | 1.07 |
| 16:I:222:TYR:OH | 16:I:349:LEU:HB3 | 1.54 | 1.07 |
| 16:I:253:ILE:CD1 | 16:I:287:ILE:HG22 | 1.84 | 1.07 |
| 17:J:167:PRO:N | 17:J:174:PHE:CZ | 2.22 | 1.07 |
| 22:O:47:LYS:NZ | 22:O:62:TYR:OH | 1.88 | 1.07 |
| 22:O:235:HIS:HD2 | 22:O:236:HIS:CE1 | 1.72 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:P:332:GLU:CB | 23:P:337:HIS:CE1 | 2.38 | 1.07 |
| 26:S:315:LYS:CD | 26:S:345:TYR:CE1 | 2.37 | 1.07 |
| 15:H:284:VAL:HB | 20:M:254:MET:HB3 | 1.26 | 1.07 |
| 21:N:329:HIS:HB3 | 29:V:182:LYS:NZ | 1.54 | 1.07 |
| 21:N:596:LEU:HD22 | 21:N:717:LEU:HD11 | 1.17 | 1.07 |
| 24:Q:273:ASN:CG | 24:Q:306:TYR:OH | 1.92 | 1.07 |
| 31:X:48:PHE:CE2 | 31:X:68:LEU:HD21 | 1.88 | 1.07 |
| 33:Z:278:LEU:CD2 | 33:Z:297:VAL:HG13 | 1.85 | 1.07 |
| 15:H:59:ILE:HD13 | 16:I:92:GLU:OE1 | 1.54 | 1.07 |
| 16:I:207:LEU:HD22 | 33:Z:930:GLY:HA3 | 1.36 | 1.07 |
| 21:N:282:TYR:OH | 21:N:286:LEU:HD13 | 1.52 | 1.07 |
| 23:P:72:TRP:HH2 | 23:P:103:TYR:CB | 1.68 | 1.07 |
| 25:R:63:TYR:HE2 | 25:R:94:PHE:HA | 1.20 | 1.07 |
| 25:R:266:LEU:HA | 25:R:270:VAL:CG2 | 1.85 | 1.07 |
| 28:U:283:ARG:NH1 | 29:V:291:ASN:ND2 | 2.02 | 1.07 |
| 33:Z:106:TRP:HA | 33:Z:112:LYS:HD3 | 1.36 | 1.07 |
| 11:D:97:ARG:NH1 | 11:D:103:PRO:HG3 | 1.69 | 1.07 |
| 13:F:84:LEU:CD2 | 13:F:132:LEU:HD12 | 1.85 | 1.07 |
| 13:F:105:VAL:HG22 | 13:F:145:LEU:HD13 | 1.35 | 1.07 |
| 14:G:121:ALA:O | 14:G:125:TYR:HD1 | 1.34 | 1.07 |
| 21:N:327:LEU:CD2 | 21:N:743:PHE:HE1 | 1.68 | 1.07 |
| 7:7:88:LEU:HD21 | 7:7:106:ILE:HD13 | 1.36 | 1.06 |
| 21:N:330:THR:HG21 | 21:N:739:PHE:HE1 | 1.12 | 1.06 |
| 23:P:144:VAL:HG21 | 23:P:160:LEU:HD21 | 1.33 | 1.06 |
| 8:A:153:SER:HB3 | 8:A:155:TYR:CE1 | 1.90 | 1.06 |
| 10:C:40:ALA:HA | 10:C:184:MET:SD | 1.95 | 1.06 |
| 14:G:215:ILE:HG23 | 14:G:230:VAL:HB | 1.35 | 1.06 |
| 19:L:365:THR:OG1 | 19:L:376:PHE:HE1 | 1.36 | 1.06 |
| 21:N:293:LEU:HD22 | 21:N:379:LEU:HD13 | 1.37 | 1.06 |
| 2:2:50:ALA:HB2 | 3:3:118:ILE:HG22 | 1.35 | 1.06 |
| 23:P:203:ILE:CG1 | 23:P:220:TYR:OH | 2.04 | 1.06 |
| 30:W:152:GLU:OE1 | 30:W:155:ASP:HB2 | 1.53 | 1.06 |
| 8:A:252:ASP:CG | 23:P:85:LYS:HE3 | 1.72 | 1.06 |
| 17:J:337:LEU:HB2 | 25:R:204:TRP:HZ2 | 0.89 | 1.06 |
| 26:S:192:GLU:HG3 | 26:S:239:ARG:HH12 | 1.13 | 1.06 |
| 26:S:461:PHE:CE1 | 28:U:278:ILE:HB | 1.91 | 1.06 |
| 33:Z:301:THR:HG22 | 33:Z:307:HIS:CE1 | 1.90 | 1.06 |
| 2:2:8:PHE:CZ | 2:2:11:GLY:HA3 | 1.91 | 1.06 |
| 2:2:124:TYR:OH | 2:2:139:GLU:HB3 | 1.56 | 1.06 |
| 6:6:91:LYS:HB3 | 6:6:96:TYR:HE1 | 1.15 | 1.06 |
| 7:7:129:TYR:CE1 | 7:7:134:LEU:HD22 | 1.91 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:E:15:PHE:CE1 | 12:E:21:LEU:CD1 | 2.37 | 1.06 |
| 12:E:165:TYR:HB2 | 12:E:167:TYR:CE1 | 1.89 | 1.06 |
| 18:K:272:ASP:HB2 | 19:L:306:MET:HE2 | 1.33 | 1.06 |
| 21:N:329:HIS:CB | 29:V:182:LYS:CE | 2.34 | 1.06 |
| 22:O:62:TYR:CD2 | 22:O:82:LEU:HD13 | 1.91 | 1.06 |
| 33:Z:89:LEU:HD22 | 33:Z:125:THR:HG21 | 1.08 | 1.06 |
| 14:G:7:TYR:CE1 | 14:G:13:VAL:CG2 | 2.39 | 1.05 |
| 15:H:101:ARG:NH2 | 15:H:150:LYS:HE2 | 1.71 | 1.05 |
| 25:R:137:LEU:HB3 | 25:R:141:TYR:CE2 | 1.90 | 1.05 |
| 12:E:15:PHE:CD1 | 12:E:21:LEU:CD1 | 2.38 | 1.05 |
| 14:G:106:ILE:HG12 | 14:G:114:ARG:HH21 | 1.21 | 1.05 |
| 15:H:174:VAL:CG1 | 15:H:183:ILE:HG21 | 1.87 | 1.05 |
| 25:R:363:PHE:CE1 | 32:Y:78:LYS:HD3 | 1.91 | 1.05 |
| 27:T:86:LYS:HE2 | 27:T:128:TYR:CE2 | 1.91 | 1.05 |
| 2:2:50:ALA:CB | 3:3:118:ILE:CG2 | 2.35 | 1.05 |
| 15:H:173:ARG:HB2 | 16:I:129:TYR:OH | 1.55 | 1.05 |
| 19:L:125:PRO:HB2 | 19:L:127:TYR:CE2 | 1.91 | 1.05 |
| 20:M:251:LEU:CA | 20:M:252:VAL:N | 2.18 | 1.05 |
| 27:T:86:LYS:HE3 | 27:T:128:TYR:HE2 | 0.90 | 1.05 |
| 28:U:189:ARG:HH12 | 29:V:296:LEU:HD13 | 1.12 | 1.05 |
| 15:H:456:LYS:HE2 | 16:I:332:GLU:O | 1.57 | 1.05 |
| 22:O:116:ASN:HB3 | 22:O:127:LEU:HD12 | 1.35 | 1.05 |
| 25:R:137:LEU:HB3 | 25:R:141:TYR:HE2 | 1.20 | 1.05 |
| 15:H:156:VAL:HG22 | 15:H:181:TYR:CZ | 1.90 | 1.05 |
| 22:O:62:TYR:HD2 | 22:O:82:LEU:HD13 | 1.11 | 1.05 |
| 22:O:266:PHE:HZ | 22:O:280:LEU:CD2 | 1.70 | 1.05 |
| 26:S:286:TYR:CE1 | 26:S:323:LEU:HB3 | 1.92 | 1.05 |
| 30:W:186:ALA:HB2 | 30:W:191:ILE:HG21 | 1.34 | 1.05 |
| 31:X:75:TRP:CE2 | 31:X:125:MET:CB | 2.39 | 1.05 |
| 6:6:91:LYS:CD | 6:6:96:TYR:OH | 2.05 | 1.04 |
| 21:N:162:ARG:HD3 | 21:N:165:ILE:HG12 | 1.35 | 1.04 |
| 1:1:83:LYS:HZ3 | 1:1:118:SER:CA | 1.70 | 1.04 |
| 9:B:65:SER:HB2 | 9:B:90:ARG:HH21 | 1.18 | 1.04 |
| 23:P:130:ILE:C | 23:P:136:ARG:HH12 | 1.59 | 1.04 |
| 23:P:131:PHE:CA | 23:P:136:ARG:NH1 | 2.20 | 1.04 |
| 23:P:259:PRO:HB2 | 23:P:327:LEU:HD12 | 1.37 | 1.04 |
| 25:R:105:LYS:HE2 | 25:R:109:LYS:NZ | 1.72 | 1.04 |
| 13:F:84:LEU:CD2 | 13:F:132:LEU:CD1 | 2.35 | 1.04 |
| 21:N:584:ARG:NH1 | 21:N:614:ASN:HD22 | 1.54 | 1.04 |
| 25:R:209:ARG:NH2 | 25:R:243:LEU:CD1 | 2.19 | 1.04 |
| 15:H:340:LEU:HD13 | 15:H:370:ARG:HG3 | 1.35 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:293:LEU:CD2 | 21:N:379:LEU:HD13 | 1.87 | 1.04 |
| 33:Z:321:PHE:CE2 | 33:Z:351:PRO:HG3 | 1.92 | 1.04 |
| 16:I:175:LYS:O | 17:J:282:PHE:CD1 | 2.11 | 1.04 |
| 22:O:250:TRP:CB | 22:O:269:LEU:HD21 | 1.87 | 1.04 |
| 31:X:75:TRP:CH2 | 31:X:125:MET:CE | 2.41 | 1.04 |
| 31:X:91:PHE:H | 31:X:96:ARG:HG2 | 1.16 | 1.04 |
| 2:2:124:TYR:OH | 2:2:139:GLU:CB | 2.06 | 1.03 |
| 5:5:135:PHE:CE2 | 5:5:163:ALA:HB1 | 1.92 | 1.03 |
| 21:N:588:VAL:CG1 | 21:N:621:THR:HG22 | 1.88 | 1.03 |
| 22:O:185:PHE:CD2 | 22:O:223:LEU:HD13 | 1.93 | 1.03 |
| 23:P:308:LEU:HD13 | 23:P:349:ASN:ND2 | 1.73 | 1.03 |
| 28:U:92:TRP:HZ2 | 28:U:120:LEU:HD12 | 1.22 | 1.03 |
| 11:D:10:ILE:HD11 | 12:E:10:ARG:HD2 | 1.38 | 1.03 |
| 13:F:120:THR:O | 14:G:129:ARG:HD2 | 1.56 | 1.03 |
| 16:I:380:LEU:HD22 | 16:I:420:LYS:HG3 | 1.40 | 1.03 |
| 24:Q:309:ARG:NH2 | 24:Q:345:SER:CA | 2.18 | 1.03 |
| 16:I:320:GLY:HA2 | 16:I:323:LYS:HE2 | 1.39 | 1.03 |
| 22:O:342:ASP:OD1 | 23:P:358:SER:CB | 2.06 | 1.03 |
| 33:Z:865:ASP:CG | 33:Z:909:ARG:NH2 | 2.09 | 1.03 |
| 4:4:66:TYR:CE2 | 10:C:102:TYR:OH | 2.12 | 1.03 |
| 15:H:323:ALA:C | 20:M:290:ARG:HH21 | 1.62 | 1.03 |
| 21:N:330:THR:HG21 | 21:N:739:PHE:CE1 | 1.91 | 1.03 |
| 21:N:584:ARG:HH11 | 21:N:614:ASN:ND2 | 1.56 | 1.03 |
| 25:R:408:ASP:HB2 | 26:S:464:ARG:HH22 | 1.10 | 1.03 |
| 33:Z:53:VAL:CG1 | 33:Z:95:THR:HG21 | 1.83 | 1.03 |
| 33:Z:923:ILE:HD11 | 33:Z:985:LYS:HE2 | 1.40 | 1.03 |
| 15:H:206:VAL:HG21 | 15:H:261:ARG:HE | 1.23 | 1.03 |
| 25:R:70:TYR:OH | 25:R:75:GLY:C | 1.97 | 1.03 |
| 28:U:203:LYS:CE | 28:U:229:LEU:CD2 | 2.36 | 1.03 |
| 15:H:174:VAL:HG13 | 15:H:183:ILE:HG21 | 1.34 | 1.02 |
| 15:H:329:VAL:HG21 | 16:I:300:ARG:HH12 | 1.20 | 1.02 |
| 18:K:346:ARG:HG2 | 18:K:349:ARG:NH2 | 1.74 | 1.02 |
| 29:V:107:TRP:CZ3 | 29:V:109:HIS:HD2 | 1.70 | 1.02 |
| 7:7:33:ARG:HH21 | 7:7:46:SER:HA | 1.17 | 1.02 |
| 8:A:128:TYR:CZ | 8:A:134:MET:HE1 | 1.94 | 1.02 |
| 14:G:122:HIS:CD2 | 14:G:128:VAL:CG1 | 2.42 | 1.02 |
| 15:H:156:VAL:CG2 | 15:H:181:TYR:OH | 2.05 | 1.02 |
| 15:H:324:GLY:CA | 20:M:290:ARG:HH21 | 1.56 | 1.02 |
| 19:L:361:PHE:CZ | 19:L:391:ILE:HD12 | 1.93 | 1.02 |
| 33:Z:392:LEU:HD12 | 33:Z:424:SER:O | 1.54 | 1.02 |
| 19:L:340:PRO:HB3 | 19:L:344:ASP:OD2 | 1.58 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:327:LEU:HD23 | 21:N:743:PHE:CE1 | 1.94 | 1.02 |
| 33:Z:443:ASP:CB | 33:Z:447:VAL:HG11 | 1.89 | 1.02 |
| 15:H:102:CYS:HB2 | 15:H:105:ILE:HD11 | 1.37 | 1.02 |
| 16:I:204:HIS:CG | 16:I:207:LEU:HD12 | 1.94 | 1.02 |
| 16:I:222:TYR:CZ | 16:I:349:LEU:HB3 | 1.93 | 1.02 |
| 27:T:126:LEU:HD22 | 27:T:136:LEU:HD21 | 1.39 | 1.02 |
| 10:C:115:LEU:CD1 | 10:C:137:TYR:OH | 2.08 | 1.02 |
| 16:I:395:MET:CE | 16:I:420:LYS:HZ3 | 1.73 | 1.02 |
| 21:N:329:HIS:CG | 29:V:182:LYS:HZ1 | 1.77 | 1.02 |
| 33:Z:493:LEU:CD1 | 33:Z:497:PHE:CZ | 2.43 | 1.02 |
| 6:6:91:LYS:HB3 | 6:6:96:TYR:CE1 | 1.94 | 1.01 |
| 19:L:189:GLN:NE2 | 19:L:350:PRO:HD2 | 1.74 | 1.01 |
| 15:H:173:ARG:N | 16:I:129:TYR:CZ | 2.28 | 1.01 |
| 18:K:212:TYR:HE1 | 18:K:320:ARG:HA | 0.99 | 1.01 |
| 8:A:252:ASP:OXT | 23:P:44:LYS:NZ | 1.94 | 1.01 |
| 15:H:156:VAL:HG13 | 15:H:181:TYR:CE1 | 1.95 | 1.01 |
| 15:H:284:VAL:CB | 20:M:254:MET:CA | 2.38 | 1.01 |
| 23:P:332:GLU:HB3 | 23:P:337:HIS:NE2 | 1.74 | 1.01 |
| 30:W:20:ASP:CB | 30:W:25:ARG:NH2 | 2.23 | 1.01 |
| 30:W:21:PHE:CZ | 30:W:144:PHE:CE2 | 2.48 | 1.01 |
| 33:Z:886:VAL:HA | 33:Z:893:PHE:CE2 | 1.94 | 1.01 |
| 3:3:60:TYR:CD2 | 10:C:96:GLN:HB3 | 1.95 | 1.01 |
| 19:L:290:ARG:HD2 | 19:L:293:GLU:HA | 1.43 | 1.01 |
| 21:N:717:LEU:CD2 | 21:N:733:LEU:CD1 | 2.39 | 1.01 |
| 30:W:20:ASP:CB | 30:W:25:ARG:HH21 | 1.73 | 1.01 |
| 10:C:177:GLN:HG2 | 11:D:54:LEU:HD21 | 1.41 | 1.01 |
| 16:I:174:ASP:OD1 | 17:J:282:PHE:HB2 | 1.61 | 1.01 |
| 24:Q:36:SER:O | 24:Q:46:VAL:HG23 | 1.60 | 1.01 |
| 33:Z:68:LEU:HD12 | 33:Z:111:LEU:HD22 | 1.02 | 1.01 |
| 33:Z:138:ARG:NH2 | 33:Z:157:LEU:CD1 | 2.24 | 1.01 |
| 33:Z:863:THR:CG2 | 33:Z:911:LYS:HZ3 | 1.74 | 1.01 |
| 1:1:137:TYR:CZ | 1:1:157:HIS:CD2 | 2.49 | 1.00 |
| 4:4:45:PHE:CD2 | 4:4:101:VAL:HG12 | 1.96 | 1.00 |
| 16:I:204:HIS:CD2 | 16:I:207:LEU:HD12 | 1.96 | 1.00 |
| 23:P:366:ASN:ND2 | 23:P:373:GLU:HA | 1.74 | 1.00 |
| 28:U:16:LEU:HD23 | 28:U:19:LEU:HD12 | 1.43 | 1.00 |
| 1:1:-8:LYS:HZ3 | 2:2:117:GLY:HA3 | 1.26 | 1.00 |
| 28:U:203:LYS:HE3 | 28:U:229:LEU:CD2 | 1.91 | 1.00 |
| 30:W:21:PHE:CZ | 30:W:144:PHE:CD2 | 2.48 | 1.00 |
| 2:2:50:ALA:HB3 | 3:3:118:ILE:CG2 | 1.92 | 1.00 |
| 7:7:33:ARG:HH21 | 7:7:46:SER:CA | 1.74 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:J:340:GLY:HA2 | 25:R:238:PHE:CE1 | 1.95 | 1.00 |
| 22:O:15:ARG:NH1 | 22:O:73:ILE:CG1 | 2.23 | 1.00 |
| 29:V:145:GLN:HG2 | 29:V:148:LYS:HE3 | 1.44 | 1.00 |
| 20:M:50:ARG:NH1 | 20:M:54:GLU:OE2 | 1.95 | 1.00 |
| 25:R:167:LYS:HE2 | 25:R:197:MET:HE2 | 1.43 | 1.00 |
| 16:I:395:MET:HE2 | 16:I:420:LYS:HZ3 | 0.83 | 1.00 |
| 33:Z:385:PHE:CZ | 33:Z:389:PHE:CZ | 2.50 | 1.00 |
| 16:I:204:HIS:CG | 16:I:207:LEU:CD1 | 2.45 | 0.99 |
| 28:U:67:PHE:CE1 | 30:W:97:THR:OG1 | 2.13 | 0.99 |
| 19:L:290:ARG:NH1 | 19:L:293:GLU:HB3 | 1.77 | 0.99 |
| 26:S:428:ARG:HA | 27:T:195:LEU:CD2 | 1.91 | 0.99 |
| 21:N:362:TRP:CZ2 | 29:V:23:THR:HG21 | 1.97 | 0.99 |
| 14:G:173:ALA:CB | 19:L:420:ARG:NH2 | 2.23 | 0.99 |
| 33:Z:154:ILE:CG2 | 33:Z:211:PHE:CZ | 2.45 | 0.99 |
| 25:R:335:ARG:CD | 25:R:376:GLN:HB3 | 1.90 | 0.99 |
| 14:G:200:TYR:CE1 | 14:G:246:ILE:CG2 | 2.45 | 0.99 |
| 31:X:75:TRP:CE2 | 31:X:125:MET:CG | 2.40 | 0.99 |
| 33:Z:246:CYS:SG | 33:Z:271:ILE:CG2 | 2.50 | 0.99 |
| 21:N:53:ASP:CA | 21:N:58:ARG:HH21 | 1.75 | 0.99 |
| 25:R:241:ILE:HG22 | 25:R:242:GLU:HG3 | 1.41 | 0.99 |
| 28:U:203:LYS:HE3 | 28:U:229:LEU:HD21 | 1.02 | 0.99 |
| 33:Z:562:TRP:HE1 | 33:Z:566:LEU:HD21 | 1.21 | 0.99 |
| 14:G:111:PHE:CD1 | 14:G:114:ARG:NH2 | 2.27 | 0.99 |
| 17:J:62:LEU:HD11 | 18:K:89:ILE:HG13 | 1.41 | 0.99 |
| 23:P:272:PRO:O | 23:P:273:TYR:CD1 | 2.15 | 0.99 |
| 1:1:-8:LYS:NZ | 2:2:117:GLY:HA3 | 1.78 | 0.99 |
| 12:E:87:SER:O | 12:E:91:HIS:ND1 | 1.94 | 0.99 |
| 14:G:168:ARG:HE | 14:G:172:LYS:NZ | 1.59 | 0.99 |
| 22:O:15:ARG:NH1 | 22:O:73:ILE:HD11 | 1.77 | 0.99 |
| 22:O:377:VAL:HG21 | 28:U:200:LEU:HD11 | 1.45 | 0.99 |
| 33:Z:884:THR:O | 33:Z:888:LEU:HD12 | 1.61 | 0.99 |
| 15:H:323:ALA:C | 20:M:290:ARG:NH2 | 2.14 | 0.99 |
| 19:L:88:TYR:CD1 | 20:M:62:ILE:HB | 1.97 | 0.99 |
| 24:Q:418:GLN:HB2 | 29:V:262:THR:HG21 | 1.40 | 0.99 |
| 22:O:228:TYR:HA | 22:O:290:LYS:NZ | 1.76 | 0.98 |
| 13:F:101:ARG:HH12 | 13:F:103:LEU:HD12 | 1.26 | 0.98 |
| 18:K:280:LYS:NZ | 18:K:296:LEU:HD23 | 1.78 | 0.98 |
| 27:T:126:LEU:HD22 | 27:T:136:LEU:CD2 | 1.93 | 0.98 |
| 33:Z:64:TYR:CD2 | 33:Z:111:LEU:CD1 | 1.87 | 0.98 |
| 33:Z:886:VAL:HG13 | 33:Z:893:PHE:CZ | 1.98 | 0.98 |
| 15:H:172:MET:HB3 | 16:I:129:TYR:CD2 | 1.66 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:K:242:PHE:C | 18:K:243:VAL:N | 2.17 | 0.98 |
| 3:3:37:TYR:OH | 3:3:59:ARG:HB2 | 1.64 | 0.98 |
| 17:J:337:LEU:CB | 25:R:204:TRP:HZ2 | 1.76 | 0.98 |
| 21:N:593:PHE:CZ | 21:N:734:VAL:HG22 | 1.97 | 0.98 |
| 33:Z:188:ALA:H | 33:Z:201:LEU:HD11 | 1.24 | 0.98 |
| 16:I:126:PRO:HG2 | 16:I:154:MET:CE | 1.93 | 0.98 |
| 17:J:340:GLY:CA | 25:R:238:PHE:CE1 | 2.46 | 0.98 |
| 2:2:160:GLN:NE2 | 2:2:164:TRP:NE1 | 2.10 | 0.98 |
| 20:M:196:ALA:HB2 | 20:M:345:ARG:HE | 1.24 | 0.98 |
| 24:Q:299:MET:CE | 24:Q:335:PHE:HZ | 1.77 | 0.98 |
| 33:Z:74:SER:HB2 | 33:Z:79:THR:HG22 | 1.45 | 0.98 |
| 8:A:164:VAL:HB | 9:B:61:LEU:HD21 | 1.44 | 0.98 |
| 12:E:165:TYR:HB2 | 12:E:167:TYR:HE1 | 1.27 | 0.98 |
| 19:L:365:THR:OG1 | 19:L:376:PHE:CE1 | 2.11 | 0.98 |
| 33:Z:929:VAL:O | 33:Z:955:VAL:HG22 | 1.63 | 0.98 |
| 1:1:83:LYS:HD2 | 1:1:119:VAL:HG23 | 1.00 | 0.98 |
| 11:D:10:ILE:H | 11:D:18:PHE:HE2 | 1.05 | 0.98 |
| 15:H:172:MET:C | 16:I:129:TYR:CE2 | 2.36 | 0.98 |
| 23:P:344:ARG:O | 23:P:348:HIS:ND1 | 1.97 | 0.98 |
| 14:G:7:TYR:HE1 | 14:G:13:VAL:HG21 | 1.26 | 0.97 |
| 25:R:158:LEU:HD11 | 25:R:197:MET:HE1 | 1.46 | 0.97 |
| 33:Z:68:LEU:HD12 | 33:Z:111:LEU:CD2 | 1.93 | 0.97 |
| 12:E:15:PHE:HE1 | 12:E:21:LEU:HD11 | 1.21 | 0.97 |
| 17:J:167:PRO:CB | 17:J:174:PHE:CE2 | 2.47 | 0.97 |
| 19:L:336:ALA:HB1 | 19:L:342:ARG:HH12 | 1.05 | 0.97 |
| 9:B:218:ASN:O | 9:B:222:LEU:HG | 1.64 | 0.97 |
| 26:S:141:LEU:O | 26:S:145:PHE:HD1 | 1.47 | 0.97 |
| 33:Z:805:LEU:HD22 | 33:Z:841:GLU:CD | 1.83 | 0.97 |
| 15:H:101:ARG:HH22 | 15:H:150:LYS:HE2 | 1.29 | 0.97 |
| 15:H:379:LEU:CD2 | 15:H:415:THR:HG22 | 1.94 | 0.97 |
| 17:J:277:ASN:HD21 | 17:J:309:ARG:CZ | 1.76 | 0.97 |
| 17:J:134:VAL:HG12 | 17:J:135:SER:H | 0.82 | 0.97 |
| 21:N:329:HIS:HB3 | 29:V:182:LYS:HZ1 | 0.80 | 0.97 |
| 21:N:424:LYS:HZ1 | 21:N:461:GLU:HB3 | 0.82 | 0.97 |
| 22:O:190:TYR:HD1 | 22:O:227:ILE:HD11 | 1.30 | 0.97 |
| 26:S:286:TYR:CZ | 26:S:323:LEU:HB3 | 2.00 | 0.97 |
| 11:D:193:LYS:HG3 | 11:D:197:ARG:NH1 | 1.80 | 0.97 |
| 15:H:396:MET:CE | 15:H:438:ALA:HB3 | 1.94 | 0.97 |
| 30:W:141:ILE:HD13 | 30:W:154:LEU:HD22 | 1.45 | 0.97 |
| 3:3:60:TYR:HA | 10:C:96:GLN:OE1 | 1.65 | 0.97 |
| 16:I:310:LEU:HD11 | 16:I:337:ALA:O | 1.65 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:396:MET:HE2 | 15:H:438:ALA:HB1 | 1.14 | 0.97 |
| 17:J:228:ARG:NH1 | 17:J:232:GLU:OE2 | 1.97 | 0.97 |
| 24:Q:418:GLN:CB | 29:V:262:THR:CG2 | 2.33 | 0.97 |
| 28:U:32:ARG:CB | 28:U:94:HIS:CE1 | 2.45 | 0.97 |
| 33:Z:769:ASN:HB3 | 33:Z:772:ILE:HD12 | 1.47 | 0.97 |
| 10:C:3:SER:HB3 | 11:D:6:ARG:NH2 | 1.78 | 0.97 |
| 13:F:179:PHE:CZ | 13:F:192:ALA:CB | 2.47 | 0.96 |
| 16:I:104:LEU:CD2 | 16:I:149:LEU:O | 2.13 | 0.96 |
| 20:M:148:VAL:HG22 | 20:M:155:ILE:HG12 | 1.46 | 0.96 |
| 28:U:21:HIS:CE1 | 28:U:93:TYR:OH | 2.18 | 0.96 |
| 30:W:103:ASN:HB2 | 30:W:106:GLN:HE21 | 1.30 | 0.96 |
| 33:Z:474:LEU:HD23 | 33:Z:493:LEU:HD22 | 0.99 | 0.96 |
| 33:Z:835:ALA:O | 33:Z:838:TYR:CD2 | 2.19 | 0.96 |
| 33:Z:290:GLU:HG3 | 33:Z:293:MET:CE | 1.95 | 0.96 |
| 7:7:93:TYR:HE1 | 7:7:96:ARG:HH21 | 1.04 | 0.96 |
| 24:Q:309:ARG:HE | 24:Q:345:SER:HB3 | 1.22 | 0.96 |
| 24:Q:429:LYS:HB2 | 29:V:269:ARG:HH21 | 1.30 | 0.96 |
| 30:W:9:VAL:HG22 | 30:W:52:ILE:HD11 | 0.98 | 0.96 |
| 15:H:59:ILE:HD13 | 16:I:92:GLU:CD | 1.85 | 0.96 |
| 18:K:272:ASP:CB | 19:L:306:MET:HE2 | 1.87 | 0.96 |
| 1:1:83:LYS:NZ | 1:1:118:SER:CA | 2.28 | 0.96 |
| 3:3:129:VAL:HG22 | 3:3:138:PHE:CD1 | 1.99 | 0.96 |
| 7:7:93:TYR:CE1 | 7:7:96:ARG:NH2 | 2.32 | 0.96 |
| 20:M:75:LEU:HA | 20:M:77:TYR:HD1 | 1.30 | 0.96 |
| 21:N:318:LYS:HA | 29:V:180:LEU:HG | 1.46 | 0.96 |
| 25:R:70:TYR:OH | 25:R:75:GLY:O | 1.82 | 0.96 |
| 33:Z:394:TYR:HD2 | 33:Z:396:ASN:ND2 | 1.62 | 0.96 |
| 16:I:207:LEU:HD22 | 33:Z:930:GLY:CA | 1.95 | 0.96 |
| 21:N:329:HIS:CB | 29:V:182:LYS:HE3 | 1.93 | 0.96 |
| 28:U:119:LEU:HD12 | 28:U:137:TYR:O | 1.65 | 0.96 |
| 19:L:159:LEU:HD12 | 19:L:160:PRO:O | 1.64 | 0.96 |
| 21:N:588:VAL:HG11 | 21:N:621:THR:HG22 | 1.45 | 0.96 |
| 1:1:14:LEU:HD11 | 1:1:100:ALA:HB1 | 1.48 | 0.96 |
| 18:K:159:SER:CB | 18:K:244:HIS:HE2 | 1.79 | 0.96 |
| 22:O:59:LEU:HD21 | 22:O:85:SER:CB | 1.95 | 0.96 |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:HD11 | 1.20 | 0.96 |
| 33:Z:208:VAL:HG21 | 33:Z:236:PHE:CE2 | 2.01 | 0.96 |
| 2:2:82:MET:O | 2:2:86:HIS:ND1 | 1.97 | 0.96 |
| 28:U:92:TRP:CZ2 | 28:U:120:LEU:HD12 | 2.01 | 0.96 |
| 15:H:249:TYR:CE1 | 15:H:376:GLU:HA | 2.01 | 0.95 |
| 21:N:162:ARG:CD | 21:N:165:ILE:HG12 | 1.95 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:I:172:LYS:HG2 | 17:J:278:GLN:HG3 | 1.49 | 0.95 |
| 28:U:32:ARG:CG | 28:U:94:HIS:CE1 | 2.48 | 0.95 |
| 28:U:92:TRP:CZ2 | 28:U:120:LEU:CD1 | 2.49 | 0.95 |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:CE2 | 2.01 | 0.95 |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:HD22 | 1.49 | 0.95 |
| 19:L:336:ALA:C | 19:L:342:ARG:HH11 | 1.69 | 0.95 |
| 23:P:141:LYS:HB2 | 23:P:179:PHE:HE1 | 1.30 | 0.95 |
| 2:2:8:PHE:CZ | 2:2:11:GLY:CA | 2.49 | 0.95 |
| 14:G:200:TYR:CE1 | 14:G:246:ILE:HG21 | 2.01 | 0.95 |
| 15:H:306:ILE:HG22 | 15:H:308:PHE:CE1 | 2.01 | 0.95 |
| 33:Z:89:LEU:HD22 | 33:Z:125:THR:CB | 1.94 | 0.95 |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:HA | 1.45 | 0.95 |
| 15:H:172:MET:CB | 16:I:129:TYR:HD2 | 1.75 | 0.95 |
| 15:H:324:GLY:CA | 20:M:290:ARG:HH22 | 1.54 | 0.95 |
| 25:R:209:ARG:HG3 | 25:R:213:TYR:CE2 | 2.02 | 0.95 |
| 33:Z:322:GLU:HG2 | 33:Z:464:ASP:OD2 | 1.67 | 0.95 |
| 7:7:193:ASP:HB3 | 7:7:196:THR:OG1 | 1.64 | 0.95 |
| 15:H:436:LYS:HE2 | 33:Z:365:SER:CB | 1.97 | 0.95 |
| 21:N:346:ASN:HB3 | 21:N:350:LYS:HE3 | 1.47 | 0.95 |
| 22:O:266:PHE:HZ | 22:O:280:LEU:HD22 | 1.31 | 0.95 |
| 23:P:131:PHE:N | 23:P:136:ARG:HH12 | 1.64 | 0.95 |
| 33:Z:64:TYR:CE2 | 33:Z:68:LEU:HD11 | 2.01 | 0.95 |
| 14:G:53:ILE:HD11 | 14:G:212:GLU:HB2 | 1.46 | 0.95 |
| 21:N:424:LYS:NZ | 21:N:461:GLU:CB | 2.30 | 0.95 |
| 28:U:67:PHE:CZ | 30:W:97:THR:HA | 2.00 | 0.95 |
| 29:V:131:GLN:HE22 | 29:V:194:ARG:HH21 | 1.12 | 0.95 |
| 24:Q:309:ARG:HH21 | 24:Q:345:SER:HA | 1.28 | 0.95 |
| 33:Z:884:THR:O | 33:Z:888:LEU:CD1 | 2.13 | 0.95 |
| 7:7:68:TYR:OH | 14:G:70:ASP:N | 1.99 | 0.95 |
| 23:P:131:PHE:HA | 23:P:136:ARG:HH11 | 1.25 | 0.95 |
| 28:U:67:PHE:CE2 | 30:W:97:THR:HA | 2.02 | 0.95 |
| 29:V:135:ARG:HA | 29:V:157:ARG:CZ | 1.97 | 0.95 |
| 33:Z:748:LEU:CD2 | 33:Z:783:VAL:CG1 | 2.45 | 0.95 |
| 14:G:146:HIS:CB | 14:G:148:TYR:HE1 | 1.79 | 0.95 |
| 23:P:366:ASN:HD21 | 23:P:373:GLU:HA | 1.28 | 0.95 |
| 33:Z:64:TYR:CZ | 33:Z:68:LEU:HD11 | 2.02 | 0.95 |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:CG1 | 1.96 | 0.95 |
| 19:L:336:ALA:CB | 19:L:342:ARG:HH12 | 1.80 | 0.94 |
| 24:Q:146:TYR:HE1 | 24:Q:184:VAL:HA | 1.15 | 0.94 |
| 16:I:204:HIS:HD2 | 16:I:207:LEU:HD11 | 1.28 | 0.94 |
| 20:M:197:ILE:HB | 20:M:322:LYS:HD3 | 1.46 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:290:GLU:HG3 | 33:Z:293:MET:HE1 | 1.46 | 0.94 |
| 16:I:253:ILE:HD13 | 16:I:287:ILE:HG22 | 1.48 | 0.94 |
| 7:7:145:PRO:HA | 7:7:148:ARG:HE | 1.32 | 0.94 |
| 15:H:172:MET:HB2 | 16:I:129:TYR:CG | 2.01 | 0.94 |
| 18:K:137:VAL:HB | 18:K:146:LEU:CD1 | 1.98 | 0.94 |
| 22:O:59:LEU:HD21 | 22:O:85:SER:HB3 | 1.48 | 0.94 |
| 15:H:59:ILE:CD1 | 16:I:92:GLU:OE1 | 2.15 | 0.94 |
| 33:Z:562:TRP:NE1 | 33:Z:566:LEU:CD2 | 2.29 | 0.94 |
| 14:G:122:HIS:NE2 | 14:G:128:VAL:HG11 | 1.82 | 0.94 |
| 15:H:284:VAL:CG2 | 20:M:254:MET:HA | 1.98 | 0.94 |
| 18:K:135:MET:HG2 | 18:K:259:ARG:HH22 | 1.31 | 0.94 |
| 33:Z:165:TYR:HE1 | 33:Z:190:THR:HG1 | 0.96 | 0.94 |
| 33:Z:327:GLN:HG2 | 33:Z:349:THR:HB | 1.47 | 0.94 |
| 8:A:205:PHE:CZ | 8:A:209:HIS:HE1 | 1.82 | 0.94 |
| 26:S:343:LEU:CD1 | 26:S:347:HIS:HE1 | 1.81 | 0.94 |
| 30:W:158:ILE:HG13 | 30:W:171:LEU:HB2 | 1.50 | 0.94 |
| 1:1:83:LYS:HD2 | 1:1:119:VAL:CG2 | 1.95 | 0.94 |
| 4:4:129:TYR:OH | 4:4:144:ASP:OD1 | 1.86 | 0.94 |
| 14:G:173:ALA:HA | 19:L:420:ARG:NH2 | 1.83 | 0.94 |
| 16:I:310:LEU:HD13 | 16:I:338:LEU:HA | 1.50 | 0.94 |
| 18:K:224:LYS:CE | 18:K:236:ARG:NH2 | 2.30 | 0.94 |
| 20:M:74:GLN:O | 20:M:77:TYR:HE1 | 1.49 | 0.94 |
| 25:R:411:LEU:CD2 | 26:S:464:ARG:HH11 | 1.81 | 0.94 |
| 28:U:283:ARG:HH12 | 29:V:291:ASN:ND2 | 1.60 | 0.94 |
| 33:Z:205:LEU:CG | 33:Z:236:PHE:HE1 | 1.80 | 0.94 |
| 33:Z:497:PHE:CE2 | 33:Z:505:VAL:HG12 | 2.02 | 0.94 |
| 19:L:336:ALA:CB | 19:L:342:ARG:NH1 | 2.30 | 0.94 |
| 6:6:91:LYS:HD3 | 6:6:96:TYR:HH | 1.25 | 0.94 |
| 13:F:13:PHE:HE1 | 14:G:130:PRO:HD2 | 1.32 | 0.93 |
| 15:H:172:MET:CG | 16:I:129:TYR:CD2 | 2.51 | 0.93 |
| 33:Z:863:THR:CG2 | 33:Z:911:LYS:NZ | 2.31 | 0.93 |
| 13:F:120:THR:CB | 14:G:129:ARG:NH1 | 2.27 | 0.93 |
| 21:N:536:ILE:HD13 | 21:N:555:ILE:CG1 | 1.98 | 0.93 |
| 23:P:308:LEU:CD1 | 23:P:349:ASN:OD1 | 2.16 | 0.93 |
| 30:W:44:ASN:HB2 | 30:W:47:ASN:HD21 | 1.32 | 0.93 |
| 33:Z:56:LEU:CD2 | 33:Z:68:LEU:HD23 | 1.99 | 0.93 |
| 33:Z:385:PHE:CE2 | 33:Z:389:PHE:HE2 | 1.79 | 0.93 |
| 33:Z:562:TRP:CD1 | 33:Z:566:LEU:HG | 2.02 | 0.93 |
| 25:R:130:GLN:HE21 | 25:R:134:TRP:HE1 | 1.12 | 0.93 |
| 22:O:356:ARG:HH12 | 28:U:234:ASN:HB2 | 1.32 | 0.93 |
| 17:J:337:LEU:HD23 | 17:J:377:VAL:HB | 1.49 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:299:MET:CE | 24:Q:335:PHE:CZ | 2.52 | 0.93 |
| 33:Z:427:GLN:HG2 | 33:Z:428:TRP:CD1 | 2.03 | 0.93 |
| 25:R:50:VAL:HG13 | 25:R:54:ILE:HD12 | 1.50 | 0.93 |
| 26:S:461:PHE:CD2 | 28:U:277:TYR:HB2 | 2.03 | 0.93 |
| 26:S:141:LEU:O | 26:S:145:PHE:CD1 | 2.21 | 0.93 |
| 30:W:139:VAL:HG11 | 30:W:157:PHE:CE2 | 2.04 | 0.93 |
| 1:1:57:ASP:HB3 | 8:A:106:TYR:CE1 | 2.02 | 0.93 |
| 14:G:121:ALA:O | 14:G:125:TYR:CD1 | 2.22 | 0.93 |
| 19:L:88:TYR:CE1 | 20:M:62:ILE:HB | 2.02 | 0.93 |
| 21:N:329:HIS:CG | 29:V:182:LYS:NZ | 2.34 | 0.93 |
| 33:Z:546:ILE:CG2 | 33:Z:550:PHE:CE2 | 2.51 | 0.93 |
| 1:1:19:ARG:HH21 | 1:1:171:GLY:CA | 1.80 | 0.93 |
| 7:7:129:TYR:HE1 | 7:7:134:LEU:CD2 | 1.82 | 0.93 |
| 10:C:44:ILE:HB | 10:C:216:ILE:HD12 | 1.51 | 0.93 |
| 14:G:146:HIS:HB3 | 14:G:148:TYR:HE1 | 1.10 | 0.93 |
| 21:N:536:ILE:HD13 | 21:N:555:ILE:HG12 | 1.48 | 0.93 |
| 22:O:15:ARG:NH1 | 22:O:73:ILE:CD1 | 2.32 | 0.93 |
| 1:1:174:ARG:NH1 | 1:1:185:ARG:NH2 | 2.17 | 0.92 |
| 15:H:65:GLU:O | 15:H:69:VAL:HG23 | 1.69 | 0.92 |
| 15:H:396:MET:HE3 | 15:H:438:ALA:HB2 | 0.94 | 0.92 |
| 16:I:75:PHE:HD2 | 16:I:76:VAL:HG23 | 1.33 | 0.92 |
| 23:P:184:MET:CB | 23:P:223:LEU:HD13 | 1.98 | 0.92 |
| 23:P:342:GLN:HE21 | 23:P:346:ILE:HD11 | 1.31 | 0.92 |
| 32:Y:80:GLU:CD | 32:Y:83:ARG:HH21 | 1.73 | 0.92 |
| 13:F:84:LEU:HD21 | 13:F:132:LEU:HD12 | 1.47 | 0.92 |
| 13:F:105:VAL:CG2 | 13:F:145:LEU:HB2 | 1.99 | 0.92 |
| 18:K:212:TYR:CE1 | 18:K:321:ALA:N | 2.38 | 0.92 |
| 30:W:21:PHE:CZ | 30:W:25:ARG:NH1 | 2.36 | 0.92 |
| 31:X:75:TRP:HZ3 | 31:X:125:MET:HE2 | 1.31 | 0.92 |
| 16:I:126:PRO:HG2 | 16:I:154:MET:HE3 | 1.52 | 0.92 |
| 24:Q:309:ARG:NH2 | 24:Q:345:SER:HA | 1.83 | 0.92 |
| 31:X:75:TRP:HZ2 | 31:X:125:MET:HG3 | 1.26 | 0.92 |
| 15:H:173:ARG:HA | 16:I:129:TYR:OH | 1.66 | 0.92 |
| 18:K:224:LYS:HE2 | 18:K:236:ARG:NH2 | 1.84 | 0.92 |
| 21:N:717:LEU:HD23 | 21:N:733:LEU:CD1 | 1.99 | 0.92 |
| 22:O:15:ARG:HH12 | 22:O:73:ILE:HG12 | 1.34 | 0.92 |
| 24:Q:329:GLU:OE1 | 24:Q:332:ARG:NH2 | 2.03 | 0.92 |
| 33:Z:443:ASP:CB | 33:Z:447:VAL:CG1 | 2.47 | 0.92 |
| 20:M:290:ARG:HD3 | 20:M:294:GLU:HB3 | 1.49 | 0.92 |
| 23:P:308:LEU:HD13 | 23:P:349:ASN:OD1 | 1.70 | 0.92 |
| 28:U:32:ARG:HH22 | 28:U:106:ILE:HD12 | 1.33 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:562:TRP:CD2 | 33:Z:566:LEU:HD11 | 2.05 | 0.92 |
| 14:G:192:VAL:HG13 | 14:G:215:ILE:HD13 | 1.50 | 0.92 |
| 24:Q:299:MET:HE3 | 24:Q:335:PHE:CZ | 2.04 | 0.92 |
| 25:R:105:LYS:HE2 | 25:R:109:LYS:HZ2 | 1.23 | 0.92 |
| 10:C:13:PHE:CZ | 11:D:127:ARG:NH1 | 2.37 | 0.92 |
| 13:F:3:ARG:NH2 | 15:H:359:ASN:ND2 | 2.18 | 0.92 |
| 16:I:126:PRO:HB3 | 16:I:128:TYR:HE2 | 0.75 | 0.92 |
| 16:I:204:HIS:CB | 16:I:207:LEU:HD12 | 1.99 | 0.92 |
| 21:N:273:LEU:O | 21:N:277:LEU:HG | 1.68 | 0.92 |
| 22:O:15:ARG:NH1 | 22:O:73:ILE:HG12 | 1.82 | 0.92 |
| 33:Z:53:VAL:HG23 | 33:Z:91:PHE:CE2 | 2.05 | 0.92 |
| 9:B:65:SER:HB2 | 9:B:90:ARG:NH2 | 1.83 | 0.92 |
| 12:E:165:TYR:CB | 12:E:167:TYR:CE1 | 2.53 | 0.92 |
| 16:I:207:LEU:CD1 | 33:Z:930:GLY:HA2 | 2.00 | 0.92 |
| 25:R:50:VAL:HG13 | 25:R:54:ILE:CD1 | 2.00 | 0.92 |
| 26:S:461:PHE:HZ | 28:U:274:MET:O | 1.52 | 0.92 |
| 19:L:88:TYR:CD1 | 20:M:62:ILE:HD13 | 2.04 | 0.92 |
| 23:P:202:LYS:HE2 | 23:P:206:LYS:NZ | 1.85 | 0.92 |
| 25:R:50:VAL:CG1 | 25:R:54:ILE:HD12 | 2.00 | 0.92 |
| 26:S:461:PHE:HE1 | 28:U:278:ILE:HB | 1.34 | 0.92 |
| 33:Z:165:TYR:OH | 33:Z:188:ALA:HB1 | 1.70 | 0.92 |
| 4:4:81:SER:HA | 4:4:124:LYS:HZ3 | 1.33 | 0.91 |
| 9:B:66:LEU:HD11 | 9:B:235:PHE:CE2 | 2.04 | 0.91 |
| 21:N:221:ASP:HA | 21:N:894:ARG:HH22 | 1.32 | 0.91 |
| 25:R:63:TYR:CE2 | 25:R:94:PHE:HA | 2.04 | 0.91 |
| 29:V:53:MET:CE | 29:V:65:VAL:HG11 | 2.00 | 0.91 |
| 8:A:56:GLN:NE2 | 8:A:214:LEU:HD13 | 1.84 | 0.91 |
| 15:H:284:VAL:CB | 20:M:254:MET:HB3 | 2.00 | 0.91 |
| 33:Z:53:VAL:HG13 | 33:Z:95:THR:HG21 | 0.92 | 0.91 |
| 33:Z:188:ALA:N | 33:Z:201:LEU:HD12 | 1.79 | 0.91 |
| 4:4:3:ILE:CG2 | 4:4:102:LEU:HD12 | 1.98 | 0.91 |
| 21:N:207:LEU:HB2 | 21:N:232:LEU:HD21 | 1.51 | 0.91 |
| 33:Z:574:TYR:OH | 33:Z:584:VAL:CG2 | 2.19 | 0.91 |
| 8:A:156:LYS:HB3 | 8:A:166:TYR:CE1 | 2.04 | 0.91 |
| 14:G:173:ALA:HB1 | 19:L:420:ARG:HH21 | 1.32 | 0.91 |
| 18:K:70:ASP:OD1 | 18:K:73:ARG:NH2 | 2.03 | 0.91 |
| 19:L:357:ARG:HH12 | 19:L:386:PHE:HB2 | 1.34 | 0.91 |
| 7:7:187:PHE:CZ | 7:7:204:LEU:HB3 | 2.06 | 0.91 |
| 11:D:7:ALA:HB2 | 12:E:125:GLU:OE2 | 1.71 | 0.91 |
| 12:E:208:MET:HG2 | 12:E:210:GLU:H | 1.36 | 0.91 |
| 18:K:159:SER:HG | 18:K:244:HIS:HE2 | 0.96 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:8:PHE:CE2 | 2:2:11:GLY:N | 2.37 | 0.91 |
| 17:J:167:PRO:HA | 17:J:174:PHE:CZ | 2.06 | 0.91 |
| 33:Z:562:TRP:HE1 | 33:Z:566:LEU:CD2 | 1.84 | 0.91 |
| 5:5:38:ASN:HD21 | 5:5:41:LEU:HD12 | 1.36 | 0.91 |
| 10:C:115:LEU:HD12 | 10:C:137:TYR:OH | 1.71 | 0.91 |
| 13:F:12:THR:CG2 | 13:F:19:LEU:CD1 | 2.49 | 0.91 |
| 15:H:351:VAL:HG12 | 15:H:353:PHE:CE1 | 2.04 | 0.91 |
| 23:P:267:PHE:HE1 | 23:P:329:PHE:CE2 | 1.65 | 0.91 |
| 31:X:100:TRP:CZ3 | 31:X:102:GLN:HA | 2.06 | 0.91 |
| 5:5:159:ARG:HH12 | 5:5:200:VAL:HA | 1.35 | 0.91 |
| 14:G:48:ALA:HB1 | 14:G:199:ILE:HD11 | 1.53 | 0.90 |
| 24:Q:311:LEU:HD22 | 24:Q:343:LEU:CD1 | 1.99 | 0.90 |
| 28:U:32:ARG:CG | 28:U:94:HIS:HE1 | 1.84 | 0.90 |
| 22:O:250:TRP:O | 22:O:269:LEU:CD1 | 2.16 | 0.90 |
| 23:P:72:TRP:CH2 | 23:P:103:TYR:CB | 2.48 | 0.90 |
| 23:P:332:GLU:HB2 | 23:P:337:HIS:CE1 | 2.06 | 0.90 |
| 15:H:340:LEU:CD1 | 15:H:370:ARG:HG3 | 2.00 | 0.90 |
| 17:J:377:VAL:HG12 | 17:J:382:PHE:CE2 | 2.05 | 0.90 |
| 22:O:266:PHE:CZ | 22:O:280:LEU:CD2 | 2.54 | 0.90 |
| 30:W:31:ASP:O | 30:W:35:PHE:HD1 | 1.55 | 0.90 |
| 31:X:79:LYS:HE2 | 31:X:98:PHE:HE2 | 1.35 | 0.90 |
| 15:H:206:VAL:CG2 | 15:H:261:ARG:HE | 1.83 | 0.90 |
| 21:N:211:PHE:CD2 | 21:N:237:LEU:HD22 | 2.07 | 0.90 |
| 24:Q:146:TYR:OH | 24:Q:183:LYS:O | 1.89 | 0.90 |
| 25:R:411:LEU:HD23 | 26:S:464:ARG:NH1 | 1.87 | 0.90 |
| 28:U:203:LYS:HE2 | 28:U:229:LEU:CD2 | 1.99 | 0.90 |
| 5:5:135:PHE:HB2 | 5:5:167:ARG:NH2 | 1.87 | 0.90 |
| 13:F:101:ARG:HG2 | 13:F:103:LEU:H | 1.36 | 0.90 |
| 15:H:284:VAL:HB | 20:M:254:MET:N | 1.86 | 0.90 |
| 22:O:377:VAL:HG11 | 28:U:200:LEU:HD12 | 1.52 | 0.90 |
| 33:Z:562:TRP:CE2 | 33:Z:566:LEU:CD1 | 2.53 | 0.90 |
| 4:4:3:ILE:HG22 | 4:4:102:LEU:CD1 | 2.02 | 0.90 |
| 4:4:26:VAL:HG11 | 4:4:29:ASP:HB3 | 1.49 | 0.90 |
| 23:P:131:PHE:CA | 23:P:136:ARG:HH11 | 1.83 | 0.90 |
| 28:U:32:ARG:HG2 | 28:U:94:HIS:CE1 | 2.05 | 0.90 |
| 29:V:107:TRP:HZ3 | 29:V:109:HIS:CD2 | 1.77 | 0.90 |
| 21:N:327:LEU:HD21 | 21:N:743:PHE:CE1 | 2.01 | 0.90 |
| 3:3:125:LYS:O | 3:3:126:ASP:OD1 | 1.89 | 0.90 |
| 5:5:111:THR:HG21 | 5:5:113:TYR:CZ | 2.06 | 0.90 |
| 15:H:172:MET:HB3 | 16:I:129:TYR:HE2 | 1.31 | 0.90 |
| 15:H:251:PRO:HD2 | 15:H:377:PHE:CD2 | 2.06 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:284:VAL:CB | 20:M:254:MET:HA | 2.02 | 0.90 |
| 20:M:290:ARG:HD3 | 20:M:294:GLU:CB | 2.02 | 0.90 |
| 21:N:75:TYR:OH | 26:S:223:LEU:HD12 | 1.72 | 0.90 |
| 27:T:47:GLN:O | 27:T:48:ASN:CG | 2.10 | 0.90 |
| 33:Z:574:TYR:HE2 | 33:Z:584:VAL:CG1 | 1.70 | 0.90 |
| 9:B:219:PRO:HA | 9:B:222:LEU:HD12 | 1.53 | 0.90 |
| 19:L:222:GLY:HA3 | 19:L:349:ILE:HD12 | 1.51 | 0.90 |
| 27:T:136:LEU:HD22 | 27:T:146:ILE:HD11 | 1.52 | 0.90 |
| 33:Z:888:LEU:HB3 | 33:Z:901:PHE:HE1 | 1.35 | 0.90 |
| 16:I:204:HIS:HB3 | 16:I:207:LEU:CB | 2.02 | 0.89 |
| 24:Q:275:ILE:HD11 | 24:Q:306:TYR:HD2 | 1.32 | 0.89 |
| 26:S:218:LEU:HG | 26:S:256:LYS:NZ | 1.87 | 0.89 |
| 4:4:166:GLU:HB3 | 4:4:170:ARG:HH21 | 1.36 | 0.89 |
| 18:K:71:GLU:OE2 | 21:N:576:VAL:HG22 | 1.72 | 0.89 |
| 20:M:119:VAL:HG11 | 20:M:155:ILE:HD11 | 1.55 | 0.89 |
| 33:Z:64:TYR:OH | 33:Z:115:LEU:CD2 | 2.19 | 0.89 |
| 33:Z:154:ILE:HG21 | 33:Z:211:PHE:CE1 | 2.06 | 0.89 |
| 22:O:228:TYR:HA | 22:O:290:LYS:HZ1 | 1.35 | 0.89 |
| 25:R:334:ARG:NH1 | 25:R:363:PHE:HZ | 1.70 | 0.89 |
| 26:S:188:TYR:HE2 | 26:S:239:ARG:HH11 | 1.20 | 0.89 |
| 21:N:585:ARG:NH2 | 21:N:623:PHE:CE2 | 2.39 | 0.89 |
| 18:K:137:VAL:HB | 18:K:146:LEU:HD11 | 1.53 | 0.89 |
| 24:Q:343:LEU:HD11 | 24:Q:368:LEU:HD11 | 1.54 | 0.89 |
| 33:Z:813:PHE:CZ | 33:Z:847:ILE:HG12 | 2.07 | 0.89 |
| 6:6:196:LEU:CD2 | 6:6:205:LYS:HG2 | 2.02 | 0.89 |
| 33:Z:74:SER:CB | 33:Z:79:THR:HG22 | 2.02 | 0.89 |
| 11:D:11:PHE:HE2 | 12:E:26:TYR:CB | 1.85 | 0.89 |
| 16:I:214:LYS:NZ | 16:I:318:ASP:C | 2.26 | 0.89 |
| 14:G:122:HIS:CG | 14:G:128:VAL:HG12 | 2.07 | 0.89 |
| 19:L:167:VAL:HG23 | 20:M:142:PRO:HG3 | 1.55 | 0.89 |
| 24:Q:165:PHE:CZ | 24:Q:173:SER:OG | 2.26 | 0.89 |
| 33:Z:138:ARG:HH21 | 33:Z:157:LEU:CD1 | 1.81 | 0.89 |
| 33:Z:863:THR:CB | 33:Z:911:LYS:NZ | 2.35 | 0.89 |
| 33:Z:888:LEU:HB3 | 33:Z:901:PHE:CE1 | 2.07 | 0.89 |
| 13:F:7:ASP:CA | 13:F:21:GLN:HE21 | 1.86 | 0.89 |
| 16:I:395:MET:CE | 16:I:420:LYS:NZ | 2.32 | 0.89 |
| 20:M:251:LEU:C | 20:M:252:VAL:N | 0.84 | 0.89 |
| 31:X:67:ILE:HD12 | 31:X:69:ILE:HD11 | 1.54 | 0.89 |
| 33:Z:205:LEU:HG | 33:Z:236:PHE:HE1 | 1.28 | 0.89 |
| 33:Z:763:HIS:CG | 33:Z:766:HIS:CE1 | 2.61 | 0.89 |
| 26:S:428:ARG:HA | 27:T:195:LEU:HD23 | 1.54 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:155:PHE:CE1 | 3:3:189:ARG:HD2 | 2.08 | 0.88 |
| 15:H:351:VAL:HG11 | 15:H:353:PHE:CZ | 2.08 | 0.88 |
| 21:N:596:LEU:HD13 | 21:N:717:LEU:HD13 | 1.55 | 0.88 |
| 22:O:116:ASN:CB | 22:O:127:LEU:HD12 | 2.03 | 0.88 |
| 23:P:167:THR:CB | 23:P:168:TYR:CD1 | 2.56 | 0.88 |
| 33:Z:484:LYS:HB2 | 33:Z:521:GLU:OE1 | 1.71 | 0.88 |
| 6:6:66:TYR:CE2 | 6:6:73:LYS:O | 2.25 | 0.88 |
| 19:L:157:ARG:HH21 | 20:M:128:PHE:HD2 | 1.17 | 0.88 |
| 30:W:20:ASP:HB3 | 30:W:25:ARG:HH21 | 1.30 | 0.88 |
| 33:Z:111:LEU:O | 33:Z:115:LEU:HG | 1.73 | 0.88 |
| 16:I:317:ASP:HB3 | 16:I:343:ARG:NH2 | 1.88 | 0.88 |
| 23:P:131:PHE:HZ | 23:P:167:THR:HG22 | 1.09 | 0.88 |
| 33:Z:546:ILE:HG22 | 33:Z:550:PHE:CE2 | 2.08 | 0.88 |
| 11:D:208:LYS:HE2 | 11:D:226:SER:HB3 | 1.54 | 0.88 |
| 18:K:212:TYR:CE1 | 18:K:320:ARG:CA | 2.40 | 0.88 |
| 25:R:209:ARG:O | 25:R:213:TYR:HD2 | 1.56 | 0.88 |
| 27:T:15:PHE:CZ | 27:T:67:LEU:HB3 | 2.09 | 0.88 |
| 11:D:92:GLU:OE2 | 11:D:108:TYR:HE2 | 1.55 | 0.88 |
| 13:F:159:THR:HA | 13:F:169:LYS:HZ3 | 1.27 | 0.88 |
| 23:P:125:VAL:HG23 | 23:P:126:THR:HG23 | 1.54 | 0.88 |
| 23:P:245:TYR:CZ | 23:P:257:TRP:NE1 | 2.40 | 0.88 |
| 28:U:67:PHE:CZ | 30:W:97:THR:HG23 | 2.08 | 0.88 |
| 33:Z:75:ILE:O | 33:Z:75:ILE:HG22 | 1.72 | 0.88 |
| 33:Z:138:ARG:CZ | 33:Z:157:LEU:CG | 2.52 | 0.88 |
| 33:Z:387:ASN:HD22 | 33:Z:400:ILE:HD11 | 1.36 | 0.88 |
| 33:Z:763:HIS:HA | 33:Z:766:HIS:ND1 | 1.88 | 0.88 |
| 17:J:337:LEU:HD22 | 17:J:382:PHE:HZ | 0.73 | 0.88 |
| 21:N:588:VAL:HG11 | 21:N:621:THR:HG23 | 1.54 | 0.88 |
| 24:Q:61:LEU:HG | 24:Q:65:TYR:CZ | 2.08 | 0.88 |
| 33:Z:812:ILE:HG12 | 33:Z:834:LEU:HD22 | 1.54 | 0.88 |
| 33:Z:473:LEU:O | 33:Z:477:TYR:CD2 | 2.26 | 0.88 |
| 7:7:118:PHE:CE2 | 7:7:120:ARG:HD2 | 2.08 | 0.88 |
| 16:I:384:LYS:NZ | 16:I:420:LYS:NZ | 2.11 | 0.88 |
| 26:S:461:PHE:HE2 | 28:U:274:MET:CA | 1.86 | 0.88 |
| 1:1:66:TYR:CE2 | 1:1:73:PRO:HB3 | 2.08 | 0.88 |
| 13:F:105:VAL:HG22 | 13:F:145:LEU:HD12 | 1.55 | 0.88 |
| 23:P:167:THR:OG1 | 23:P:168:TYR:CD1 | 2.07 | 0.88 |
| 25:R:316:LEU:HD11 | 25:R:329:PHE:CE1 | 2.09 | 0.88 |
| 33:Z:154:ILE:HG22 | 33:Z:211:PHE:HZ | 1.33 | 0.88 |
| 33:Z:208:VAL:HG11 | 33:Z:236:PHE:CD2 | 2.08 | 0.88 |
| 33:Z:463:HIS:O | 33:Z:466:GLU:HG2 | 1.74 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:249:TYR:CZ | 15:H:376:GLU:HA | 2.08 | 0.87 |
| 19:L:88:TYR:CE1 | 20:M:62:ILE:CB | 2.55 | 0.87 |
| 33:Z:750:GLU:HG2 | 33:Z:753:GLY:H | 1.37 | 0.87 |
| 1:1:98:ILE:HD11 | 1:1:127:ALA:HB3 | 1.56 | 0.87 |
| 3:3:60:TYR:CE2 | 10:C:96:GLN:HB3 | 2.09 | 0.87 |
| 18:K:241:GLU:HA | 19:L:303:ARG:NH1 | 1.90 | 0.87 |
| 4:4:109:LYS:HG3 | 4:4:110:LYS:HG3 | 1.55 | 0.87 |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:HG22 | 1.56 | 0.87 |
| 17:J:337:LEU:H | 25:R:204:TRP:HE1 | 1.16 | 0.87 |
| 21:N:162:ARG:HD3 | 21:N:165:ILE:CG1 | 2.03 | 0.87 |
| 1:1:30:VAL:HG23 | 1:1:172:VAL:CG2 | 2.03 | 0.87 |
| 12:E:17:PRO:HA | 13:F:24:TYR:CE2 | 2.09 | 0.87 |
| 20:M:331:ASP:OD1 | 20:M:332:VAL:HG23 | 1.75 | 0.87 |
| 21:N:361:ASN:HB3 | 21:N:399:PHE:CD2 | 2.10 | 0.87 |
| 24:Q:322:GLU:HG3 | 24:Q:326:MET:CE | 2.03 | 0.87 |
| 27:T:11:LEU:HD22 | 27:T:30:ILE:HD13 | 1.56 | 0.87 |
| 19:L:289:ARG:NH1 | 19:L:333:LEU:O | 2.07 | 0.87 |
| 22:O:178:TYR:CZ | 22:O:182:LYS:NZ | 2.42 | 0.87 |
| 25:R:266:LEU:HD21 | 25:R:293:THR:HG23 | 1.56 | 0.87 |
| 13:F:72:LEU:HD13 | 13:F:132:LEU:HD22 | 1.54 | 0.87 |
| 19:L:95:ILE:HG23 | 20:M:68:LYS:NZ | 1.89 | 0.87 |
| 25:R:158:LEU:HD11 | 25:R:197:MET:CE | 2.04 | 0.87 |
| 27:T:206:LYS:NZ | 27:T:214:GLU:OE2 | 2.07 | 0.87 |
| 33:Z:795:THR:HG22 | 33:Z:799:PHE:HE2 | 1.38 | 0.87 |
| 1:1:94:THR:CG2 | 1:1:115:LEU:HD22 | 2.05 | 0.87 |
| 21:N:207:LEU:CB | 21:N:232:LEU:HD21 | 2.04 | 0.87 |
| 33:Z:250:VAL:HG21 | 33:Z:272:TYR:OH | 1.73 | 0.87 |
| 8:A:205:PHE:CE2 | 8:A:209:HIS:CE1 | 2.62 | 0.87 |
| 11:D:8:LEU:O | 11:D:18:PHE:HZ | 1.58 | 0.87 |
| 21:N:444:HIS:ND1 | 21:N:476:THR:O | 2.08 | 0.87 |
| 30:W:115:CYS:SG | 30:W:144:PHE:CZ | 2.68 | 0.87 |
| 11:D:11:PHE:HE2 | 12:E:26:TYR:HB3 | 1.40 | 0.87 |
| 11:D:68:ASP:CG | 11:D:97:ARG:HH21 | 1.77 | 0.87 |
| 23:P:267:PHE:CE1 | 23:P:329:PHE:CD2 | 2.63 | 0.87 |
| 24:Q:11:ALA:HB2 | 24:Q:26:VAL:HG11 | 1.54 | 0.86 |
| 16:I:126:PRO:CB | 16:I:128:TYR:CE2 | 2.30 | 0.86 |
| 17:J:218:LEU:HD21 | 17:J:230:VAL:HA | 1.57 | 0.86 |
| 21:N:770:LYS:HE3 | 21:N:917:ILE:HG21 | 1.55 | 0.86 |
| 24:Q:382:LEU:HB3 | 25:R:263:ARG:NH1 | 1.90 | 0.86 |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:C | 1.95 | 0.86 |
| 17:J:329:ARG:HH11 | 17:J:333:ARG:CZ | 1.88 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:53:ASP:HA | 21:N:58:ARG:NH2 | 1.90 | 0.86 |
| 21:N:315:ASN:HA | 21:N:318:LYS:NZ | 1.90 | 0.86 |
| 21:N:596:LEU:CD2 | 21:N:717:LEU:HD11 | 2.05 | 0.86 |
| 23:P:332:GLU:CB | 23:P:337:HIS:NE2 | 2.36 | 0.86 |
| 26:S:461:PHE:HE2 | 28:U:274:MET:O | 1.56 | 0.86 |
| 33:Z:221:VAL:HG22 | 33:Z:245:VAL:HG13 | 1.56 | 0.86 |
| 33:Z:394:TYR:HD2 | 33:Z:396:ASN:HD21 | 0.87 | 0.86 |
| 17:J:167:PRO:HA | 17:J:174:PHE:CE1 | 2.10 | 0.86 |
| 19:L:263:ILE:O | 19:L:267:PHE:HD1 | 1.58 | 0.86 |
| 31:X:79:LYS:HE2 | 31:X:98:PHE:CD2 | 2.10 | 0.86 |
| 18:K:371:LEU:HD21 | 18:K:407:LEU:HD13 | 1.55 | 0.86 |
| 26:S:399:TYR:HD2 | 26:S:401:LYS:O | 1.58 | 0.86 |
| 2:2:42:TRP:HD1 | 2:2:178:MET:SD | 1.98 | 0.86 |
| 15:H:172:MET:CA | 16:I:129:TYR:CE2 | 2.58 | 0.86 |
| 16:I:384:LYS:HD3 | 16:I:420:LYS:HD2 | 1.55 | 0.86 |
| 16:I:331:ILE:HD13 | 16:I:347:LYS:HE2 | 1.56 | 0.86 |
| 27:T:2:PRO:O | 27:T:9:LYS:CD | 2.22 | 0.86 |
| 13:F:157:TYR:HD2 | 14:G:57:LEU:O | 1.59 | 0.86 |
| 15:H:351:VAL:CG1 | 15:H:353:PHE:CE1 | 2.58 | 0.86 |
| 22:O:253:GLN:HB2 | 22:O:269:LEU:HD12 | 1.55 | 0.86 |
| 23:P:95:TYR:CD2 | 23:P:96:MET:CE | 2.59 | 0.86 |
| 4:4:45:PHE:CD2 | 4:4:101:VAL:CG1 | 2.58 | 0.86 |
| 16:I:163:ASP:HB2 | 17:J:76:ILE:HD13 | 1.56 | 0.86 |
| 20:M:236:ALA:HB2 | 20:M:277:ILE:HD12 | 1.57 | 0.86 |
| 21:N:599:TYR:HE1 | 21:N:634:LEU:HD13 | 1.39 | 0.86 |
| 23:P:259:PRO:CB | 23:P:327:LEU:HD12 | 2.06 | 0.86 |
| 15:H:396:MET:HE2 | 15:H:438:ALA:HB3 | 1.48 | 0.85 |
| 17:J:26:LYS:HE2 | 18:K:51:LEU:HD21 | 1.58 | 0.85 |
| 24:Q:141:LEU:HD11 | 24:Q:145:HIS:NE2 | 1.91 | 0.85 |
| 25:R:301:TYR:CE1 | 25:R:305:PHE:CE1 | 2.64 | 0.85 |
| 28:U:32:ARG:HG2 | 28:U:94:HIS:NE2 | 1.91 | 0.85 |
| 33:Z:126:TYR:HD2 | 33:Z:128:GLU:HB2 | 1.37 | 0.85 |
| 33:Z:748:LEU:CD2 | 33:Z:783:VAL:O | 2.23 | 0.85 |
| 15:H:97:LEU:HD11 | 15:H:176:VAL:H | 1.42 | 0.85 |
| 15:H:284:VAL:HG21 | 20:M:254:MET:HA | 1.57 | 0.85 |
| 24:Q:10:GLU:O | 24:Q:14:LEU:HG | 1.76 | 0.85 |
| 31:X:37:PRO:HB3 | 31:X:46:TRP:CZ3 | 2.11 | 0.85 |
| 22:O:178:TYR:OH | 22:O:182:LYS:NZ | 2.08 | 0.85 |
| 28:U:32:ARG:NH2 | 28:U:106:ILE:HD12 | 1.91 | 0.85 |
| 10:C:13:PHE:CE2 | 11:D:127:ARG:NH1 | 2.44 | 0.85 |
| 13:F:7:ASP:HA | 13:F:21:GLN:NE2 | 1.90 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:M:195:GLU:HA | 20:M:199:LEU:HD12 | 1.56 | 0.85 |
| 23:P:167:THR:HB | 23:P:168:TYR:CE1 | 2.11 | 0.85 |
| 25:R:134:TRP:CH2 | 25:R:156:LYS:NZ | 2.44 | 0.85 |
| 15:H:97:LEU:HD21 | 15:H:175:GLY:HA3 | 1.55 | 0.85 |
| 21:N:326:SER:HA | 29:V:182:LYS:HE2 | 1.59 | 0.85 |
| 21:N:717:LEU:HD23 | 21:N:733:LEU:HD11 | 1.57 | 0.85 |
| 23:P:131:PHE:HZ | 23:P:167:THR:CG2 | 1.75 | 0.85 |
| 1:1:61:TYR:HE1 | 8:A:103:GLU:HA | 1.42 | 0.85 |
| 5:5:81:LYS:HG2 | 11:D:101:GLU:OE2 | 1.77 | 0.85 |
| 15:H:306:ILE:CG2 | 15:H:308:PHE:CE1 | 2.60 | 0.85 |
| 19:L:401:PHE:CD1 | 19:L:404:ARG:NH1 | 2.44 | 0.85 |
| 22:O:235:HIS:CD2 | 22:O:236:HIS:CE1 | 2.63 | 0.85 |
| 24:Q:311:LEU:HD22 | 24:Q:343:LEU:HD13 | 1.56 | 0.85 |
| 24:Q:382:LEU:HD13 | 25:R:263:ARG:CZ | 2.07 | 0.85 |
| 7:7:42:VAL:HG23 | 7:7:192:ILE:HD11 | 1.59 | 0.85 |
| 33:Z:205:LEU:CD2 | 33:Z:236:PHE:HE1 | 1.89 | 0.85 |
| 15:H:389:PHE:CZ | 15:H:419:LEU:CD2 | 2.59 | 0.85 |
| 17:J:114:CYS:SG | 18:K:119:VAL:HG21 | 2.17 | 0.85 |
| 22:O:15:ARG:NH2 | 22:O:73:ILE:HD11 | 1.91 | 0.85 |
| 23:P:95:TYR:HD2 | 23:P:96:MET:HE3 | 1.40 | 0.85 |
| 31:X:48:PHE:CZ | 31:X:68:LEU:HD21 | 2.11 | 0.85 |
| 33:Z:763:HIS:HA | 33:Z:766:HIS:CE1 | 2.11 | 0.85 |
| 12:E:86:ARG:NH1 | 12:E:90:GLU:HB2 | 1.92 | 0.85 |
| 23:P:184:MET:HB2 | 23:P:223:LEU:HD13 | 1.59 | 0.85 |
| 24:Q:426:LEU:HD22 | 28:U:293:GLU:OE1 | 1.76 | 0.85 |
| 13:F:159:THR:HA | 13:F:169:LYS:HZ2 | 1.38 | 0.84 |
| 14:G:200:TYR:CE1 | 14:G:246:ILE:HG22 | 2.09 | 0.84 |
| 15:H:101:ARG:NH2 | 15:H:150:LYS:CE | 2.38 | 0.84 |
| 15:H:329:VAL:HG21 | 16:I:300:ARG:NH1 | 1.91 | 0.84 |
| 23:P:130:ILE:C | 23:P:136:ARG:NH1 | 2.30 | 0.84 |
| 33:Z:75:ILE:HG21 | 33:Z:121:ILE:HG21 | 0.89 | 0.84 |
| 33:Z:763:HIS:O | 33:Z:766:HIS:CE1 | 2.30 | 0.84 |
| 18:K:258:PHE:CG | 18:K:302:GLN:HB3 | 2.12 | 0.84 |
| 14:G:173:ALA:CA | 19:L:420:ARG:NH2 | 2.39 | 0.84 |
| 3:3:37:TYR:CE1 | 3:3:59:ARG:HG3 | 2.13 | 0.84 |
| 15:H:284:VAL:CG1 | 20:M:254:MET:N | 2.39 | 0.84 |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:CG2 | 2.07 | 0.84 |
| 19:L:157:ARG:NH2 | 20:M:128:PHE:CD2 | 2.46 | 0.84 |
| 23:P:229:LEU:HD22 | 23:P:332:GLU:HG3 | 1.59 | 0.84 |
| 25:R:170:VAL:HG12 | 25:R:194:VAL:HG21 | 1.59 | 0.84 |
| 1:1:-4:VAL:CG1 | 1:1:49:ALA:HB3 | 2.08 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:J:219:VAL:HB | 18:K:281:ARG:HD2 | 1.57 | 0.84 |
| 33:Z:562:TRP:NE1 | 33:Z:566:LEU:CG | 2.39 | 0.84 |
| 16:I:208:TYR:CE1 | 16:I:209:GLU:HG3 | 2.12 | 0.84 |
| 18:K:386:ILE:HA | 18:K:414:GLN:HE22 | 1.43 | 0.84 |
| 21:N:282:TYR:CZ | 21:N:286:LEU:CD1 | 2.59 | 0.84 |
| 24:Q:289:GLU:HB2 | 24:Q:291:TYR:HD1 | 1.42 | 0.84 |
| 31:X:48:PHE:CZ | 31:X:68:LEU:CD2 | 2.61 | 0.84 |
| 33:Z:493:LEU:HD11 | 33:Z:497:PHE:CE1 | 2.12 | 0.84 |
| 13:F:105:VAL:HG21 | 13:F:145:LEU:CB | 2.08 | 0.84 |
| 15:H:249:TYR:OH | 15:H:376:GLU:HB2 | 1.78 | 0.84 |
| 21:N:579:SER:HA | 21:N:584:ARG:NH2 | 1.92 | 0.84 |
| 31:X:75:TRP:CH2 | 31:X:125:MET:SD | 2.70 | 0.84 |
| 33:Z:53:VAL:CG1 | 33:Z:95:THR:HG22 | 2.06 | 0.84 |
| 13:F:13:PHE:CE1 | 14:G:130:PRO:HD2 | 2.11 | 0.84 |
| 20:M:116:ALA:HB1 | 20:M:128:PHE:CE1 | 2.12 | 0.84 |
| 21:N:749:LEU:HG | 21:N:753:PHE:CZ | 2.13 | 0.84 |
| 23:P:95:TYR:HD2 | 23:P:96:MET:CE | 1.90 | 0.84 |
| 26:S:397:LEU:HD22 | 26:S:402:ILE:HG21 | 1.58 | 0.84 |
| 30:W:139:VAL:HG11 | 30:W:157:PHE:HE2 | 1.43 | 0.84 |
| 33:Z:574:TYR:CZ | 33:Z:584:VAL:CG2 | 2.61 | 0.84 |
| 5:5:111:THR:CG2 | 5:5:113:TYR:CZ | 2.61 | 0.84 |
| 12:E:20:ARG:HD3 | 20:M:432:PHE:CZ | 2.12 | 0.84 |
| 10:C:161:LYS:CD | 11:D:56:ASP:HB2 | 2.07 | 0.84 |
| 24:Q:48:ASP:OD1 | 24:Q:92:LYS:HE3 | 1.77 | 0.84 |
| 33:Z:574:TYR:CZ | 33:Z:584:VAL:CG1 | 2.56 | 0.83 |
| 21:N:223:LEU:HD11 | 21:N:722:THR:HG22 | 1.59 | 0.83 |
| 31:X:27:ILE:HB | 31:X:59:ARG:NH2 | 1.92 | 0.83 |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:CD2 | 2.14 | 0.83 |
| 5:5:6:PHE:CZ | 5:5:13:ILE:HB | 2.11 | 0.83 |
| 25:R:158:LEU:CD1 | 25:R:197:MET:HE1 | 2.07 | 0.83 |
| 13:F:120:THR:O | 14:G:129:ARG:CD | 2.25 | 0.83 |
| 23:P:144:VAL:HG21 | 23:P:160:LEU:CD2 | 2.08 | 0.83 |
| 26:S:192:GLU:HG3 | 26:S:239:ARG:NH1 | 1.94 | 0.83 |
| 28:U:32:ARG:NE | 28:U:94:HIS:CE1 | 2.45 | 0.83 |
| 28:U:46:ILE:HD13 | 28:U:119:LEU:HD22 | 1.58 | 0.83 |
| 5:5:8:PHE:CZ | 5:5:13:ILE:HD11 | 2.14 | 0.83 |
| 10:C:4:ARG:HG3 | 11:D:6:ARG:HD2 | 1.59 | 0.83 |
| 15:H:206:VAL:HG21 | 15:H:261:ARG:NE | 1.92 | 0.83 |
| 19:L:145:ARG:HE | 19:L:162:GLU:HG3 | 1.44 | 0.83 |
| 12:E:86:ARG:HH12 | 12:E:90:GLU:HB2 | 1.43 | 0.83 |
| 14:G:217:TRP:HE1 | 14:G:228:LYS:HB2 | 1.42 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:88:TYR:HE1 | 20:M:62:ILE:HG12 | 1.43 | 0.83 |
| 33:Z:138:ARG:HH21 | 33:Z:157:LEU:HD12 | 1.38 | 0.83 |
| 5:5:100:MET:SD | 5:5:127:PHE:HB2 | 2.19 | 0.83 |
| 18:K:48:TYR:CZ | 21:N:156:ILE:HD11 | 2.14 | 0.83 |
| 19:L:369:LYS:HE3 | 20:M:209:ASP:O | 1.79 | 0.83 |
| 25:R:209:ARG:HE | 25:R:243:LEU:HD22 | 1.41 | 0.83 |
| 29:V:53:MET:HE2 | 29:V:65:VAL:HG11 | 1.58 | 0.83 |
| 31:X:38:ASN:HD22 | 31:X:42:GLU:H | 1.25 | 0.83 |
| 33:Z:443:ASP:HB3 | 33:Z:447:VAL:CB | 2.08 | 0.83 |
| 33:Z:463:HIS:NE2 | 33:Z:497:PHE:CD1 | 2.47 | 0.83 |
| 33:Z:886:VAL:HG13 | 33:Z:893:PHE:CE1 | 2.13 | 0.83 |
| 11:D:11:PHE:CE2 | 12:E:26:TYR:HB3 | 2.13 | 0.83 |
| 23:P:426:ILE:O | 29:V:230:TYR:OH | 1.97 | 0.83 |
| 17:J:241:ALA:HB2 | 17:J:288:ILE:HD11 | 1.59 | 0.83 |
| 17:J:329:ARG:NH1 | 17:J:333:ARG:CZ | 2.42 | 0.83 |
| 18:K:98:GLN:HE22 | 18:K:136:SER:CB | 1.90 | 0.83 |
| 19:L:290:ARG:NH1 | 19:L:293:GLU:CB | 2.41 | 0.83 |
| 21:N:406:TYR:CD1 | 21:N:448:LEU:HB3 | 2.13 | 0.83 |
| 25:R:137:LEU:O | 25:R:141:TYR:CD2 | 2.31 | 0.83 |
| 33:Z:985:LYS:HE3 | 33:Z:991:GLU:HB2 | 1.61 | 0.83 |
| 15:H:168:ILE:HD12 | 15:H:187:LEU:HD12 | 1.59 | 0.83 |
| 19:L:357:ARG:HH22 | 19:L:386:PHE:H | 1.27 | 0.83 |
| 22:O:185:PHE:CG | 22:O:223:LEU:HD13 | 2.13 | 0.83 |
| 1:1:83:LYS:HZ2 | 1:1:118:SER:HA | 1.42 | 0.82 |
| 5:5:40:PHE:HB3 | 5:5:73:ARG:NH2 | 1.94 | 0.82 |
| 9:B:239:THR:HG22 | 9:B:241:GLN:H | 1.42 | 0.82 |
| 21:N:222:TYR:H | 21:N:894:ARG:CZ | 1.91 | 0.82 |
| 21:N:717:LEU:CD2 | 21:N:733:LEU:HD12 | 2.07 | 0.82 |
| 22:O:253:GLN:CB | 22:O:269:LEU:HD12 | 2.10 | 0.82 |
| 1:1:-2:LEU:HD12 | 1:1:1:THR:H | 1.44 | 0.82 |
| 19:L:167:VAL:CG2 | 20:M:142:PRO:HG3 | 2.09 | 0.82 |
| 21:N:424:LYS:HZ1 | 21:N:461:GLU:CB | 1.79 | 0.82 |
| 4:4:109:LYS:HE3 | 4:4:110:LYS:HE3 | 1.61 | 0.82 |
| 15:H:299:ARG:NH2 | 15:H:345:PRO:HD3 | 1.94 | 0.82 |
| 15:H:323:ALA:O | 20:M:290:ARG:NH2 | 2.12 | 0.82 |
| 15:H:324:GLY:HA3 | 20:M:290:ARG:HH22 | 0.71 | 0.82 |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:CG2 | 2.09 | 0.82 |
| 25:R:408:ASP:CB | 26:S:464:ARG:NH2 | 2.33 | 0.82 |
| 31:X:75:TRP:CH2 | 31:X:125:MET:CG | 2.49 | 0.82 |
| 33:Z:119:LEU:HB3 | 33:Z:137:TYR:CD2 | 2.14 | 0.82 |
| 16:I:281:ILE:HG21 | 16:I:284:ILE:HD11 | 1.62 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:K:216:GLY:HA3 | 19:L:342:ARG:NH2 | 1.94 | 0.82 |
| 26:S:425:ARG:NH2 | 27:T:153:MET:O | 2.12 | 0.82 |
| 31:X:66:LEU:HD22 | 31:X:97:TYR:CD1 | 2.14 | 0.82 |
| 24:Q:311:LEU:CD2 | 24:Q:343:LEU:HD13 | 2.09 | 0.82 |
| 28:U:203:LYS:HE2 | 28:U:229:LEU:HD21 | 1.54 | 0.82 |
| 33:Z:53:VAL:HG13 | 33:Z:95:THR:HG22 | 1.61 | 0.82 |
| 9:B:174:PHE:HB3 | 9:B:178:ARG:HH12 | 1.45 | 0.82 |
| 15:H:102:CYS:HB3 | 15:H:105:ILE:CD1 | 2.10 | 0.82 |
| 22:O:377:VAL:HG21 | 28:U:200:LEU:CD1 | 2.08 | 0.82 |
| 23:P:267:PHE:CZ | 23:P:329:PHE:CD2 | 2.68 | 0.82 |
| 25:R:266:LEU:CA | 25:R:270:VAL:HG22 | 2.09 | 0.82 |
| 26:S:461:PHE:CE2 | 28:U:274:MET:C | 2.52 | 0.82 |
| 4:4:107:ASP:OD1 | 4:4:109:LYS:HG2 | 1.78 | 0.82 |
| 13:F:201:LEU:O | 13:F:202:ARG:HG3 | 1.80 | 0.82 |
| 15:H:59:ILE:CG2 | 16:I:92:GLU:OE2 | 2.27 | 0.82 |
| 17:J:305:LEU:HD22 | 17:J:313:LYS:CE | 2.07 | 0.82 |
| 31:X:36:LYS:NZ | 31:X:49:GLU:OE1 | 2.12 | 0.82 |
| 6:6:66:TYR:OH | 6:6:73:LYS:HG2 | 1.80 | 0.82 |
| 13:F:65:LYS:HG3 | 13:F:222:PHE:CD2 | 2.15 | 0.82 |
| 18:K:167:PRO:HG2 | 18:K:228:ASN:HB2 | 1.62 | 0.82 |
| 22:O:219:ILE:HG23 | 22:O:274:ILE:CD1 | 2.10 | 0.82 |
| 31:X:100:TRP:HZ3 | 31:X:102:GLN:HA | 1.43 | 0.82 |
| 33:Z:900:LEU:HD22 | 33:Z:903:MET:CE | 2.09 | 0.82 |
| 10:C:115:LEU:HD13 | 10:C:137:TYR:OH | 1.80 | 0.81 |
| 10:C:137:TYR:O | 10:C:148:LEU:HD12 | 1.80 | 0.81 |
| 13:F:157:TYR:OH | 14:G:59:VAL:HG23 | 1.80 | 0.81 |
| 29:V:135:ARG:HD2 | 29:V:157:ARG:HH22 | 0.73 | 0.81 |
| 33:Z:89:LEU:HD21 | 33:Z:125:THR:HG21 | 0.82 | 0.81 |
| 5:5:83:LEU:O | 5:5:87:VAL:HG23 | 1.79 | 0.81 |
| 33:Z:64:TYR:HD2 | 33:Z:111:LEU:HD11 | 1.40 | 0.81 |
| 33:Z:321:PHE:HE2 | 33:Z:351:PRO:CG | 1.89 | 0.81 |
| 33:Z:550:PHE:CZ | 33:Z:566:LEU:CB | 2.61 | 0.81 |
| 33:Z:550:PHE:CE1 | 33:Z:566:LEU:HB3 | 2.14 | 0.81 |
| 6:6:43:MET:HG3 | 6:6:102:ILE:HG22 | 1.61 | 0.81 |
| 14:G:122:HIS:CG | 14:G:128:VAL:CG1 | 2.62 | 0.81 |
| 17:J:167:PRO:CD | 17:J:174:PHE:CZ | 2.64 | 0.81 |
| 18:K:49:PHE:CE2 | 18:K:53:LYS:HE3 | 2.15 | 0.81 |
| 21:N:77:SER:O | 21:N:81:TYR:HD1 | 1.62 | 0.81 |
| 21:N:615:ALA:HB3 | 21:N:651:PHE:HZ | 1.44 | 0.81 |
| 26:S:435:LYS:HD3 | 27:T:198:ASP:OD2 | 1.80 | 0.81 |
| 27:T:112:ASN:HB2 | 27:T:177:PHE:HZ | 1.45 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:509:LEU:HB2 | 33:Z:530:LEU:HD21 | 1.62 | 0.81 |
| 1:1:1:THR:HG22 | 1:1:129:SER:H | 1.45 | 0.81 |
| 7:7:192:ILE:HG12 | 7:7:198:LEU:HD13 | 1.60 | 0.81 |
| 17:J:167:PRO:CD | 17:J:174:PHE:HZ | 1.92 | 0.81 |
| 24:Q:151:TYR:OH | 24:Q:187:LYS:HG2 | 1.79 | 0.81 |
| 6:6:91:LYS:CB | 6:6:96:TYR:CE1 | 2.63 | 0.81 |
| 20:M:282:GLU:OE2 | 20:M:328:ASN:ND2 | 2.14 | 0.81 |
| 21:N:67:LYS:HG2 | 21:N:97:PHE:CD1 | 2.15 | 0.81 |
| 23:P:274:GLY:O | 23:P:277:GLN:HG2 | 1.79 | 0.81 |
| 33:Z:550:PHE:HZ | 33:Z:566:LEU:HB3 | 1.41 | 0.81 |
| 33:Z:562:TRP:CZ2 | 33:Z:566:LEU:HD11 | 2.16 | 0.81 |
| 8:A:220:LYS:HD3 | 8:A:242:GLU:HB2 | 0.84 | 0.81 |
| 10:C:194:LEU:HD12 | 10:C:242:THR:HG21 | 1.62 | 0.81 |
| 11:D:159:TRP:CZ2 | 12:E:59:LEU:HD13 | 2.14 | 0.81 |
| 15:H:389:PHE:CE1 | 15:H:419:LEU:HD22 | 2.16 | 0.81 |
| 22:O:72:LYS:O | 30:W:18:ASN:CB | 2.29 | 0.81 |
| 22:O:356:ARG:NH1 | 28:U:234:ASN:HB2 | 1.94 | 0.81 |
| 8:A:19:PHE:HA | 8:A:25:LEU:HD21 | 1.63 | 0.81 |
| 15:H:69:VAL:HG11 | 16:I:133:LEU:HD21 | 1.62 | 0.81 |
| 16:I:175:LYS:O | 17:J:282:PHE:CZ | 2.33 | 0.81 |
| 22:O:157:LEU:HD22 | 22:O:171:PHE:CD1 | 2.16 | 0.81 |
| 27:T:89:TYR:CE1 | 27:T:102:LYS:HD3 | 2.15 | 0.81 |
| 1:1:8:PHE:CE1 | 1:1:13:ILE:HG13 | 2.16 | 0.81 |
| 9:B:44:VAL:HG22 | 9:B:213:ILE:HG22 | 1.60 | 0.81 |
| 14:G:106:ILE:HG12 | 14:G:114:ARG:NH2 | 1.94 | 0.81 |
| 16:I:103:PRO:HB3 | 17:J:120:TYR:CZ | 2.15 | 0.81 |
| 18:K:224:LYS:NZ | 18:K:236:ARG:HH22 | 1.78 | 0.81 |
| 24:Q:61:LEU:CG | 24:Q:65:TYR:CZ | 2.64 | 0.81 |
| 25:R:209:ARG:CG | 25:R:213:TYR:HE2 | 1.92 | 0.81 |
| 33:Z:51:LEU:HB3 | 33:Z:91:PHE:HZ | 1.44 | 0.81 |
| 33:Z:182:SER:O | 33:Z:183:LYS:HB2 | 1.79 | 0.81 |
| 10:C:161:LYS:HD2 | 11:D:56:ASP:CB | 2.08 | 0.81 |
| 18:K:132:LYS:HB2 | 18:K:135:MET:HG3 | 1.63 | 0.81 |
| 19:L:88:TYR:CE1 | 20:M:62:ILE:HG12 | 2.16 | 0.81 |
| 23:P:344:ARG:HH21 | 23:P:347:GLU:CD | 1.85 | 0.81 |
| 25:R:399:GLN:O | 25:R:403:LEU:HG | 1.81 | 0.81 |
| 14:G:173:ALA:HB1 | 19:L:420:ARG:NH2 | 1.91 | 0.81 |
| 21:N:549:TYR:OH | 21:N:738:GLN:NE2 | 2.12 | 0.81 |
| 26:S:461:PHE:CE1 | 28:U:278:ILE:CB | 2.64 | 0.81 |
| 6:6:73:LYS:HD2 | 12:E:108:ASN:HD21 | 1.45 | 0.80 |
| 12:E:20:ARG:HD3 | 20:M:432:PHE:HZ | 1.44 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:F:84:LEU:CD2 | 13:F:132:LEU:HD11 | 2.07 | 0.80 |
| 17:J:116:ARG:HB3 | 17:J:118:ASP:OD1 | 1.82 | 0.80 |
| 22:O:250:TRP:HZ2 | 22:O:271:LYS:CG | 1.95 | 0.80 |
| 8:A:128:TYR:CZ | 8:A:134:MET:CE | 2.63 | 0.80 |
| 9:B:43:VAL:HG11 | 9:B:137:ALA:HB1 | 1.63 | 0.80 |
| 13:F:179:PHE:CE2 | 13:F:192:ALA:HB1 | 2.16 | 0.80 |
| 19:L:178:ILE:HD13 | 19:L:230:LEU:CD2 | 2.11 | 0.80 |
| 23:P:154:ASP:OD1 | 23:P:190:LYS:NZ | 2.14 | 0.80 |
| 29:V:107:TRP:HZ3 | 29:V:109:HIS:CG | 1.97 | 0.80 |
| 33:Z:574:TYR:OH | 33:Z:584:VAL:HG21 | 1.80 | 0.80 |
| 3:3:129:VAL:CG2 | 3:3:138:PHE:CD1 | 2.62 | 0.80 |
| 23:P:202:LYS:HE2 | 23:P:206:LYS:HZ1 | 1.44 | 0.80 |
| 15:H:156:VAL:HG22 | 15:H:181:TYR:HH | 1.46 | 0.80 |
| 15:H:392:HIS:CE1 | 15:H:420:ARG:HG3 | 2.16 | 0.80 |
| 33:Z:158:ALA:HB2 | 33:Z:207:ILE:HD13 | 1.63 | 0.80 |
| 7:7:118:PHE:CZ | 7:7:120:ARG:HD2 | 2.15 | 0.80 |
| 10:C:66:LEU:CD1 | 10:C:212:GLU:HG2 | 2.11 | 0.80 |
| 17:J:156:GLN:HE21 | 17:J:160:ILE:HB | 1.45 | 0.80 |
| 19:L:362:LYS:HA | 19:L:376:PHE:CZ | 2.16 | 0.80 |
| 14:G:173:ALA:HB2 | 19:L:420:ARG:HH21 | 1.43 | 0.80 |
| 15:H:254:THR:OG1 | 15:H:377:PHE:CE1 | 2.35 | 0.80 |
| 19:L:117:TYR:CE1 | 19:L:131:VAL:HG11 | 2.17 | 0.80 |
| 19:L:178:ILE:HD13 | 19:L:230:LEU:HD22 | 1.61 | 0.80 |
| 23:P:79:LEU:CD1 | 23:P:100:VAL:HG21 | 2.11 | 0.80 |
| 25:R:105:LYS:CE | 25:R:109:LYS:NZ | 2.44 | 0.80 |
| 33:Z:338:HIS:HD2 | 33:Z:339:PHE:CE2 | 2.00 | 0.80 |
| 33:Z:863:THR:OG1 | 33:Z:911:LYS:NZ | 2.14 | 0.80 |
| 1:1:57:ASP:O | 8:A:106:TYR:CE1 | 2.34 | 0.80 |
| 14:G:108:ILE:CG2 | 14:G:148:TYR:CE1 | 2.64 | 0.80 |
| 18:K:126:LEU:HD22 | 18:K:149:ILE:CD1 | 2.12 | 0.80 |
| 21:N:502:PHE:CZ | 21:N:538:LYS:HB3 | 2.17 | 0.80 |
| 24:Q:99:THR:HG22 | 24:Q:103:LYS:HE3 | 1.62 | 0.80 |
| 29:V:186:GLN:O | 29:V:190:HIS:CD2 | 2.35 | 0.80 |
| 33:Z:763:HIS:O | 33:Z:766:HIS:ND1 | 2.15 | 0.80 |
| 6:6:48:PHE:CE2 | 6:6:50:ALA:HB3 | 2.17 | 0.80 |
| 18:K:280:LYS:HZ2 | 18:K:296:LEU:HD23 | 1.44 | 0.80 |
| 21:N:549:TYR:CD2 | 21:N:586:ALA:HB2 | 2.17 | 0.80 |
| 23:P:431:HIS:ND1 | 28:U:156:HIS:HB2 | 1.97 | 0.80 |
| 24:Q:51:ARG:NH1 | 24:Q:55:GLU:OE2 | 2.13 | 0.80 |
| 24:Q:146:TYR:CE1 | 24:Q:151:TYR:HE1 | 2.00 | 0.80 |
| 24:Q:415:LEU:HD13 | 28:U:282:VAL:HG11 | 1.61 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:F:137:TYR:CZ | 13:F:218:LYS:HA | 2.16 | 0.80 |
| 15:H:102:CYS:CB | 15:H:105:ILE:CD1 | 2.59 | 0.80 |
| 15:H:147:ILE:HD12 | 15:H:181:TYR:HB3 | 1.64 | 0.80 |
| 16:I:317:ASP:HB3 | 16:I:343:ARG:HH21 | 1.47 | 0.80 |
| 19:L:117:TYR:CE1 | 19:L:131:VAL:CG1 | 2.64 | 0.80 |
| 21:N:362:TRP:CH2 | 29:V:23:THR:CG2 | 2.65 | 0.80 |
| 26:S:315:LYS:NZ | 26:S:345:TYR:CE1 | 2.50 | 0.80 |
| 33:Z:866:VAL:HB | 33:Z:873:LEU:HG | 1.63 | 0.80 |
| 1:1:137:TYR:OH | 1:1:157:HIS:CD2 | 2.35 | 0.80 |
| 12:E:15:PHE:CZ | 13:F:126:ARG:NH2 | 2.49 | 0.80 |
| 22:O:373:TRP:CZ2 | 28:U:200:LEU:HD21 | 2.16 | 0.80 |
| 24:Q:232:TYR:HB2 | 24:Q:272:LEU:HD21 | 1.61 | 0.80 |
| 24:Q:348:CYS:HB3 | 24:Q:386:PHE:CE1 | 2.17 | 0.80 |
| 11:D:70:HIS:HE1 | 11:D:97:ARG:HH22 | 1.30 | 0.79 |
| 15:H:102:CYS:HB3 | 15:H:105:ILE:HD11 | 1.62 | 0.79 |
| 22:O:185:PHE:CE2 | 22:O:223:LEU:HD13 | 2.16 | 0.79 |
| 31:X:75:TRP:NE1 | 31:X:125:MET:HB2 | 1.97 | 0.79 |
| 30:W:46:GLU:O | 30:W:47:ASN:CG | 2.19 | 0.79 |
| 33:Z:833:GLN:NE2 | 33:Z:837:TYR:OH | 2.16 | 0.79 |
| 5:5:81:LYS:HD3 | 5:5:121:ARG:HE | 1.45 | 0.79 |
| 19:L:145:ARG:HH21 | 19:L:163:THR:CA | 1.95 | 0.79 |
| 20:M:196:ALA:HB2 | 20:M:345:ARG:NE | 1.96 | 0.79 |
| 29:V:107:TRP:CH2 | 29:V:109:HIS:CD2 | 2.70 | 0.79 |
| 33:Z:900:LEU:HD22 | 33:Z:903:MET:HE1 | 1.63 | 0.79 |
| 6:6:58:ARG:HD3 | 6:6:87:LEU:HD22 | 1.63 | 0.79 |
| 21:N:406:TYR:CE1 | 21:N:448:LEU:HB3 | 2.17 | 0.79 |
| 23:P:119:ILE:HG21 | 23:P:143:LEU:HD22 | 1.65 | 0.79 |
| 6:6:66:TYR:HE2 | 6:6:73:LYS:O | 1.65 | 0.79 |
| 9:B:174:PHE:HB3 | 9:B:178:ARG:NH1 | 1.97 | 0.79 |
| 19:L:88:TYR:CE1 | 20:M:62:ILE:CG1 | 2.65 | 0.79 |
| 20:M:59:LEU:O | 20:M:63:LYS:HG3 | 1.83 | 0.79 |
| 20:M:394:VAL:HA | 20:M:423:GLN:HE22 | 1.46 | 0.79 |
| 24:Q:249:LEU:O | 24:Q:250:THR:CG2 | 2.29 | 0.79 |
| 2:2:160:GLN:HE21 | 2:2:164:TRP:HE1 | 1.31 | 0.79 |
| 11:D:11:PHE:CE2 | 12:E:26:TYR:CB | 2.65 | 0.79 |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:HA | 1.65 | 0.79 |
| 21:N:315:ASN:HA | 21:N:318:LYS:HZ3 | 1.46 | 0.79 |
| 22:O:190:TYR:HD1 | 22:O:227:ILE:CD1 | 1.95 | 0.79 |
| 25:R:70:TYR:CE2 | 25:R:76:GLN:HA | 2.17 | 0.79 |
| 33:Z:394:TYR:CD2 | 33:Z:396:ASN:ND2 | 2.45 | 0.79 |
| 21:N:398:ARG:HD2 | 21:N:438:ASP:CB | 2.08 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:P:131:PHE:N | 23:P:136:ARG:NH1 | 2.28 | 0.79 |
| 27:T:89:TYR:CD1 | 27:T:102:LYS:CD | 2.63 | 0.79 |
| 30:W:141:ILE:HG21 | 30:W:154:LEU:HD13 | 1.64 | 0.79 |
| 14:G:64:VAL:HG12 | 14:G:66:ILE:H | 1.45 | 0.79 |
| 15:H:217:GLN:NE2 | 15:H:248:LEU:HD13 | 1.98 | 0.79 |
| 26:S:360:PHE:O | 26:S:364:ILE:HG12 | 1.83 | 0.79 |
| 26:S:461:PHE:HE2 | 28:U:274:MET:C | 1.85 | 0.79 |
| 17:J:167:PRO:N | 17:J:174:PHE:HZ | 1.81 | 0.79 |
| 20:M:218:ALA:HB3 | 20:M:324:LEU:CD2 | 2.13 | 0.79 |
| 24:Q:74:LEU:HD23 | 24:Q:104:PHE:CD1 | 2.17 | 0.79 |
| 24:Q:74:LEU:HD23 | 24:Q:104:PHE:CE1 | 2.17 | 0.79 |
| 14:G:183:PRO:O | 14:G:184:GLU:HG2 | 1.82 | 0.79 |
| 16:I:174:ASP:OD2 | 16:I:177:PRO:HB3 | 1.83 | 0.79 |
| 20:M:47:GLU:CD | 20:M:50:ARG:NH2 | 2.37 | 0.79 |
| 25:R:63:TYR:OH | 25:R:93:LYS:O | 2.01 | 0.79 |
| 25:R:410:LEU:HD21 | 28:U:285:ILE:HG21 | 1.65 | 0.79 |
| 30:W:186:ALA:HB1 | 30:W:191:ILE:CG2 | 2.13 | 0.79 |
| 3:3:37:TYR:CZ | 3:3:59:ARG:HB2 | 2.18 | 0.78 |
| 4:4:45:PHE:CE2 | 4:4:101:VAL:HG11 | 2.18 | 0.78 |
| 12:E:15:PHE:CD1 | 12:E:21:LEU:HD12 | 2.16 | 0.78 |
| 12:E:20:ARG:CD | 20:M:432:PHE:HZ | 1.95 | 0.78 |
| 16:I:104:LEU:HD21 | 16:I:149:LEU:O | 1.83 | 0.78 |
| 33:Z:518:LEU:HD11 | 33:Z:562:TRP:CE3 | 2.19 | 0.78 |
| 10:C:3:SER:HB3 | 11:D:6:ARG:CZ | 2.13 | 0.78 |
| 11:D:97:ARG:HH12 | 11:D:103:PRO:HG3 | 1.45 | 0.78 |
| 15:H:147:ILE:HG13 | 15:H:183:ILE:CG1 | 2.13 | 0.78 |
| 26:S:343:LEU:HD11 | 26:S:347:HIS:HE1 | 1.45 | 0.78 |
| 27:T:139:ASP:OD2 | 27:T:142:LEU:HG | 1.83 | 0.78 |
| 10:C:3:SER:CB | 11:D:6:ARG:NH2 | 2.45 | 0.78 |
| 12:E:207:VAL:HA | 15:H:409:ARG:HH12 | 1.47 | 0.78 |
| 15:H:97:LEU:HB3 | 15:H:173:ARG:HG3 | 1.64 | 0.78 |
| 20:M:203:ARG:HD3 | 20:M:206:LYS:HD2 | 1.65 | 0.78 |
| 25:R:334:ARG:NH1 | 25:R:363:PHE:CZ | 2.49 | 0.78 |
| 18:K:98:GLN:HE22 | 18:K:136:SER:HB2 | 1.47 | 0.78 |
| 21:N:315:ASN:O | 21:N:318:LYS:HG2 | 1.84 | 0.78 |
| 21:N:328:PHE:HZ | 21:N:693:GLY:HA2 | 1.47 | 0.78 |
| 24:Q:36:SER:O | 24:Q:46:VAL:CG2 | 2.31 | 0.78 |
| 33:Z:224:LEU:HD13 | 33:Z:233:LEU:CD2 | 2.08 | 0.78 |
| 5:5:35:ILE:HD11 | 5:5:45:MET:HE3 | 1.64 | 0.78 |
| 25:R:411:LEU:CD2 | 26:S:464:ARG:NH1 | 2.43 | 0.78 |
| 30:W:133:LYS:CE | 30:W:163:ASN:HD21 | 1.97 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:474:LEU:CD2 | 33:Z:493:LEU:HD23 | 2.12 | 0.78 |
| 3:3:60:TYR:CE2 | 10:C:96:GLN:CB | 2.66 | 0.78 |
| 7:7:33:ARG:NH2 | 7:7:46:SER:HA | 1.96 | 0.78 |
| 10:C:158:THR:HG1 | 10:C:160:TRP:HE1 | 1.30 | 0.78 |
| 23:P:440:HIS:CE1 | 28:U:209:GLU:HB3 | 2.18 | 0.78 |
| 29:V:57:PHE:HZ | 29:V:135:ARG:NH1 | 1.81 | 0.78 |
| 33:Z:119:LEU:HD13 | 33:Z:137:TYR:CZ | 2.19 | 0.78 |
| 8:A:164:VAL:CB | 9:B:61:LEU:HD21 | 2.13 | 0.78 |
| 13:F:3:ARG:HH21 | 15:H:359:ASN:HD21 | 1.31 | 0.78 |
| 20:M:119:VAL:CG1 | 20:M:155:ILE:HD11 | 2.12 | 0.78 |
| 20:M:197:ILE:HB | 20:M:322:LYS:CD | 2.13 | 0.78 |
| 22:O:233:LEU:HD22 | 22:O:238:ILE:CD1 | 2.11 | 0.78 |
| 23:P:131:PHE:CE2 | 23:P:167:THR:CG2 | 2.59 | 0.78 |
| 31:X:104:LYS:HE3 | 31:X:108:ASN:ND2 | 1.99 | 0.78 |
| 1:1:30:VAL:HG23 | 1:1:172:VAL:HG21 | 1.65 | 0.78 |
| 19:L:389:ALA:CB | 20:M:339:ARG:HE | 1.97 | 0.78 |
| 27:T:70:ILE:HD11 | 27:T:78:PHE:CE1 | 2.18 | 0.78 |
| 33:Z:169:VAL:HG11 | 33:Z:183:LYS:HG2 | 1.65 | 0.78 |
| 18:K:280:LYS:HZ1 | 18:K:296:LEU:HD23 | 1.49 | 0.78 |
| 25:R:219:LEU:O | 25:R:325:HIS:CE1 | 2.36 | 0.78 |
| 25:R:301:TYR:HE1 | 25:R:305:PHE:HZ | 1.29 | 0.78 |
| 6:6:10:ASP:OD2 | 6:6:165:TYR:OH | 2.01 | 0.78 |
| 15:H:183:ILE:HG22 | 15:H:183:ILE:O | 1.81 | 0.78 |
| 17:J:146:THR:HG23 | 17:J:148:ASP:H | 1.48 | 0.78 |
| 19:L:290:ARG:HH12 | 19:L:293:GLU:HB3 | 1.48 | 0.78 |
| 25:R:209:ARG:HE | 25:R:243:LEU:CD2 | 1.96 | 0.78 |
| 27:T:8:THR:HG23 | 27:T:61:ILE:HG12 | 1.65 | 0.78 |
| 29:V:53:MET:HE2 | 29:V:65:VAL:CG1 | 2.14 | 0.78 |
| 1:1:8:PHE:HE2 | 1:1:10:ASP:HB2 | 1.49 | 0.77 |
| 17:J:305:LEU:CD2 | 17:J:313:LYS:HE3 | 2.07 | 0.77 |
| 26:S:464:ARG:HB3 | 28:U:281:LEU:HD22 | 1.65 | 0.77 |
| 7:7:-7:GLN:HG3 | 7:7:101:PRO:HD2 | 1.64 | 0.77 |
| 9:B:70:ASP:OD1 | 9:B:71:ILE:HG13 | 1.83 | 0.77 |
| 16:I:314:ASP:OD1 | 16:I:340:ARG:NE | 2.16 | 0.77 |
| 26:S:461:PHE:HE1 | 28:U:278:ILE:CB | 1.96 | 0.77 |
| 29:V:57:PHE:HZ | 29:V:135:ARG:CZ | 1.96 | 0.77 |
| 13:F:144:LEU:O | 13:F:155:GLU:HG3 | 1.84 | 0.77 |
| 13:F:157:TYR:CD2 | 14:G:57:LEU:O | 2.38 | 0.77 |
| 23:P:413:ASN:OD1 | 29:V:245:VAL:HG13 | 1.83 | 0.77 |
| 25:R:209:ARG:O | 25:R:213:TYR:CD2 | 2.36 | 0.77 |
| 26:S:461:PHE:CZ | 28:U:278:ILE:HB | 2.19 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:T:186:ARG:NH1 | 27:T:220:PHE:CE2 | 2.53 | 0.77 |
| 11:D:159:TRP:CZ3 | 12:E:59:LEU:HD13 | 2.18 | 0.77 |
| 18:K:212:TYR:CZ | 18:K:320:ARG:HA | 2.18 | 0.77 |
| 18:K:280:LYS:NZ | 18:K:296:LEU:CD2 | 2.47 | 0.77 |
| 19:L:401:PHE:CE1 | 19:L:404:ARG:NH1 | 2.52 | 0.77 |
| 23:P:203:ILE:HG12 | 23:P:220:TYR:HH | 1.48 | 0.77 |
| 25:R:315:VAL:O | 25:R:319:CYS:SG | 2.40 | 0.77 |
| 26:S:464:ARG:CB | 28:U:281:LEU:HD22 | 2.14 | 0.77 |
| 33:Z:865:ASP:OD2 | 33:Z:909:ARG:CZ | 2.32 | 0.77 |
| 16:I:320:GLY:HA2 | 16:I:323:LYS:CE | 2.13 | 0.77 |
| 13:F:101:ARG:NH1 | 13:F:103:LEU:HD12 | 2.00 | 0.77 |
| 27:T:256:LYS:HE3 | 29:V:298:ALA:O | 1.85 | 0.77 |
| 33:Z:829:GLN:HG2 | 33:Z:832:ARG:NH2 | 2.00 | 0.77 |
| 13:F:65:LYS:HE2 | 13:F:222:PHE:HD2 | 1.49 | 0.77 |
| 16:I:264:CYS:SG | 16:I:305:THR:HG23 | 2.24 | 0.77 |
| 25:R:170:VAL:CG1 | 25:R:194:VAL:HG21 | 2.14 | 0.77 |
| 31:X:27:ILE:HB | 31:X:59:ARG:HH22 | 1.50 | 0.77 |
| 31:X:91:PHE:N | 31:X:96:ARG:HG2 | 1.97 | 0.77 |
| 33:Z:562:TRP:CE2 | 33:Z:566:LEU:HD21 | 2.19 | 0.77 |
| 1:1:66:TYR:CD2 | 1:1:73:PRO:HB3 | 2.20 | 0.77 |
| 16:I:395:MET:HG3 | 16:I:420:LYS:HD3 | 1.65 | 0.77 |
| 21:N:362:TRP:CH2 | 29:V:23:THR:HG21 | 2.20 | 0.77 |
| 33:Z:126:TYR:CD2 | 33:Z:128:GLU:HB2 | 2.19 | 0.77 |
| 13:F:158:GLY:O | 14:G:57:LEU:HD13 | 1.85 | 0.77 |
| 21:N:145:LEU:HD22 | 21:N:173:LYS:HZ1 | 1.50 | 0.77 |
| 21:N:222:TYR:N | 21:N:894:ARG:NH2 | 2.32 | 0.77 |
| 25:R:246:TYR:OH | 25:R:275:GLU:OE2 | 2.02 | 0.77 |
| 30:W:7:VAL:HG23 | 30:W:98:LEU:CD2 | 2.15 | 0.77 |
| 33:Z:812:ILE:CG1 | 33:Z:834:LEU:HD22 | 2.14 | 0.77 |
| 33:Z:924:LYS:NZ | 33:Z:993:GLU:HG3 | 2.00 | 0.77 |
| 1:1:57:ASP:C | 8:A:106:TYR:HE1 | 1.88 | 0.77 |
| 19:L:227:GLY:HA2 | 19:L:230:LEU:HD12 | 1.66 | 0.77 |
| 20:M:303:ARG:NH1 | 20:M:307:GLU:HB2 | 1.99 | 0.77 |
| 26:S:218:LEU:HG | 26:S:256:LYS:HZ3 | 1.50 | 0.77 |
| 15:H:436:LYS:CE | 33:Z:365:SER:HB2 | 2.09 | 0.76 |
| 16:I:148:LEU:CD2 | 16:I:160:LEU:HD22 | 2.16 | 0.76 |
| 33:Z:382:ALA:HB1 | 33:Z:849:ARG:HG2 | 1.67 | 0.76 |
| 33:Z:392:LEU:HD13 | 33:Z:424:SER:O | 1.84 | 0.76 |
| 3:3:52:THR:CB | 4:4:84:ARG:NH2 | 2.48 | 0.76 |
| 6:6:39:ASP:O | 6:6:40:ASN:HB2 | 1.83 | 0.76 |
| 7:7:174:ARG:NE | 7:7:207:GLU:O | 2.17 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:95:ILE:HG23 | 20:M:68:LYS:HZ2 | 1.47 | 0.76 |
| 19:L:357:ARG:O | 19:L:361:PHE:CD2 | 2.38 | 0.76 |
| 26:S:151:GLU:OE2 | 26:S:153:GLU:HB3 | 1.84 | 0.76 |
| 28:U:277:TYR:OH | 29:V:295:VAL:CG1 | 2.32 | 0.76 |
| 28:U:283:ARG:NH1 | 29:V:291:ASN:HD22 | 1.82 | 0.76 |
| 2:2:42:TRP:CD1 | 2:2:178:MET:SD | 2.78 | 0.76 |
| 10:C:33:GLY:HA2 | 10:C:51:LYS:HE3 | 1.67 | 0.76 |
| 17:J:224:GLY:C | 17:J:225:GLU:CA | 2.53 | 0.76 |
| 19:L:283:VAL:HG22 | 19:L:286:ILE:HD11 | 1.68 | 0.76 |
| 22:O:15:ARG:CZ | 22:O:73:ILE:CD1 | 2.55 | 0.76 |
| 28:U:21:HIS:CE1 | 28:U:93:TYR:HH | 2.02 | 0.76 |
| 23:P:130:ILE:HG22 | 23:P:136:ARG:HH22 | 1.50 | 0.76 |
| 28:U:67:PHE:HE2 | 30:W:100:HIS:ND1 | 1.82 | 0.76 |
| 29:V:57:PHE:CE2 | 29:V:59:ASP:O | 2.39 | 0.76 |
| 21:N:158:LEU:HD12 | 21:N:202:PHE:HE2 | 1.49 | 0.76 |
| 21:N:315:ASN:CA | 21:N:318:LYS:HZ3 | 1.97 | 0.76 |
| 23:P:94:GLN:OE1 | 23:P:136:ARG:HG2 | 1.86 | 0.76 |
| 23:P:167:THR:HB | 23:P:168:TYR:CD1 | 2.21 | 0.76 |
| 24:Q:141:LEU:HG | 24:Q:145:HIS:CD2 | 2.20 | 0.76 |
| 24:Q:299:MET:HE1 | 24:Q:335:PHE:CZ | 2.20 | 0.76 |
| 25:R:202:GLY:HA2 | 25:R:207:ARG:HH21 | 1.51 | 0.76 |
| 31:X:75:TRP:CD2 | 31:X:125:MET:HB3 | 2.20 | 0.76 |
| 5:5:158:LYS:HE3 | 5:5:196:LEU:HD11 | 1.68 | 0.76 |
| 8:A:205:PHE:CZ | 8:A:209:HIS:NE2 | 2.53 | 0.76 |
| 14:G:108:ILE:HG22 | 14:G:148:TYR:CE1 | 2.21 | 0.76 |
| 14:G:111:PHE:HD1 | 14:G:114:ARG:HH22 | 0.81 | 0.76 |
| 20:M:384:ASP:H | 20:M:386:PHE:HE1 | 1.34 | 0.76 |
| 24:Q:61:LEU:CD2 | 24:Q:65:TYR:OH | 2.32 | 0.76 |
| 29:V:57:PHE:CZ | 29:V:135:ARG:NH1 | 2.54 | 0.76 |
| 33:Z:188:ALA:HB3 | 33:Z:201:LEU:HD11 | 1.65 | 0.76 |
| 33:Z:363:ASP:O | 33:Z:366:LYS:NZ | 2.17 | 0.76 |
| 1:1:-4:VAL:HG12 | 1:1:49:ALA:HB3 | 1.66 | 0.76 |
| 4:4:102:LEU:HD22 | 4:4:117:GLN:HG2 | 1.67 | 0.76 |
| 8:A:31:ALA:HA | 14:G:14:PHE:CZ | 2.19 | 0.76 |
| 8:A:220:LYS:CG | 8:A:242:GLU:HB2 | 2.15 | 0.76 |
| 10:C:144:TYR:HB2 | 10:C:147:GLN:HE21 | 1.49 | 0.76 |
| 14:G:108:ILE:CG2 | 14:G:148:TYR:CD1 | 2.69 | 0.76 |
| 17:J:214:SER:HB3 | 17:J:217:GLU:OE1 | 1.86 | 0.76 |
| 19:L:107:GLU:OE2 | 19:L:145:ARG:NH2 | 2.19 | 0.76 |
| 19:L:401:PHE:CD1 | 19:L:404:ARG:CZ | 2.69 | 0.76 |
| 22:O:219:ILE:HG23 | 22:O:274:ILE:HD13 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:348:LEU:HD23 | 33:Z:353:VAL:HB | 1.66 | 0.76 |
| 18:K:141:ARG:NH1 | 19:L:153:LEU:HD11 | 2.00 | 0.76 |
| 30:W:133:LYS:HE3 | 30:W:163:ASN:HD21 | 1.48 | 0.76 |
| 33:Z:106:TRP:HB2 | 33:Z:112:LYS:NZ | 2.00 | 0.76 |
| 33:Z:443:ASP:HB3 | 33:Z:447:VAL:HB | 1.66 | 0.76 |
| 33:Z:975:SER:O | 33:Z:977:ILE:HG23 | 1.86 | 0.76 |
| 1:1:94:THR:HG23 | 1:1:115:LEU:HD22 | 1.66 | 0.76 |
| 7:7:145:PRO:CB | 7:7:148:ARG:HH21 | 1.99 | 0.76 |
| 10:C:46:LEU:HD11 | 10:C:138:ALA:HB3 | 1.67 | 0.76 |
| 11:D:19:GLN:NE2 | 11:D:121:THR:HA | 2.01 | 0.76 |
| 16:I:253:ILE:HD11 | 16:I:287:ILE:CA | 2.16 | 0.76 |
| 21:N:490:LEU:HD21 | 21:N:526:TYR:CD2 | 2.21 | 0.76 |
| 2:2:7:LYS:O | 2:2:146:LEU:HD23 | 1.86 | 0.76 |
| 7:7:33:ARG:NH2 | 7:7:46:SER:CA | 2.49 | 0.76 |
| 15:H:172:MET:C | 16:I:129:TYR:HE2 | 1.88 | 0.76 |
| 25:R:411:LEU:HD22 | 26:S:464:ARG:HH11 | 1.50 | 0.76 |
| 33:Z:89:LEU:HD13 | 33:Z:125:THR:HB | 1.67 | 0.76 |
| 33:Z:363:ASP:O | 33:Z:366:LYS:CE | 2.34 | 0.76 |
| 33:Z:509:LEU:CD1 | 33:Z:530:LEU:HD23 | 2.16 | 0.76 |
| 33:Z:776:VAL:HG13 | 33:Z:777:PRO:HD3 | 1.65 | 0.76 |
| 33:Z:813:PHE:CE1 | 33:Z:847:ILE:HG23 | 2.21 | 0.76 |
| 2:2:104:ASP:HB3 | 2:2:105:PRO:HD2 | 1.68 | 0.75 |
| 9:B:190:HIS:NE2 | 24:Q:94:VAL:HG21 | 2.01 | 0.75 |
| 22:O:228:TYR:CD2 | 22:O:229:ASN:N | 2.49 | 0.75 |
| 24:Q:232:TYR:HB2 | 24:Q:272:LEU:CD2 | 2.15 | 0.75 |
| 26:S:163:VAL:HA | 26:S:167:LEU:HD23 | 1.66 | 0.75 |
| 26:S:184:TRP:CH2 | 26:S:217:PHE:HE2 | 2.02 | 0.75 |
| 27:T:86:LYS:HE2 | 27:T:128:TYR:CD2 | 2.21 | 0.75 |
| 27:T:226:TRP:CZ3 | 27:T:235:PHE:HE2 | 2.04 | 0.75 |
| 33:Z:763:HIS:CA | 33:Z:766:HIS:CE1 | 2.69 | 0.75 |
| 2:2:59:ILE:HD12 | 2:2:82:MET:HB3 | 1.67 | 0.75 |
| 6:6:10:ASP:OD1 | 6:6:11:PHE:HD1 | 1.69 | 0.75 |
| 12:E:98:THR:CG2 | 12:E:102:TYR:CE2 | 2.69 | 0.75 |
| 16:I:75:PHE:CD2 | 16:I:76:VAL:HG23 | 2.20 | 0.75 |
| 16:I:200:LEU:HB3 | 33:Z:931:GLN:HG2 | 1.68 | 0.75 |
| 18:K:159:SER:OG | 18:K:244:HIS:NE2 | 2.08 | 0.75 |
| 24:Q:38:SER:OG | 24:Q:88:PHE:CE1 | 2.39 | 0.75 |
| 24:Q:263:LYS:HE2 | 24:Q:295:GLY:HA3 | 1.67 | 0.75 |
| 33:Z:74:SER:CB | 33:Z:79:THR:CG2 | 2.64 | 0.75 |
| 25:R:130:GLN:NE2 | 25:R:134:TRP:HE1 | 1.84 | 0.75 |
| 27:T:221:ALA:CB | 27:T:228:ILE:HD11 | 2.17 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:443:ASP:HB3 | 33:Z:447:VAL:CG1 | 2.13 | 0.75 |
| 5:5:145:LYS:HE3 | 5:5:147:ASP:HB2 | 1.68 | 0.75 |
| 9:B:67:LEU:HD11 | 9:B:73:ALA:HB2 | 1.69 | 0.75 |
| 13:F:105:VAL:CG2 | 13:F:145:LEU:CB | 2.63 | 0.75 |
| 23:P:308:LEU:HD22 | 23:P:369:LEU:CD2 | 2.15 | 0.75 |
| 33:Z:428:TRP:CZ3 | 33:Z:461:GLY:CA | 2.63 | 0.75 |
| 33:Z:428:TRP:CE3 | 33:Z:461:GLY:HA3 | 2.20 | 0.75 |
| 33:Z:463:HIS:NE2 | 33:Z:497:PHE:HD1 | 1.82 | 0.75 |
| 7:7:88:LEU:HD21 | 7:7:106:ILE:CD1 | 2.16 | 0.75 |
| 10:C:4:ARG:CG | 11:D:6:ARG:HD2 | 2.16 | 0.75 |
| 10:C:207:THR:HG23 | 10:C:210:ARG:HH21 | 1.51 | 0.75 |
| 18:K:159:SER:HB3 | 18:K:244:HIS:HE2 | 1.52 | 0.75 |
| 22:O:190:TYR:CD1 | 22:O:227:ILE:HD11 | 2.18 | 0.75 |
| 24:Q:146:TYR:CE1 | 24:Q:184:VAL:CA | 2.63 | 0.75 |
| 29:V:127:LYS:HE3 | 29:V:194:ARG:NE | 2.01 | 0.75 |
| 8:A:81:MET:SD | 8:A:143:PHE:CE1 | 2.79 | 0.75 |
| 16:I:245:LEU:HG | 16:I:247:ILE:HD11 | 1.67 | 0.75 |
| 21:N:424:LYS:HA | 21:N:427:ILE:HD12 | 1.68 | 0.75 |
| 24:Q:146:TYR:CE1 | 24:Q:151:TYR:CE1 | 2.75 | 0.75 |
| 9:B:139:HIS:CD2 | 9:B:234:ARG:HD3 | 2.22 | 0.75 |
| 18:K:126:LEU:HD22 | 18:K:149:ILE:HD11 | 1.66 | 0.75 |
| 21:N:163:LEU:HB3 | 21:N:209:LYS:NZ | 2.02 | 0.75 |
| 22:O:116:ASN:HB3 | 22:O:127:LEU:CD1 | 2.14 | 0.75 |
| 33:Z:863:THR:CB | 33:Z:911:LYS:HZ2 | 1.98 | 0.75 |
| 2:2:8:PHE:CE2 | 2:2:10:ASN:C | 2.60 | 0.75 |
| 6:6:85:GLN:HG3 | 6:6:122:TYR:HD1 | 1.51 | 0.75 |
| 10:C:46:LEU:HD11 | 10:C:138:ALA:CB | 2.16 | 0.75 |
| 16:I:340:ARG:NH1 | 16:I:343:ARG:HG2 | 2.01 | 0.75 |
| 18:K:205:PRO:HD2 | 18:K:207:ARG:NH2 | 2.01 | 0.75 |
| 23:P:184:MET:HB3 | 23:P:223:LEU:HD13 | 1.67 | 0.75 |
| 24:Q:389:VAL:HG13 | 24:Q:400:TYR:HB2 | 1.66 | 0.75 |
| 25:R:378:ASN:HB3 | 25:R:391:ASN:OD1 | 1.86 | 0.75 |
| 33:Z:338:HIS:HD2 | 33:Z:339:PHE:CZ | 2.05 | 0.75 |
| 1:1:190:PRO:HA | 1:1:193:TYR:CE2 | 2.22 | 0.75 |
| 3:3:155:PHE:HD1 | 3:3:180:ILE:HD11 | 1.52 | 0.75 |
| 7:7:103:TRP:O | 7:7:103:TRP:CD1 | 2.39 | 0.75 |
| 19:L:219:LEU:HD23 | 19:L:346:LYS:HG3 | 1.68 | 0.75 |
| 21:N:654:GLN:NE2 | 21:N:697:PHE:HD2 | 1.85 | 0.75 |
| 21:N:909:GLU:HB3 | 21:N:911:LYS:NZ | 2.01 | 0.75 |
| 29:V:135:ARG:HA | 29:V:157:ARG:NH2 | 2.02 | 0.75 |
| 30:W:35:PHE:CE2 | 30:W:182:TYR:CD2 | 2.75 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:481:PRO:O | 33:Z:482:ASP:CG | 2.25 | 0.75 |
| 33:Z:493:LEU:HG | 33:Z:497:PHE:CE2 | 2.22 | 0.75 |
| 33:Z:574:TYR:OH | 33:Z:584:VAL:CG1 | 2.35 | 0.75 |
| 33:Z:823:ASN:CB | 33:Z:856:HIS:CE1 | 2.65 | 0.75 |
| 16:I:310:LEU:CD1 | 16:I:338:LEU:HA | 2.17 | 0.74 |
| 21:N:16:ASN:O | 21:N:17:GLN:HG2 | 1.87 | 0.74 |
| 24:Q:50:ARG:NH2 | 24:Q:53:GLU:HB3 | 2.02 | 0.74 |
| 26:S:378:GLN:HB3 | 26:S:382:ARG:NH1 | 2.02 | 0.74 |
| 33:Z:748:LEU:CD2 | 33:Z:783:VAL:HA | 2.16 | 0.74 |
| 7:7:193:ASP:CB | 7:7:196:THR:OG1 | 2.35 | 0.74 |
| 8:A:83:VAL:HG22 | 8:A:141:LEU:CD2 | 2.17 | 0.74 |
| 11:D:53:LYS:HG3 | 11:D:55:GLN:HG2 | 1.67 | 0.74 |
| 14:G:7:TYR:CE1 | 14:G:13:VAL:HG23 | 2.20 | 0.74 |
| 14:G:168:ARG:HE | 14:G:172:LYS:HZ1 | 1.34 | 0.74 |
| 14:G:173:ALA:HA | 19:L:420:ARG:CZ | 2.16 | 0.74 |
| 15:H:59:ILE:HD13 | 16:I:92:GLU:OE2 | 1.87 | 0.74 |
| 16:I:281:ILE:CG2 | 16:I:284:ILE:HD11 | 2.16 | 0.74 |
| 22:O:30:GLU:CG | 22:O:58:ARG:NH1 | 2.50 | 0.74 |
| 30:W:21:PHE:CE1 | 30:W:144:PHE:CE2 | 2.74 | 0.74 |
| 33:Z:443:ASP:HB3 | 33:Z:447:VAL:HG11 | 1.67 | 0.74 |
| 9:B:159:TRP:CZ3 | 10:C:57:LEU:HB2 | 2.22 | 0.74 |
| 15:H:284:VAL:CB | 20:M:254:MET:CB | 2.55 | 0.74 |
| 19:L:290:ARG:NH1 | 19:L:293:GLU:CA | 2.50 | 0.74 |
| 19:L:357:ARG:O | 19:L:361:PHE:HD2 | 1.71 | 0.74 |
| 20:M:81:ASN:HD21 | 20:M:143:ASN:H | 1.35 | 0.74 |
| 24:Q:289:GLU:HB2 | 24:Q:291:TYR:CD1 | 2.23 | 0.74 |
| 33:Z:154:ILE:CG2 | 33:Z:211:PHE:CE1 | 2.70 | 0.74 |
| 1:1:-2:LEU:CD1 | 1:1:1:THR:H | 2.01 | 0.74 |
| 6:6:48:PHE:HE2 | 6:6:50:ALA:HB3 | 1.52 | 0.74 |
| 6:6:58:ARG:HH12 | 6:6:91:LYS:HD2 | 1.52 | 0.74 |
| 8:A:220:LYS:HG3 | 8:A:242:GLU:OE1 | 1.87 | 0.74 |
| 13:F:91:GLN:NE2 | 13:F:111:LEU:HD23 | 2.03 | 0.74 |
| 15:H:284:VAL:CB | 20:M:254:MET:N | 2.48 | 0.74 |
| 17:J:212:ARG:NH1 | 17:J:246:PHE:HE2 | 1.83 | 0.74 |
| 23:P:141:LYS:HB2 | 23:P:179:PHE:CE1 | 2.20 | 0.74 |
| 25:R:353:MET:HA | 25:R:357:PHE:HD2 | 1.52 | 0.74 |
| 3:3:52:THR:HG21 | 4:4:84:ARG:CZ | 2.17 | 0.74 |
| 22:O:71:ASP:O | 30:W:18:ASN:HB2 | 1.86 | 0.74 |
| 26:S:256:LYS:O | 26:S:259:TYR:CE1 | 2.39 | 0.74 |
| 26:S:343:LEU:CD1 | 26:S:347:HIS:CE1 | 2.70 | 0.74 |
| 33:Z:604:GLY:O | 33:Z:608:TYR:HD2 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:5:40:PHE:HB3 | 5:5:73:ARG:HH21 | 1.46 | 0.74 |
| 14:G:61:GLN:HA | 14:G:64:VAL:HG23 | 1.69 | 0.74 |
| 16:I:103:PRO:HB3 | 17:J:120:TYR:CE2 | 2.22 | 0.74 |
| 17:J:337:LEU:CD2 | 17:J:377:VAL:HB | 2.16 | 0.74 |
| 21:N:386:MET:O | 21:N:390:LEU:HG | 1.87 | 0.74 |
| 24:Q:50:ARG:HH21 | 24:Q:53:GLU:CB | 2.00 | 0.74 |
| 24:Q:50:ARG:HH21 | 24:Q:53:GLU:HB3 | 1.51 | 0.74 |
| 33:Z:748:LEU:HD22 | 33:Z:783:VAL:O | 1.88 | 0.74 |
| 23:P:344:ARG:NH2 | 23:P:347:GLU:OE1 | 2.20 | 0.74 |
| 24:Q:353:PRO:O | 24:Q:354:PHE:HD1 | 1.71 | 0.74 |
| 22:O:15:ARG:HH12 | 22:O:73:ILE:HG13 | 1.52 | 0.74 |
| 22:O:266:PHE:CZ | 22:O:280:LEU:HD22 | 2.18 | 0.74 |
| 22:O:373:TRP:CH2 | 28:U:200:LEU:HD21 | 2.22 | 0.74 |
| 27:T:157:TYR:OH | 27:T:188:GLU:CG | 2.30 | 0.74 |
| 31:X:12:ALA:HB3 | 31:X:33:ILE:HG23 | 1.70 | 0.74 |
| 8:A:232:LYS:HD2 | 8:A:234:PHE:HE1 | 1.52 | 0.74 |
| 17:J:219:VAL:HG11 | 18:K:284:ALA:HA | 1.68 | 0.74 |
| 24:Q:11:ALA:HB2 | 24:Q:26:VAL:CG1 | 2.16 | 0.74 |
| 33:Z:135:LEU:O | 33:Z:139:LEU:HG | 1.88 | 0.74 |
| 7:7:154:GLU:HA | 7:7:157:ILE:HD12 | 1.68 | 0.74 |
| 15:H:156:VAL:HG13 | 15:H:181:TYR:HE1 | 1.53 | 0.74 |
| 16:I:148:LEU:HD21 | 16:I:160:LEU:HD22 | 1.70 | 0.74 |
| 16:I:310:LEU:CD1 | 16:I:337:ALA:O | 2.36 | 0.74 |
| 18:K:186:GLU:HA | 18:K:190:LEU:HD12 | 1.70 | 0.74 |
| 19:L:290:ARG:CD | 19:L:293:GLU:HA | 2.18 | 0.74 |
| 21:N:762:ARG:HG3 | 21:N:890:PHE:HE2 | 1.52 | 0.74 |
| 23:P:353:ILE:HG23 | 23:P:357:TYR:CD2 | 2.23 | 0.74 |
| 29:V:131:GLN:NE2 | 29:V:194:ARG:NH2 | 2.32 | 0.74 |
| 33:Z:217:GLU:CD | 33:Z:244:ARG:NH2 | 2.31 | 0.74 |
| 33:Z:272:TYR:HE2 | 33:Z:284:LEU:HD11 | 1.53 | 0.74 |
| 3:3:155:PHE:CD1 | 3:3:180:ILE:HD11 | 2.23 | 0.73 |
| 9:B:119:GLN:OE1 | 10:C:82:ALA:HB1 | 1.87 | 0.73 |
| 9:B:139:HIS:ND1 | 9:B:145:PHE:CD1 | 2.56 | 0.73 |
| 17:J:241:ALA:CB | 17:J:288:ILE:HD11 | 2.17 | 0.73 |
| 24:Q:104:PHE:CD2 | 24:Q:114:GLN:OE1 | 2.41 | 0.73 |
| 33:Z:829:GLN:HG2 | 33:Z:832:ARG:HH22 | 1.53 | 0.73 |
| 21:N:424:LYS:HZ2 | 21:N:461:GLU:HB3 | 1.52 | 0.73 |
| 24:Q:74:LEU:CD2 | 24:Q:104:PHE:CD1 | 2.71 | 0.73 |
| 26:S:315:LYS:CD | 26:S:345:TYR:CZ | 2.63 | 0.73 |
| 31:X:75:TRP:CE2 | 31:X:125:MET:HB3 | 2.21 | 0.73 |
| 33:Z:190:THR:HG21 | 33:Z:195:PHE:HB2 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:30:VAL:HG22 | 1:1:174:ARG:HH21 | 1.53 | 0.73 |
| 4:4:81:SER:HA | 4:4:124:LYS:NZ | 2.03 | 0.73 |
| 15:H:147:ILE:HB | 15:H:183:ILE:HD11 | 1.70 | 0.73 |
| 17:J:27:ILE:HD13 | 18:K:50:LYS:HD3 | 1.69 | 0.73 |
| 18:K:307:ASP:OD1 | 18:K:312:VAL:O | 2.05 | 0.73 |
| 22:O:23:HIS:ND1 | 22:O:24:PRO:HD2 | 2.02 | 0.73 |
| 24:Q:250:THR:HG23 | 24:Q:251:THR:N | 2.03 | 0.73 |
| 29:V:53:MET:HE2 | 29:V:65:VAL:HG21 | 1.70 | 0.73 |
| 29:V:131:GLN:HE22 | 29:V:194:ARG:NH2 | 1.85 | 0.73 |
| 33:Z:562:TRP:NE1 | 33:Z:566:LEU:HG | 2.03 | 0.73 |
| 9:B:139:HIS:ND1 | 9:B:145:PHE:CE1 | 2.56 | 0.73 |
| 19:L:159:LEU:CD1 | 19:L:160:PRO:O | 2.37 | 0.73 |
| 23:P:130:ILE:O | 23:P:136:ARG:NH1 | 2.22 | 0.73 |
| 33:Z:221:VAL:HG11 | 33:Z:248:TYR:HD2 | 1.54 | 0.73 |
| 8:A:64:LEU:HD13 | 14:G:157:TRP:CD1 | 2.22 | 0.73 |
| 15:H:351:VAL:CG1 | 15:H:353:PHE:CZ | 2.71 | 0.73 |
| 22:O:233:LEU:CD2 | 22:O:238:ILE:HD11 | 2.16 | 0.73 |
| 22:O:266:PHE:CZ | 22:O:280:LEU:HD21 | 2.22 | 0.73 |
| 24:Q:141:LEU:CD1 | 24:Q:145:HIS:NE2 | 2.51 | 0.73 |
| 25:R:239:THR:HG22 | 25:R:246:TYR:HB2 | 1.69 | 0.73 |
| 25:R:366:ASN:O | 25:R:370:LYS:HG3 | 1.88 | 0.73 |
| 33:Z:64:TYR:CZ | 33:Z:115:LEU:HD21 | 2.23 | 0.73 |
| 33:Z:557:GLU:OE1 | 33:Z:562:TRP:CZ3 | 2.40 | 0.73 |
| 33:Z:776:VAL:CG1 | 33:Z:777:PRO:CD | 2.63 | 0.73 |
| 2:2:8:PHE:CE1 | 2:2:11:GLY:C | 2.62 | 0.73 |
| 17:J:162:GLU:HA | 17:J:166:LEU:HD12 | 1.70 | 0.73 |
| 18:K:346:ARG:HG2 | 18:K:349:ARG:HH22 | 1.53 | 0.73 |
| 19:L:362:LYS:HA | 19:L:376:PHE:CE2 | 2.24 | 0.73 |
| 24:Q:61:LEU:HD11 | 24:Q:65:TYR:CE1 | 2.23 | 0.73 |
| 25:R:378:ASN:ND2 | 25:R:393:PRO:HA | 2.03 | 0.73 |
| 33:Z:92:LEU:O | 33:Z:95:THR:OG1 | 2.05 | 0.73 |
| 33:Z:165:TYR:OH | 33:Z:188:ALA:CB | 2.36 | 0.73 |
| 33:Z:497:PHE:CD2 | 33:Z:505:VAL:CG1 | 2.71 | 0.73 |
| 33:Z:812:ILE:HG12 | 33:Z:834:LEU:CD2 | 2.18 | 0.73 |
| 5:5:8:PHE:CZ | 5:5:13:ILE:CD1 | 2.71 | 0.73 |
| 16:I:171:MET:HB3 | 16:I:245:LEU:HD11 | 1.71 | 0.73 |
| 16:I:229:LYS:NZ | 16:I:283:GLU:OE2 | 2.21 | 0.73 |
| 21:N:75:TYR:O | 21:N:79:VAL:HG23 | 1.88 | 0.73 |
| 25:R:55:LYS:NZ | 25:R:91:TRP:CE2 | 2.57 | 0.73 |
| 26:S:286:TYR:CE1 | 26:S:323:LEU:CB | 2.70 | 0.73 |
| 10:C:144:TYR:HB2 | 10:C:147:GLN:NE2 | 2.03 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:I:253:ILE:CD1 | 16:I:287:ILE:CG2 | 2.64 | 0.73 |
| 16:I:428:VAL:HG12 | 16:I:428:VAL:O | 1.87 | 0.73 |
| 20:M:59:LEU:HG | 20:M:63:LYS:HE3 | 1.69 | 0.73 |
| 21:N:536:ILE:CD1 | 21:N:555:ILE:HG12 | 2.19 | 0.73 |
| 26:S:428:ARG:HA | 27:T:195:LEU:HD22 | 1.69 | 0.73 |
| 27:T:112:ASN:HB2 | 27:T:177:PHE:CZ | 2.23 | 0.73 |
| 29:V:53:MET:CE | 29:V:65:VAL:HG21 | 2.19 | 0.73 |
| 33:Z:312:TYR:CE1 | 33:Z:348:LEU:HD22 | 2.23 | 0.73 |
| 33:Z:761:PHE:CD2 | 33:Z:780:MET:CE | 2.70 | 0.73 |
| 17:J:167:PRO:HD3 | 17:J:174:PHE:HZ | 1.50 | 0.73 |
| 23:P:271:SER:C | 23:P:344:ARG:HD2 | 2.09 | 0.73 |
| 25:R:252:TYR:HE1 | 25:R:319:CYS:SG | 2.11 | 0.73 |
| 26:S:461:PHE:CE2 | 28:U:277:TYR:HB2 | 2.24 | 0.73 |
| 28:U:277:TYR:HE1 | 29:V:295:VAL:HG11 | 0.95 | 0.73 |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:O | 1.85 | 0.73 |
| 11:D:120:TYR:CD1 | 11:D:126:VAL:HG21 | 2.24 | 0.73 |
| 15:H:295:PHE:CZ | 15:H:336:LEU:HD12 | 2.23 | 0.73 |
| 21:N:282:TYR:CE2 | 21:N:286:LEU:HB3 | 2.24 | 0.73 |
| 21:N:460:ILE:HG22 | 21:N:494:LYS:HE3 | 1.70 | 0.73 |
| 21:N:596:LEU:CD2 | 21:N:717:LEU:CD1 | 2.57 | 0.73 |
| 22:O:72:LYS:O | 30:W:18:ASN:HB2 | 1.89 | 0.73 |
| 6:6:-5:TYR:CE1 | 6:6:97:TYR:CB | 2.72 | 0.72 |
| 8:A:64:LEU:HD12 | 14:G:158:GLY:O | 1.88 | 0.72 |
| 8:A:154:ILE:HD11 | 8:A:169:THR:HG22 | 1.68 | 0.72 |
| 12:E:207:VAL:HA | 15:H:409:ARG:NH1 | 2.04 | 0.72 |
| 15:H:49:LEU:HD22 | 33:Z:758:LEU:O | 1.89 | 0.72 |
| 19:L:336:ALA:O | 19:L:342:ARG:HD2 | 1.89 | 0.72 |
| 21:N:300:ASN:HD22 | 21:N:920:VAL:HG21 | 1.54 | 0.72 |
| 21:N:579:SER:HA | 21:N:584:ARG:HH21 | 1.52 | 0.72 |
| 21:N:615:ALA:CB | 21:N:651:PHE:CZ | 2.72 | 0.72 |
| 23:P:212:LYS:HD3 | 23:P:247:THR:HG23 | 1.70 | 0.72 |
| 25:R:55:LYS:NZ | 25:R:91:TRP:CZ2 | 2.57 | 0.72 |
| 26:S:184:TRP:CH2 | 26:S:217:PHE:CE2 | 2.78 | 0.72 |
| 26:S:286:TYR:HE1 | 26:S:323:LEU:HD13 | 1.53 | 0.72 |
| 28:U:293:GLU:HG2 | 29:V:277:LYS:CE | 2.18 | 0.72 |
| 33:Z:550:PHE:CE1 | 33:Z:566:LEU:CB | 2.71 | 0.72 |
| 8:A:232:LYS:HD2 | 8:A:234:PHE:CE1 | 2.24 | 0.72 |
| 21:N:36:TRP:HZ3 | 26:S:252:ASP:HB3 | 1.53 | 0.72 |
| 26:S:461:PHE:CE1 | 28:U:278:ILE:CA | 2.72 | 0.72 |
| 30:W:172:LEU:HD11 | 30:W:190:ILE:HB | 1.70 | 0.72 |
| 17:J:221:LYS:HD3 | 18:K:288:SER:HA | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:386:PHE:HE1 | 19:L:422:VAL:HG12 | 1.54 | 0.72 |
| 21:N:162:ARG:NH1 | 21:N:165:ILE:HD11 | 2.04 | 0.72 |
| 25:R:214:TYR:CD2 | 25:R:230:LEU:HD12 | 2.23 | 0.72 |
| 31:X:9:LYS:HG2 | 31:X:34:GLU:HG2 | 1.69 | 0.72 |
| 31:X:75:TRP:CE3 | 31:X:125:MET:CE | 2.43 | 0.72 |
| 31:X:75:TRP:CH2 | 31:X:125:MET:HE2 | 2.17 | 0.72 |
| 33:Z:912:PHE:HE2 | 33:Z:980:VAL:HG23 | 1.55 | 0.72 |
| 1:1:114:PRO:HG2 | 1:1:118:SER:HB2 | 1.71 | 0.72 |
| 3:3:68:LYS:HG2 | 10:C:92:ARG:NH1 | 2.05 | 0.72 |
| 4:4:38:SER:HB3 | 4:4:39:PRO:HD2 | 1.72 | 0.72 |
| 14:G:98:PHE:CE2 | 14:G:106:ILE:HA | 2.25 | 0.72 |
| 22:O:253:GLN:HB2 | 22:O:269:LEU:CD1 | 2.19 | 0.72 |
| 25:R:266:LEU:HD21 | 25:R:293:THR:CG2 | 2.19 | 0.72 |
| 26:S:315:LYS:HD3 | 26:S:345:TYR:OH | 1.89 | 0.72 |
| 1:1:175:MET:CE | 1:1:188:PHE:HE1 | 2.01 | 0.72 |
| 9:B:66:LEU:HD11 | 9:B:235:PHE:CD2 | 2.24 | 0.72 |
| 16:I:204:HIS:HB3 | 16:I:207:LEU:CD1 | 2.20 | 0.72 |
| 16:I:246:ARG:HD2 | 17:J:278:GLN:NE2 | 2.05 | 0.72 |
| 22:O:250:TRP:CZ2 | 22:O:271:LYS:CG | 2.71 | 0.72 |
| 31:X:104:LYS:HE3 | 31:X:108:ASN:HD21 | 1.54 | 0.72 |
| 33:Z:463:HIS:HA | 33:Z:466:GLU:OE2 | 1.89 | 0.72 |
| 33:Z:612:GLY:HA3 | 33:Z:746:ILE:CG2 | 2.20 | 0.72 |
| 19:L:196:VAL:HG23 | 19:L:197:ILE:HG13 | 1.71 | 0.72 |
| 22:O:359:SER:HB3 | 22:O:363:ILE:HG13 | 1.70 | 0.72 |
| 1:1:19:ARG:CZ | 1:1:171:GLY:N | 2.50 | 0.72 |
| 15:H:221:LEU:HD21 | 15:H:263:VAL:HB | 1.70 | 0.72 |
| 20:M:264:ARG:HA | 20:M:311:GLN:HE22 | 1.53 | 0.72 |
| 25:R:241:ILE:CG2 | 25:R:242:GLU:HG3 | 2.18 | 0.72 |
| 27:T:103:SER:CB | 27:T:141:LEU:HD12 | 2.20 | 0.72 |
| 33:Z:612:GLY:CA | 33:Z:746:ILE:HG23 | 2.20 | 0.72 |
| 4:4:103:ILE:HD12 | 4:4:118:ILE:HD12 | 1.72 | 0.72 |
| 17:J:212:ARG:NH2 | 17:J:248:ASP:OD1 | 2.22 | 0.72 |
| 20:M:50:ARG:O | 20:M:54:GLU:HG3 | 1.89 | 0.72 |
| 21:N:406:TYR:HD1 | 21:N:448:LEU:CB | 2.03 | 0.72 |
| 22:O:99:LEU:HD11 | 22:O:132:GLU:HG3 | 1.71 | 0.72 |
| 33:Z:497:PHE:HB2 | 33:Z:533:VAL:HG22 | 1.72 | 0.72 |
| 2:2:160:GLN:NE2 | 2:2:164:TRP:HE1 | 1.83 | 0.72 |
| 5:5:135:PHE:HB2 | 5:5:167:ARG:HH22 | 1.54 | 0.72 |
| 7:7:119:LEU:HG | 7:7:134:LEU:HD12 | 1.72 | 0.72 |
| 15:H:299:ARG:NH2 | 15:H:344:ASP:HA | 2.05 | 0.72 |
| 23:P:342:GLN:HE21 | 23:P:346:ILE:CD1 | 2.01 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:U:67:PHE:CD2 | 30:W:100:HIS:CE1 | 2.78 | 0.72 |
| 30:W:94:ALA:O | 30:W:98:LEU:HG | 1.89 | 0.72 |
| 10:C:14:SER:HB2 | 10:C:15:PRO:HD2 | 1.72 | 0.72 |
| 13:F:7:ASP:CA | 13:F:21:GLN:NE2 | 2.50 | 0.72 |
| 21:N:75:TYR:OH | 26:S:223:LEU:CD1 | 2.38 | 0.72 |
| 23:P:234:TYR:OH | 23:P:340:ASP:OD2 | 2.06 | 0.72 |
| 33:Z:612:GLY:HA3 | 33:Z:746:ILE:HG21 | 1.72 | 0.72 |
| 33:Z:857:LEU:HD21 | 33:Z:908:ILE:HD11 | 1.72 | 0.72 |
| 1:1:-8:LYS:NZ | 2:2:117:GLY:CA | 2.52 | 0.71 |
| 19:L:392:ARG:HH21 | 20:M:213:ARG:HG3 | 1.55 | 0.71 |
| 27:T:245:TYR:O | 27:T:246:GLU:CB | 2.38 | 0.71 |
| 33:Z:371:SER:O | 33:Z:372:ALA:CB | 2.38 | 0.71 |
| 21:N:642:ASP:HB2 | 21:N:643:PRO:HD3 | 1.73 | 0.71 |
| 21:N:712:ASN:OD1 | 21:N:873:ARG:HG2 | 1.90 | 0.71 |
| 24:Q:273:ASN:ND2 | 24:Q:306:TYR:OH | 2.22 | 0.71 |
| 5:5:34:VAL:CG1 | 5:5:42:LEU:HD22 | 2.20 | 0.71 |
| 13:F:12:THR:CG2 | 13:F:19:LEU:HD11 | 2.19 | 0.71 |
| 18:K:135:MET:CG | 18:K:259:ARG:HH22 | 2.02 | 0.71 |
| 18:K:224:LYS:CE | 18:K:236:ARG:HH22 | 1.99 | 0.71 |
| 19:L:104:LEU:HD23 | 20:M:127:VAL:HG12 | 1.71 | 0.71 |
| 20:M:75:LEU:HA | 20:M:77:TYR:CD1 | 2.21 | 0.71 |
| 21:N:318:LYS:HA | 29:V:180:LEU:CG | 2.20 | 0.71 |
| 23:P:271:SER:O | 23:P:344:ARG:HD2 | 1.91 | 0.71 |
| 25:R:62:TYR:CZ | 25:R:180:PHE:HB3 | 2.25 | 0.71 |
| 28:U:67:PHE:CE2 | 30:W:100:HIS:ND1 | 2.59 | 0.71 |
| 28:U:275:VAL:O | 28:U:278:ILE:CG2 | 2.32 | 0.71 |
| 29:V:57:PHE:CZ | 29:V:135:ARG:CZ | 2.73 | 0.71 |
| 33:Z:557:GLU:OE1 | 33:Z:562:TRP:CE3 | 2.43 | 0.71 |
| 1:1:10:ASP:O | 1:1:102:TYR:CE1 | 2.44 | 0.71 |
| 17:J:212:ARG:NH1 | 17:J:246:PHE:CD2 | 2.58 | 0.71 |
| 27:T:247:ASP:OD1 | 27:T:248:GLU:N | 2.23 | 0.71 |
| 30:W:9:VAL:HG22 | 30:W:52:ILE:CG1 | 2.19 | 0.71 |
| 7:7:145:PRO:HB3 | 7:7:148:ARG:HH21 | 1.55 | 0.71 |
| 16:I:126:PRO:HG2 | 16:I:154:MET:HE2 | 1.72 | 0.71 |
| 33:Z:574:TYR:CE1 | 33:Z:584:VAL:HG21 | 2.24 | 0.71 |
| 33:Z:795:THR:HG22 | 33:Z:799:PHE:CE2 | 2.24 | 0.71 |
| 33:Z:915:ALA:HB1 | 33:Z:983:LEU:HD12 | 1.73 | 0.71 |
| 33:Z:924:LYS:CE | 33:Z:993:GLU:HG3 | 2.20 | 0.71 |
| 16:I:230:THR:HG22 | 16:I:234:LYS:HE3 | 1.73 | 0.71 |
| 19:L:336:ALA:CA | 19:L:342:ARG:NH1 | 2.54 | 0.71 |
| 20:M:160:PRO:HB2 | 20:M:166:ARG:HH22 | 1.56 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:770:LYS:HE3 | 21:N:917:ILE:HD13 | 1.72 | 0.71 |
| 24:Q:309:ARG:HE | 24:Q:345:SER:CB | 2.02 | 0.71 |
| 24:Q:348:CYS:HG | 24:Q:386:PHE:HD1 | 1.39 | 0.71 |
| 25:R:408:ASP:CG | 26:S:464:ARG:HH22 | 1.93 | 0.71 |
| 27:T:119:THR:HG23 | 27:T:123:HIS:HE1 | 1.56 | 0.71 |
| 33:Z:303:ASP:O | 33:Z:307:HIS:CD2 | 2.43 | 0.71 |
| 33:Z:493:LEU:CG | 33:Z:497:PHE:CE2 | 2.74 | 0.71 |
| 1:1:57:ASP:O | 8:A:106:TYR:HE1 | 1.73 | 0.71 |
| 1:1:116:GLY:HA3 | 7:7:-4:ILE:HD11 | 1.73 | 0.71 |
| 1:1:177:VAL:HG12 | 1:1:179:THR:HG23 | 1.71 | 0.71 |
| 2:2:36:ARG:CZ | 2:2:38:SER:HA | 2.20 | 0.71 |
| 6:6:196:LEU:HD22 | 6:6:205:LYS:HG2 | 1.73 | 0.71 |
| 7:7:187:PHE:CE2 | 7:7:204:LEU:HB2 | 2.25 | 0.71 |
| 10:C:33:GLY:HA2 | 10:C:51:LYS:CE | 2.20 | 0.71 |
| 10:C:136:ILE:HD11 | 10:C:165:VAL:HG22 | 1.73 | 0.71 |
| 16:I:205:PRO:HA | 16:I:208:TYR:CE2 | 2.26 | 0.71 |
| 20:M:82:VAL:HG22 | 20:M:119:VAL:HG12 | 1.71 | 0.71 |
| 21:N:529:GLN:HE22 | 21:N:559:TYR:HA | 1.53 | 0.71 |
| 22:O:72:LYS:O | 30:W:18:ASN:CG | 2.28 | 0.71 |
| 26:S:461:PHE:HE2 | 28:U:274:MET:HA | 1.55 | 0.71 |
| 33:Z:139:LEU:HD11 | 33:Z:194:GLU:O | 1.90 | 0.71 |
| 33:Z:612:GLY:CA | 33:Z:746:ILE:CG2 | 2.68 | 0.71 |
| 19:L:114:GLU:HB3 | 19:L:137:ARG:HD3 | 1.70 | 0.71 |
| 24:Q:275:ILE:CD1 | 24:Q:306:TYR:HD2 | 2.03 | 0.71 |
| 4:4:13:ILE:HD11 | 4:4:153:THR:HG23 | 1.71 | 0.71 |
| 21:N:549:TYR:CE2 | 21:N:586:ALA:HB2 | 2.26 | 0.71 |
| 27:T:183:SER:HA | 27:T:186:ARG:NE | 2.06 | 0.71 |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:HE2 | 1.50 | 0.71 |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:CD2 | 2.21 | 0.71 |
| 1:1:124:TYR:OH | 1:1:139:ASP:OD1 | 2.04 | 0.71 |
| 19:L:290:ARG:HH11 | 19:L:293:GLU:C | 1.94 | 0.71 |
| 25:R:31:PHE:CG | 25:R:320:LYS:HG2 | 2.26 | 0.71 |
| 25:R:353:MET:HA | 25:R:357:PHE:CD2 | 2.26 | 0.71 |
| 33:Z:387:ASN:ND2 | 33:Z:400:ILE:HD11 | 2.05 | 0.71 |
| 33:Z:748:LEU:HD21 | 33:Z:783:VAL:CB | 2.21 | 0.71 |
| 4:4:32:ASP:HB3 | 4:4:35:ARG:HH12 | 1.56 | 0.70 |
| 9:B:231:LYS:HD3 | 9:B:234:ARG:HH22 | 1.56 | 0.70 |
| 17:J:219:VAL:HB | 18:K:281:ARG:CD | 2.20 | 0.70 |
| 18:K:242:PHE:N | 18:K:243:VAL:N | 2.39 | 0.70 |
| 20:M:148:VAL:CG2 | 20:M:155:ILE:HG12 | 2.21 | 0.70 |
| 20:M:251:LEU:O | 20:M:252:VAL:CA | 2.36 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:O:377:VAL:HG11 | 28:U:200:LEU:CD1 | 2.20 | 0.70 |
| 24:Q:94:VAL:HG22 | 24:Q:130:ARG:HH11 | 1.56 | 0.70 |
| 26:S:330:LEU:HD13 | 26:S:346:TYR:CD1 | 2.26 | 0.70 |
| 13:F:18:ARG:HH12 | 13:F:23:GLU:HB2 | 1.56 | 0.70 |
| 18:K:135:MET:HG2 | 18:K:259:ARG:NH2 | 2.05 | 0.70 |
| 18:K:242:PHE:C | 18:K:243:VAL:CA | 2.59 | 0.70 |
| 28:U:67:PHE:HZ | 30:W:97:THR:HG23 | 1.54 | 0.70 |
| 30:W:31:ASP:O | 30:W:35:PHE:CD1 | 2.40 | 0.70 |
| 33:Z:549:ASN:ND2 | 33:Z:562:TRP:HH2 | 1.89 | 0.70 |
| 33:Z:929:VAL:O | 33:Z:955:VAL:CG2 | 2.39 | 0.70 |
| 2:2:124:TYR:OH | 2:2:139:GLU:HB2 | 1.91 | 0.70 |
| 11:D:8:LEU:O | 11:D:18:PHE:CZ | 2.43 | 0.70 |
| 12:E:163:THR:HG22 | 13:F:78:ALA:HB3 | 1.71 | 0.70 |
| 25:R:29:LYS:HD2 | 25:R:49:PHE:CD2 | 2.26 | 0.70 |
| 33:Z:748:LEU:HD11 | 33:Z:783:VAL:HA | 1.71 | 0.70 |
| 7:7:93:TYR:HE1 | 7:7:96:ARG:NH2 | 1.82 | 0.70 |
| 18:K:193:VAL:HG12 | 18:K:194:GLN:HG2 | 1.72 | 0.70 |
| 21:N:183:VAL:HG11 | 21:N:221:ASP:OD2 | 1.90 | 0.70 |
| 21:N:315:ASN:CA | 21:N:318:LYS:NZ | 2.53 | 0.70 |
| 31:X:57:VAL:H | 31:X:59:ARG:NH1 | 1.88 | 0.70 |
| 1:1:175:MET:CE | 1:1:188:PHE:CE1 | 2.74 | 0.70 |
| 3:3:44:ILE:HG22 | 3:3:51:VAL:HG22 | 1.74 | 0.70 |
| 3:3:177:VAL:HG12 | 3:3:190:TYR:CD1 | 2.26 | 0.70 |
| 4:4:48:GLU:OE1 | 4:4:51:ASP:OD2 | 2.09 | 0.70 |
| 7:7:70:ASN:HD22 | 13:F:107:ARG:NH2 | 1.89 | 0.70 |
| 17:J:377:VAL:CG1 | 17:J:382:PHE:CE2 | 2.75 | 0.70 |
| 21:N:14:ARG:NH2 | 21:N:42:GLU:OE2 | 2.25 | 0.70 |
| 12:E:219:LEU:HD12 | 12:E:236:THR:HG22 | 1.71 | 0.70 |
| 15:H:396:MET:HE1 | 15:H:438:ALA:HB1 | 1.65 | 0.70 |
| 17:J:199:ALA:HB1 | 17:J:210:PHE:HE1 | 1.57 | 0.70 |
| 33:Z:103:TYR:OH | 33:Z:140:LEU:HD12 | 1.92 | 0.70 |
| 33:Z:205:LEU:CG | 33:Z:236:PHE:CE1 | 2.58 | 0.70 |
| 33:Z:299:ASP:OD1 | 33:Z:341:TYR:OH | 2.10 | 0.70 |
| 1:1:57:ASP:HB3 | 8:A:106:TYR:HE1 | 1.49 | 0.70 |
| 11:D:10:ILE:N | 11:D:18:PHE:HE2 | 1.86 | 0.70 |
| 13:F:64:ILE:HD12 | 13:F:72:LEU:HD11 | 1.73 | 0.70 |
| 16:I:204:HIS:CG | 16:I:207:LEU:HD13 | 2.18 | 0.70 |
| 21:N:94:LYS:HE2 | 21:N:143:LYS:NZ | 2.06 | 0.70 |
| 22:O:15:ARG:O | 30:W:20:ASP:HA | 1.91 | 0.70 |
| 23:P:272:PRO:O | 23:P:273:TYR:CG | 2.45 | 0.70 |
| 26:S:211:ARG:NH2 | 26:S:241:PHE:CE1 | 2.60 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:79:THR:HG23 | 3:3:115:PHE:CZ | 2.27 | 0.70 |
| 7:7:187:PHE:CZ | 7:7:204:LEU:CB | 2.74 | 0.70 |
| 13:F:65:LYS:HB2 | 13:F:222:PHE:HE2 | 1.55 | 0.70 |
| 14:G:200:TYR:HE1 | 14:G:246:ILE:CG2 | 2.05 | 0.70 |
| 16:I:128:TYR:CD2 | 16:I:154:MET:HG3 | 2.27 | 0.70 |
| 19:L:386:PHE:CE1 | 19:L:422:VAL:HG12 | 2.27 | 0.70 |
| 22:O:325:GLU:OE1 | 23:P:364:ARG:NH1 | 2.25 | 0.70 |
| 26:S:211:ARG:O | 26:S:215:MET:HG3 | 1.91 | 0.70 |
| 31:X:79:LYS:CE | 31:X:98:PHE:CD2 | 2.74 | 0.70 |
| 33:Z:56:LEU:HD23 | 33:Z:68:LEU:HD23 | 1.72 | 0.70 |
| 1:1:14:LEU:HD11 | 1:1:100:ALA:CB | 2.21 | 0.70 |
| 4:4:81:SER:CA | 4:4:124:LYS:HZ3 | 2.04 | 0.70 |
| 4:4:174:ASP:OD1 | 4:4:176:LYS:NZ | 2.24 | 0.70 |
| 10:C:224:GLU:HG3 | 10:C:225:VAL:HG23 | 1.74 | 0.70 |
| 19:L:145:ARG:HH21 | 19:L:163:THR:HA | 1.56 | 0.70 |
| 21:N:96:GLN:O | 21:N:100:THR:HG23 | 1.91 | 0.70 |
| 21:N:539:MET:CE | 21:N:551:GLY:HA2 | 2.22 | 0.70 |
| 3:3:18:LEU:HD11 | 3:3:177:VAL:HG13 | 1.72 | 0.70 |
| 4:4:77:GLN:HG2 | 4:4:116:TYR:OH | 1.92 | 0.70 |
| 8:A:162:TYR:CZ | 8:A:164:VAL:HG11 | 2.27 | 0.70 |
| 15:H:101:ARG:NH2 | 15:H:150:LYS:CD | 2.55 | 0.70 |
| 17:J:26:LYS:HE2 | 18:K:51:LEU:CD2 | 2.21 | 0.70 |
| 17:J:378:THR:O | 17:J:382:PHE:CD2 | 2.45 | 0.70 |
| 18:K:224:LYS:CE | 18:K:236:ARG:HH21 | 2.04 | 0.70 |
| 21:N:13:LEU:HD22 | 21:N:49:LEU:HD11 | 1.74 | 0.70 |
| 21:N:98:VAL:O | 21:N:102:VAL:HG23 | 1.92 | 0.70 |
| 21:N:450:ILE:HG21 | 21:N:466:LEU:HD21 | 1.72 | 0.70 |
| 24:Q:82:THR:O | 24:Q:86:MET:HG2 | 1.92 | 0.70 |
| 27:T:7:LEU:HD12 | 27:T:33:GLU:HG3 | 1.71 | 0.70 |
| 27:T:183:SER:HA | 27:T:186:ARG:HE | 1.56 | 0.70 |
| 27:T:221:ALA:HB1 | 27:T:228:ILE:HD11 | 1.74 | 0.70 |
| 1:1:-2:LEU:HB2 | 1:1:33:LYS:HE3 | 1.72 | 0.69 |
| 2:2:50:ALA:HB3 | 3:3:118:ILE:HG21 | 1.71 | 0.69 |
| 26:S:211:ARG:NE | 26:S:240:ASP:OD2 | 2.25 | 0.69 |
| 32:Y:82:ASP:HB3 | 32:Y:86:ARG:NH1 | 2.07 | 0.69 |
| 33:Z:242:PHE:HB2 | 33:Z:275:GLN:HG3 | 1.73 | 0.69 |
| 14:G:108:ILE:HG21 | 14:G:148:TYR:CD1 | 2.27 | 0.69 |
| 23:P:203:ILE:HG12 | 23:P:220:TYR:CZ | 2.26 | 0.69 |
| 25:R:363:PHE:HE1 | 32:Y:78:LYS:CD | 1.92 | 0.69 |
| 33:Z:301:THR:CG2 | 33:Z:307:HIS:CE1 | 2.73 | 0.69 |
| 1:1:8:PHE:HE1 | 1:1:13:ILE:HG13 | 1.55 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:32:ASP:O | 1:1:45:ARG:NH2 | 2.25 | 0.69 |
| 1:1:70:TYR:HD1 | 14:G:110:ALA:CB | 2.05 | 0.69 |
| 6:6:-5:TYR:CD1 | 6:6:97:TYR:CD2 | 2.81 | 0.69 |
| 23:P:154:ASP:CG | 23:P:190:LYS:HZ3 | 1.95 | 0.69 |
| 26:S:211:ARG:HD2 | 26:S:240:ASP:OD2 | 1.91 | 0.69 |
| 30:W:4:GLU:HG2 | 30:W:107:HIS:HB2 | 1.73 | 0.69 |
| 1:1:-2:LEU:HD12 | 1:1:1:THR:N | 2.06 | 0.69 |
| 7:7:7:LYS:HE3 | 7:7:119:LEU:HB3 | 1.74 | 0.69 |
| 15:H:308:PHE:CE1 | 15:H:351:VAL:HG13 | 2.28 | 0.69 |
| 21:N:390:LEU:HD23 | 21:N:404:SER:HB3 | 1.74 | 0.69 |
| 21:N:585:ARG:NH2 | 21:N:623:PHE:CD2 | 2.60 | 0.69 |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:CD1 | 1.96 | 0.69 |
| 27:T:103:SER:HB2 | 27:T:141:LEU:HD12 | 1.72 | 0.69 |
| 33:Z:442:VAL:CG1 | 33:Z:443:ASP:N | 2.20 | 0.69 |
| 33:Z:748:LEU:HD23 | 33:Z:783:VAL:CG1 | 2.13 | 0.69 |
| 5:5:8:PHE:CE1 | 5:5:13:ILE:CG1 | 2.72 | 0.69 |
| 10:C:44:ILE:HD11 | 10:C:146:TYR:HB3 | 1.74 | 0.69 |
| 18:K:139:LEU:HD23 | 18:K:146:LEU:HA | 1.74 | 0.69 |
| 18:K:244:HIS:CG | 19:L:256:ILE:HG23 | 2.28 | 0.69 |
| 21:N:406:TYR:CD1 | 21:N:448:LEU:CB | 2.74 | 0.69 |
| 23:P:72:TRP:CH2 | 23:P:103:TYR:HB2 | 2.26 | 0.69 |
| 25:R:194:VAL:HA | 25:R:197:MET:SD | 2.33 | 0.69 |
| 25:R:239:THR:HG22 | 25:R:246:TYR:CB | 2.23 | 0.69 |
| 1:1:70:TYR:CD1 | 14:G:110:ALA:HB1 | 2.28 | 0.69 |
| 1:1:98:ILE:HD11 | 1:1:127:ALA:CB | 2.22 | 0.69 |
| 15:H:365:LEU:HD22 | 15:H:370:ARG:NH2 | 2.08 | 0.69 |
| 16:I:164:ALA:O | 16:I:165:ASP:HB2 | 1.93 | 0.69 |
| 20:M:236:ALA:CB | 20:M:277:ILE:HD12 | 2.22 | 0.69 |
| 20:M:303:ARG:HH12 | 20:M:307:GLU:HB2 | 1.56 | 0.69 |
| 22:O:79:VAL:HB | 22:O:128:LEU:HD23 | 1.74 | 0.69 |
| 22:O:83:LEU:HD12 | 22:O:128:LEU:HD23 | 1.73 | 0.69 |
| 30:W:21:PHE:CE1 | 30:W:144:PHE:HE2 | 2.11 | 0.69 |
| 7:7:187:PHE:CE2 | 7:7:204:LEU:CB | 2.75 | 0.69 |
| 15:H:244:LYS:HB2 | 15:H:346:ARG:HG2 | 1.73 | 0.69 |
| 23:P:395:ARG:HD2 | 24:Q:357:VAL:HG12 | 1.74 | 0.69 |
| 26:S:343:LEU:O | 26:S:347:HIS:ND1 | 2.20 | 0.69 |
| 28:U:203:LYS:HE2 | 28:U:229:LEU:HD23 | 1.74 | 0.69 |
| 31:X:15:CYS:HB2 | 31:X:100:TRP:HB2 | 1.73 | 0.69 |
| 31:X:75:TRP:CD2 | 31:X:125:MET:HE3 | 2.27 | 0.69 |
| 2:2:50:ALA:HB2 | 3:3:118:ILE:CG2 | 2.09 | 0.69 |
| 8:A:252:ASP:OD1 | 23:P:85:LYS:NZ | 0.54 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:C:107:PRO:HB3 | 10:C:143:ARG:NH2 | 2.08 | 0.69 |
| 15:H:379:LEU:HD22 | 15:H:415:THR:HG22 | 1.74 | 0.69 |
| 16:I:205:PRO:HA | 16:I:208:TYR:CD2 | 2.27 | 0.69 |
| 16:I:222:TYR:CZ | 16:I:349:LEU:CB | 2.72 | 0.69 |
| 16:I:340:ARG:NH1 | 16:I:343:ARG:CG | 2.55 | 0.69 |
| 21:N:145:LEU:CD2 | 21:N:173:LYS:HZ1 | 2.05 | 0.69 |
| 21:N:221:ASP:CB | 21:N:894:ARG:HH22 | 2.06 | 0.69 |
| 21:N:615:ALA:CB | 21:N:651:PHE:HZ | 2.05 | 0.69 |
| 25:R:58:GLU:OE2 | 25:R:109:LYS:HD2 | 1.92 | 0.69 |
| 27:T:161:TRP:HE3 | 27:T:162:ASP:OD1 | 1.76 | 0.69 |
| 27:T:263:ALA:HA | 27:T:266:TYR:CE2 | 2.27 | 0.69 |
| 29:V:261:LEU:HD21 | 29:V:284:ALA:HB2 | 1.74 | 0.69 |
| 30:W:7:VAL:HG23 | 30:W:98:LEU:HD23 | 1.73 | 0.69 |
| 1:1:8:PHE:CE2 | 1:1:10:ASP:HB2 | 2.28 | 0.69 |
| 3:3:28:SER:HB2 | 4:4:127:LEU:HD21 | 1.74 | 0.69 |
| 4:4:38:SER:HB3 | 4:4:73:GLU:OE2 | 1.93 | 0.69 |
| 8:A:54:ILE:HG22 | 8:A:210:MET:HE1 | 1.74 | 0.69 |
| 8:A:56:GLN:HE22 | 8:A:214:LEU:HD13 | 1.54 | 0.69 |
| 14:G:111:PHE:CE2 | 14:G:115:LEU:HD11 | 2.28 | 0.69 |
| 17:J:167:PRO:CB | 17:J:174:PHE:CZ | 2.75 | 0.69 |
| 18:K:123:LEU:HG | 18:K:146:LEU:O | 1.92 | 0.69 |
| 21:N:329:HIS:HB3 | 29:V:182:LYS:CE | 2.10 | 0.69 |
| 33:Z:509:LEU:HD12 | 33:Z:530:LEU:HD23 | 1.73 | 0.69 |
| 16:I:220:ILE:HG13 | 16:I:344:ILE:HG21 | 1.75 | 0.69 |
| 17:J:163:VAL:HG21 | 17:J:314:ILE:HD11 | 1.75 | 0.69 |
| 19:L:361:PHE:CZ | 19:L:391:ILE:CD1 | 2.72 | 0.69 |
| 25:R:209:ARG:CG | 25:R:213:TYR:CE2 | 2.70 | 0.69 |
| 27:T:211:PHE:CZ | 27:T:220:PHE:CZ | 2.81 | 0.69 |
| 29:V:53:MET:HE3 | 29:V:65:VAL:HG11 | 1.75 | 0.69 |
| 33:Z:497:PHE:CE2 | 33:Z:505:VAL:CG1 | 2.76 | 0.69 |
| 5:5:7:ARG:NE | 5:5:110:PRO:HG2 | 2.09 | 0.68 |
| 11:D:19:GLN:HE22 | 11:D:121:THR:HA | 1.56 | 0.68 |
| 18:K:346:ARG:HG2 | 18:K:349:ARG:HH21 | 1.57 | 0.68 |
| 19:L:263:ILE:HG23 | 19:L:267:PHE:CE1 | 2.29 | 0.68 |
| 21:N:179:THR:HG21 | 21:N:219:ASN:ND2 | 2.08 | 0.68 |
| 21:N:221:ASP:HA | 21:N:894:ARG:NH2 | 2.05 | 0.68 |
| 21:N:599:TYR:CD1 | 21:N:634:LEU:HD22 | 2.28 | 0.68 |
| 26:S:294:ILE:HG12 | 26:S:317:HIS:HE1 | 1.56 | 0.68 |
| 33:Z:138:ARG:NE | 33:Z:157:LEU:CG | 2.45 | 0.68 |
| 33:Z:188:ALA:CB | 33:Z:201:LEU:HD11 | 2.23 | 0.68 |
| 8:A:164:VAL:HG12 | 9:B:61:LEU:HD22 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:D:39:LYS:HD2 | 11:D:186:ALA:HB2 | 1.74 | 0.68 |
| 12:E:50:VAL:HG22 | 12:E:67:ILE:HD11 | 1.75 | 0.68 |
| 14:G:108:ILE:HG21 | 14:G:148:TYR:CE1 | 2.27 | 0.68 |
| 15:H:147:ILE:HG13 | 15:H:183:ILE:HG13 | 1.75 | 0.68 |
| 16:I:126:PRO:HB3 | 16:I:128:TYR:CZ | 2.24 | 0.68 |
| 33:Z:924:LYS:HE2 | 33:Z:993:GLU:HG3 | 1.75 | 0.68 |
| 6:6:58:ARG:NH1 | 6:6:91:LYS:HD2 | 2.08 | 0.68 |
| 8:A:205:PHE:HZ | 8:A:209:HIS:HE1 | 1.38 | 0.68 |
| 10:C:18:ARG:HH21 | 11:D:29:ARG:HH22 | 1.40 | 0.68 |
| 16:I:204:HIS:HB3 | 16:I:207:LEU:HD12 | 1.73 | 0.68 |
| 21:N:759:ILE:HG23 | 21:N:871:MET:HE3 | 1.73 | 0.68 |
| 26:S:256:LYS:O | 26:S:259:TYR:HE1 | 1.75 | 0.68 |
| 26:S:397:LEU:CD2 | 26:S:402:ILE:HG21 | 2.22 | 0.68 |
| 33:Z:187:SER:HA | 33:Z:198:GLU:HG2 | 1.75 | 0.68 |
| 1:1:51:ASP:OD1 | 1:1:93:LEU:HD22 | 1.94 | 0.68 |
| 19:L:282:GLU:OE2 | 20:M:306:LEU:HD13 | 1.94 | 0.68 |
| 21:N:293:LEU:HD23 | 21:N:379:LEU:HD13 | 1.75 | 0.68 |
| 26:S:461:PHE:CE1 | 28:U:278:ILE:N | 2.61 | 0.68 |
| 33:Z:165:TYR:HE1 | 33:Z:190:THR:OG1 | 1.73 | 0.68 |
| 33:Z:552:GLU:HB3 | 33:Z:554:THR:HG23 | 1.74 | 0.68 |
| 33:Z:763:HIS:ND1 | 33:Z:766:HIS:HE1 | 1.89 | 0.68 |
| 10:C:198:SER:HA | 10:C:206:LEU:HD22 | 1.75 | 0.68 |
| 13:F:70:MET:SD | 13:F:135:ILE:O | 2.52 | 0.68 |
| 17:J:340:GLY:CA | 25:R:238:PHE:HE1 | 2.06 | 0.68 |
| 19:L:88:TYR:HD1 | 20:M:62:ILE:CD1 | 2.02 | 0.68 |
| 21:N:145:LEU:HB3 | 21:N:173:LYS:HZ1 | 1.59 | 0.68 |
| 22:O:26:PHE:HZ | 22:O:64:ASN:HD22 | 1.41 | 0.68 |
| 22:O:30:GLU:HG2 | 22:O:58:ARG:NH1 | 2.08 | 0.68 |
| 25:R:79:LEU:O | 25:R:93:LYS:HD3 | 1.93 | 0.68 |
| 26:S:343:LEU:HB3 | 26:S:344:PRO:HD3 | 1.76 | 0.68 |
| 29:V:134:SER:O | 29:V:157:ARG:NH2 | 2.27 | 0.68 |
| 16:I:362:LEU:CD2 | 16:I:377:LEU:HD22 | 2.23 | 0.68 |
| 17:J:378:THR:O | 17:J:382:PHE:HD2 | 1.76 | 0.68 |
| 22:O:30:GLU:HB3 | 22:O:58:ARG:HH12 | 1.59 | 0.68 |
| 22:O:310:PHE:CE2 | 22:O:346:GLU:HA | 2.29 | 0.68 |
| 5:5:35:ILE:HD11 | 5:5:45:MET:CE | 2.22 | 0.68 |
| 16:I:103:PRO:HD3 | 17:J:120:TYR:CE1 | 2.29 | 0.68 |
| 26:S:425:ARG:HH11 | 27:T:155:GLY:HA2 | 1.59 | 0.68 |
| 28:U:13:LEU:HD11 | 29:V:36:LYS:HG3 | 1.76 | 0.68 |
| 28:U:70:HIS:NE2 | 28:U:109:LEU:HD22 | 2.09 | 0.68 |
| 33:Z:483:THR:CG2 | 33:Z:521:GLU:HG3 | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:812:ILE:CD1 | 33:Z:834:LEU:HD22 | 2.22 | 0.68 |
| 15:H:50:LYS:HZ2 | 33:Z:791:LYS:HG2 | 1.57 | 0.68 |
| 18:K:224:LYS:HE2 | 18:K:236:ARG:HH21 | 1.56 | 0.68 |
| 19:L:88:TYR:CD1 | 20:M:62:ILE:CB | 2.75 | 0.68 |
| 19:L:336:ALA:C | 19:L:342:ARG:NH1 | 2.45 | 0.68 |
| 20:M:253:GLN:HG3 | 20:M:258:GLU:HB2 | 1.76 | 0.68 |
| 21:N:31:VAL:HG23 | 21:N:35:LEU:HD12 | 1.74 | 0.68 |
| 24:Q:50:ARG:NH2 | 24:Q:53:GLU:CB | 2.56 | 0.68 |
| 24:Q:409:TYR:HA | 25:R:403:LEU:CD2 | 2.07 | 0.68 |
| 25:R:286:LEU:HD12 | 25:R:289:ILE:HD13 | 1.75 | 0.68 |
| 27:T:126:LEU:CD2 | 27:T:136:LEU:HD21 | 2.19 | 0.68 |
| 31:X:62:ASP:OD1 | 31:X:63:PRO:O | 2.11 | 0.68 |
| 33:Z:554:THR:O | 33:Z:558:LEU:HG | 1.93 | 0.68 |
| 1:1:14:LEU:CD2 | 1:1:100:ALA:CB | 2.32 | 0.68 |
| 18:K:342:SER:O | 18:K:343:LEU:HB2 | 1.93 | 0.68 |
| 19:L:125:PRO:HB2 | 19:L:127:TYR:CZ | 2.28 | 0.68 |
| 21:N:221:ASP:CA | 21:N:894:ARG:NH2 | 2.49 | 0.68 |
| 23:P:130:ILE:CG2 | 23:P:136:ARG:HH22 | 2.07 | 0.68 |
| 23:P:323:ASN:OD1 | 23:P:324:GLU:HG2 | 1.93 | 0.68 |
| 24:Q:61:LEU:CD1 | 24:Q:65:TYR:CE1 | 2.77 | 0.68 |
| 24:Q:294:ARG:NH2 | 24:Q:324:GLU:HB2 | 2.08 | 0.68 |
| 27:T:229:VAL:HB | 27:T:234:TYR:HE1 | 1.58 | 0.68 |
| 33:Z:103:TYR:HE1 | 33:Z:116:ALA:HB2 | 1.58 | 0.68 |
| 12:E:109:VAL:HG12 | 12:E:156:PHE:CD1 | 2.29 | 0.68 |
| 17:J:363:THR:HA | 18:K:203:ILE:CD1 | 2.24 | 0.68 |
| 21:N:245:LEU:HD21 | 21:N:254:SER:HA | 1.75 | 0.68 |
| 21:N:749:LEU:CD2 | 21:N:753:PHE:CZ | 2.77 | 0.68 |
| 24:Q:382:LEU:CB | 25:R:263:ARG:NH1 | 2.57 | 0.68 |
| 26:S:181:ALA:HB2 | 26:S:232:MET:SD | 2.34 | 0.68 |
| 33:Z:761:PHE:CD2 | 33:Z:780:MET:HE1 | 2.29 | 0.68 |
| 33:Z:972:SER:O | 33:Z:984:LYS:HE2 | 1.93 | 0.68 |
| 9:B:75:TYR:CG | 9:B:82:TYR:CD1 | 2.82 | 0.67 |
| 17:J:167:PRO:CA | 17:J:174:PHE:CE2 | 2.76 | 0.67 |
| 21:N:67:LYS:HG2 | 21:N:97:PHE:CE1 | 2.29 | 0.67 |
| 24:Q:94:VAL:HG13 | 24:Q:133:LEU:HD11 | 1.74 | 0.67 |
| 24:Q:322:GLU:HG3 | 24:Q:326:MET:HE3 | 1.74 | 0.67 |
| 25:R:193:ALA:O | 25:R:197:MET:HG3 | 1.93 | 0.67 |
| 25:R:211:LYS:NZ | 25:R:234:SER:HA | 2.09 | 0.67 |
| 27:T:109:TYR:CE2 | 27:T:113:LEU:HD11 | 2.28 | 0.67 |
| 29:V:154:ASP:HB3 | 29:V:156:PHE:CZ | 2.28 | 0.67 |
| 33:Z:188:ALA:N | 33:Z:201:LEU:HD11 | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:205:LEU:CD2 | 33:Z:236:PHE:CE1 | 2.76 | 0.67 |
| 8:A:56:GLN:NE2 | 8:A:214:LEU:CD1 | 2.57 | 0.67 |
| 14:G:200:TYR:OH | 14:G:248:GLY:N | 2.28 | 0.67 |
| 15:H:244:LYS:HE2 | 15:H:340:LEU:HD22 | 1.76 | 0.67 |
| 21:N:657:MET:HG2 | 21:N:682:PHE:HE1 | 1.60 | 0.67 |
| 25:R:266:LEU:CA | 25:R:270:VAL:CG2 | 2.68 | 0.67 |
| 29:V:153:ILE:HG23 | 29:V:201:ILE:HD13 | 1.76 | 0.67 |
| 33:Z:368:VAL:HG12 | 33:Z:369:PHE:O | 1.94 | 0.67 |
| 12:E:98:THR:HG22 | 12:E:102:TYR:CE2 | 2.29 | 0.67 |
| 14:G:168:ARG:NE | 14:G:172:LYS:NZ | 2.40 | 0.67 |
| 27:T:253:GLU:O | 27:T:254:ASP:HB2 | 1.94 | 0.67 |
| 29:V:53:MET:HE2 | 29:V:65:VAL:CG2 | 2.23 | 0.67 |
| 30:W:152:GLU:HG2 | 30:W:155:ASP:H | 1.58 | 0.67 |
| 33:Z:490:ILE:HD11 | 33:Z:512:ILE:HD13 | 1.75 | 0.67 |
| 8:A:205:PHE:CE1 | 8:A:209:HIS:NE2 | 2.63 | 0.67 |
| 19:L:247:PRO:HB3 | 20:M:303:ARG:HH21 | 1.59 | 0.67 |
| 20:M:303:ARG:NH1 | 20:M:307:GLU:OE1 | 2.27 | 0.67 |
| 22:O:384:MET:HE2 | 28:U:189:ARG:C | 2.15 | 0.67 |
| 26:S:330:LEU:HB3 | 26:S:346:TYR:CE1 | 2.29 | 0.67 |
| 33:Z:81:SER:O | 33:Z:82:MET:HB2 | 1.95 | 0.67 |
| 1:1:75:THR:HG22 | 1:1:111:TYR:CD1 | 2.29 | 0.67 |
| 8:A:162:TYR:OH | 8:A:164:VAL:HG11 | 1.94 | 0.67 |
| 15:H:306:ILE:HG21 | 15:H:308:PHE:CZ | 2.29 | 0.67 |
| 21:N:282:TYR:CE2 | 21:N:286:LEU:CB | 2.78 | 0.67 |
| 21:N:325:PHE:CE1 | 29:V:167:ASN:OD1 | 2.47 | 0.67 |
| 22:O:41:LEU:HD21 | 22:O:62:TYR:HB2 | 1.75 | 0.67 |
| 22:O:366:MET:HG2 | 28:U:233:PHE:HE2 | 1.59 | 0.67 |
| 25:R:54:ILE:HG21 | 25:R:63:TYR:HB2 | 1.75 | 0.67 |
| 3:3:20:LEU:HD12 | 3:3:31:PHE:CD1 | 2.30 | 0.67 |
| 8:A:167:LYS:HE3 | 9:B:57:MET:HG2 | 1.76 | 0.67 |
| 12:E:109:VAL:CG1 | 12:E:156:PHE:CD1 | 2.78 | 0.67 |
| 20:M:362:GLN:O | 20:M:366:ARG:HG3 | 1.93 | 0.67 |
| 21:N:588:VAL:HG13 | 21:N:621:THR:HG22 | 1.73 | 0.67 |
| 23:P:130:ILE:O | 23:P:130:ILE:HG23 | 1.95 | 0.67 |
| 24:Q:11:ALA:HA | 24:Q:14:LEU:HD12 | 1.75 | 0.67 |
| 25:R:91:TRP:CH2 | 25:R:97:GLU:OE1 | 2.48 | 0.67 |
| 26:S:184:TRP:CZ2 | 26:S:217:PHE:CD2 | 2.82 | 0.67 |
| 26:S:211:ARG:CD | 26:S:240:ASP:OD2 | 2.42 | 0.67 |
| 28:U:20:ASP:OD2 | 28:U:24:ARG:NE | 2.19 | 0.67 |
| 4:4:145:HIS:HD2 | 4:4:146:HIS:CE1 | 2.11 | 0.67 |
| 19:L:157:ARG:NH2 | 20:M:128:PHE:CE2 | 2.63 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:117:TYR:OH | 21:N:202:PHE:N | 2.28 | 0.67 |
| 22:O:228:TYR:CA | 22:O:290:LYS:HZ1 | 2.07 | 0.67 |
| 23:P:306:ASN:OD1 | 23:P:352:VAL:HG21 | 1.94 | 0.67 |
| 24:Q:382:LEU:HB3 | 25:R:263:ARG:HH11 | 1.58 | 0.67 |
| 25:R:410:LEU:HD23 | 28:U:285:ILE:HD13 | 1.75 | 0.67 |
| 33:Z:205:LEU:HG | 33:Z:236:PHE:CZ | 2.28 | 0.67 |
| 33:Z:317:GLN:HG3 | 33:Z:317:GLN:O | 1.94 | 0.67 |
| 6:6:3:ILE:HG23 | 6:6:46:ASN:HD22 | 1.59 | 0.67 |
| 7:7:6:MET:HG2 | 7:7:169:ILE:HD11 | 1.77 | 0.67 |
| 13:F:74:LEU:HD22 | 13:F:81:ALA:CB | 2.24 | 0.67 |
| 21:N:47:GLU:OE2 | 21:N:69:TYR:OH | 2.12 | 0.67 |
| 27:T:47:GLN:O | 27:T:48:ASN:OD1 | 2.12 | 0.67 |
| 31:X:38:ASN:HB3 | 31:X:41:GLU:HA | 1.75 | 0.67 |
| 31:X:38:ASN:OD1 | 31:X:43:LEU:HD12 | 1.95 | 0.67 |
| 33:Z:168:GLN:OE1 | 33:Z:195:PHE:CZ | 2.47 | 0.67 |
| 33:Z:182:SER:O | 33:Z:183:LYS:CB | 2.41 | 0.67 |
| 9:B:211:LEU:HD22 | 9:B:238:LEU:HD12 | 1.76 | 0.67 |
| 16:I:310:LEU:HB2 | 16:I:338:LEU:HD13 | 1.76 | 0.67 |
| 17:J:224:GLY:CA | 17:J:225:GLU:N | 2.57 | 0.67 |
| 17:J:252:SER:HB2 | 17:J:259:GLU:HG2 | 1.77 | 0.67 |
| 19:L:145:ARG:NE | 19:L:162:GLU:HG3 | 2.08 | 0.67 |
| 29:V:145:GLN:HG2 | 29:V:148:LYS:CE | 2.22 | 0.67 |
| 33:Z:964:GLU:HG2 | 33:Z:965:LEU:HG | 1.76 | 0.67 |
| 10:C:171:ALA:HA | 16:I:425:LYS:HD2 | 1.77 | 0.67 |
| 14:G:196:ALA:HA | 14:G:213:LEU:HD11 | 1.77 | 0.67 |
| 15:H:192:ASP:HB2 | 15:H:193:PRO:HD2 | 1.76 | 0.67 |
| 22:O:269:LEU:HD23 | 22:O:269:LEU:O | 1.95 | 0.67 |
| 24:Q:409:TYR:CA | 25:R:403:LEU:HD21 | 2.07 | 0.67 |
| 26:S:399:TYR:HB3 | 26:S:402:ILE:CD1 | 2.25 | 0.67 |
| 33:Z:338:HIS:CD2 | 33:Z:339:PHE:CE2 | 2.83 | 0.67 |
| 33:Z:886:VAL:HA | 33:Z:893:PHE:HE2 | 1.58 | 0.67 |
| 11:D:208:LYS:HE2 | 11:D:226:SER:CB | 2.25 | 0.66 |
| 17:J:340:GLY:HA3 | 25:R:238:PHE:CE1 | 2.29 | 0.66 |
| 22:O:82:LEU:HD21 | 22:O:98:TYR:OH | 1.94 | 0.66 |
| 28:U:283:ARG:HD3 | 29:V:287:THR:HG22 | 1.76 | 0.66 |
| 16:I:230:THR:CG2 | 16:I:234:LYS:HE3 | 2.25 | 0.66 |
| 21:N:222:TYR:H | 21:N:894:ARG:NH2 | 1.89 | 0.66 |
| 10:C:66:LEU:HD11 | 10:C:212:GLU:HG2 | 1.77 | 0.66 |
| 11:D:18:PHE:CD1 | 11:D:19:GLN:N | 2.63 | 0.66 |
| 33:Z:850:LEU:HD21 | 33:Z:854:LEU:HD11 | 1.78 | 0.66 |
| 1:1:141:ASN:HB2 | 1:1:154:PHE:HE1 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:36:ARG:NH2 | 2:2:39:PRO:HD3 | 2.11 | 0.66 |
| 18:K:168:ASP:OD1 | 19:L:315:PHE:HE1 | 1.79 | 0.66 |
| 18:K:258:PHE:HZ | 18:K:299:LEU:HD12 | 1.61 | 0.66 |
| 19:L:290:ARG:HD2 | 19:L:293:GLU:CA | 2.22 | 0.66 |
| 21:N:717:LEU:HD21 | 21:N:733:LEU:CD1 | 2.24 | 0.66 |
| 24:Q:387:TYR:HB3 | 24:Q:400:TYR:HD2 | 1.59 | 0.66 |
| 25:R:137:LEU:HD22 | 25:R:141:TYR:CZ | 2.30 | 0.66 |
| 27:T:249:MET:O | 27:T:250:MET:HB2 | 1.94 | 0.66 |
| 33:Z:53:VAL:HG11 | 33:Z:95:THR:CG2 | 2.24 | 0.66 |
| 33:Z:463:HIS:CE1 | 33:Z:497:PHE:CE1 | 2.83 | 0.66 |
| 33:Z:481:PRO:O | 33:Z:482:ASP:CB | 2.43 | 0.66 |
| 33:Z:509:LEU:CB | 33:Z:530:LEU:HD21 | 2.25 | 0.66 |
| 8:A:128:TYR:CE2 | 8:A:134:MET:HE2 | 2.30 | 0.66 |
| 20:M:203:ARG:NH1 | 20:M:206:LYS:HZ2 | 1.94 | 0.66 |
| 21:N:362:TRP:CZ2 | 29:V:23:THR:CG2 | 2.77 | 0.66 |
| 21:N:654:GLN:NE2 | 21:N:697:PHE:CD2 | 2.64 | 0.66 |
| 23:P:267:PHE:HE1 | 23:P:329:PHE:CD2 | 2.06 | 0.66 |
| 25:R:54:ILE:O | 25:R:54:ILE:HG22 | 1.94 | 0.66 |
| 2:2:65:LEU:HD13 | 9:B:94:HIS:ND1 | 2.10 | 0.66 |
| 3:3:7:THR:HG23 | 3:3:112:ILE:CD1 | 2.26 | 0.66 |
| 6:6:196:LEU:HD23 | 6:6:205:LYS:HG2 | 1.77 | 0.66 |
| 15:H:365:LEU:CD2 | 15:H:370:ARG:NH2 | 2.59 | 0.66 |
| 18:K:212:TYR:CE1 | 18:K:320:ARG:C | 2.69 | 0.66 |
| 20:M:196:ALA:CB | 20:M:345:ARG:HE | 2.05 | 0.66 |
| 20:M:197:ILE:HB | 20:M:322:LYS:CE | 2.24 | 0.66 |
| 23:P:342:GLN:NE2 | 23:P:346:ILE:HD11 | 2.09 | 0.66 |
| 25:R:239:THR:CG2 | 25:R:246:TYR:HB2 | 2.26 | 0.66 |
| 27:T:245:TYR:HD2 | 27:T:246:GLU:H | 1.40 | 0.66 |
| 12:E:165:TYR:CB | 12:E:167:TYR:CZ | 2.78 | 0.66 |
| 17:J:199:ALA:HB1 | 17:J:210:PHE:CE1 | 2.30 | 0.66 |
| 18:K:388:GLN:HB2 | 19:L:340:PRO:HG2 | 1.77 | 0.66 |
| 24:Q:94:VAL:HG22 | 24:Q:130:ARG:NH1 | 2.10 | 0.66 |
| 24:Q:385:ILE:HG22 | 24:Q:386:PHE:CD1 | 2.31 | 0.66 |
| 26:S:365:THR:O | 26:S:368:LYS:HG3 | 1.95 | 0.66 |
| 31:X:79:LYS:CE | 31:X:98:PHE:HE2 | 1.96 | 0.66 |
| 9:B:48:GLU:HG3 | 9:B:200:VAL:HG11 | 1.78 | 0.66 |
| 9:B:57:MET:O | 9:B:61:LEU:HG | 1.96 | 0.66 |
| 11:D:193:LYS:HG3 | 11:D:197:ARG:CZ | 2.26 | 0.66 |
| 18:K:227:ALA:HB2 | 18:K:268:ILE:HD12 | 1.78 | 0.66 |
| 23:P:79:LEU:HD11 | 23:P:100:VAL:HG21 | 1.76 | 0.66 |
| 15:H:168:ILE:CG2 | 15:H:172:MET:HA | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:174:VAL:CG1 | 15:H:183:ILE:CG2 | 2.72 | 0.66 |
| 21:N:599:TYR:CE1 | 21:N:634:LEU:HD13 | 2.28 | 0.66 |
| 25:R:237:THR:HG22 | 25:R:275:GLU:OE1 | 1.96 | 0.66 |
| 33:Z:102:ILE:HG23 | 33:Z:115:LEU:HD13 | 1.77 | 0.66 |
| 4:4:45:PHE:CE2 | 4:4:101:VAL:CG1 | 2.79 | 0.66 |
| 7:7:192:ILE:HG12 | 7:7:198:LEU:CD1 | 2.26 | 0.66 |
| 13:F:117:GLN:HG3 | 13:F:121:GLN:HE21 | 1.61 | 0.66 |
| 15:H:101:ARG:HH21 | 15:H:150:LYS:CE | 2.09 | 0.66 |
| 19:L:145:ARG:NH2 | 19:L:163:THR:C | 2.49 | 0.66 |
| 19:L:263:ILE:HG23 | 19:L:267:PHE:HE1 | 1.59 | 0.66 |
| 24:Q:4:PRO:HB3 | 24:Q:50:ARG:HH11 | 1.61 | 0.66 |
| 24:Q:61:LEU:HD11 | 24:Q:65:TYR:CZ | 2.30 | 0.66 |
| 27:T:119:THR:CG2 | 27:T:123:HIS:CE1 | 2.78 | 0.66 |
| 4:4:34:THR:CG2 | 4:4:181:LYS:NZ | 2.59 | 0.65 |
| 17:J:59:LYS:HE2 | 17:J:63:ARG:NH1 | 2.11 | 0.65 |
| 17:J:305:LEU:HB3 | 17:J:313:LYS:CE | 2.26 | 0.65 |
| 22:O:48:PHE:CE1 | 22:O:80:LYS:NZ | 2.60 | 0.65 |
| 27:T:211:PHE:HZ | 27:T:220:PHE:CZ | 2.13 | 0.65 |
| 28:U:67:PHE:HD2 | 30:W:100:HIS:CE1 | 2.13 | 0.65 |
| 33:Z:250:VAL:HG21 | 33:Z:272:TYR:HH | 1.59 | 0.65 |
| 33:Z:313:ILE:HG21 | 33:Z:977:ILE:HD11 | 1.78 | 0.65 |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:HG | 1.77 | 0.65 |
| 15:H:223:GLU:HB3 | 20:M:400:MET:CE | 2.26 | 0.65 |
| 17:J:167:PRO:CA | 17:J:174:PHE:CE1 | 2.77 | 0.65 |
| 23:P:332:GLU:HB2 | 23:P:337:HIS:HE1 | 1.58 | 0.65 |
| 29:V:53:MET:HG3 | 29:V:108:TYR:HD1 | 1.61 | 0.65 |
| 31:X:38:ASN:ND2 | 31:X:42:GLU:H | 1.93 | 0.65 |
| 33:Z:761:PHE:CD2 | 33:Z:780:MET:HE2 | 2.32 | 0.65 |
| 33:Z:776:VAL:HG13 | 33:Z:777:PRO:CD | 2.25 | 0.65 |
| 33:Z:813:PHE:CD1 | 33:Z:847:ILE:HG23 | 2.32 | 0.65 |
| 1:1:30:VAL:HG23 | 1:1:172:VAL:HG22 | 1.76 | 0.65 |
| 11:D:11:PHE:HA | 11:D:17:ILE:CD1 | 2.26 | 0.65 |
| 20:M:72:ASN:HB3 | 20:M:156:LEU:CD2 | 2.26 | 0.65 |
| 22:O:250:TRP:HZ2 | 22:O:271:LYS:HG3 | 1.60 | 0.65 |
| 25:R:137:LEU:HD22 | 25:R:141:TYR:OH | 1.96 | 0.65 |
| 25:R:338:TYR:CZ | 25:R:368:LEU:HD13 | 2.31 | 0.65 |
| 26:S:188:TYR:CE2 | 26:S:239:ARG:NH1 | 2.64 | 0.65 |
| 33:Z:306:MET:CE | 33:Z:310:LEU:HD21 | 2.25 | 0.65 |
| 33:Z:553:ARG:HH12 | 33:Z:595:MET:CE | 2.10 | 0.65 |
| 1:1:57:ASP:C | 8:A:106:TYR:CE1 | 2.68 | 0.65 |
| 1:1:61:TYR:CE1 | 8:A:103:GLU:HA | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:5:100:MET:SD | 5:5:127:PHE:CB | 2.84 | 0.65 |
| 15:H:379:LEU:HD13 | 15:H:413:ASN:OD1 | 1.95 | 0.65 |
| 18:K:159:SER:CB | 18:K:244:HIS:NE2 | 2.54 | 0.65 |
| 21:N:315:ASN:CB | 21:N:318:LYS:NZ | 2.59 | 0.65 |
| 24:Q:311:LEU:HD22 | 24:Q:343:LEU:HD12 | 1.75 | 0.65 |
| 25:R:316:LEU:HD22 | 25:R:322:LEU:HB3 | 1.78 | 0.65 |
| 29:V:78:VAL:O | 29:V:121:VAL:HG22 | 1.97 | 0.65 |
| 33:Z:278:LEU:HD13 | 33:Z:297:VAL:CG1 | 2.27 | 0.65 |
| 33:Z:574:TYR:HE2 | 33:Z:584:VAL:HG11 | 0.90 | 0.65 |
| 2:2:124:TYR:CZ | 2:2:139:GLU:HB3 | 2.31 | 0.65 |
| 15:H:97:LEU:CB | 15:H:173:ARG:HG3 | 2.27 | 0.65 |
| 15:H:147:ILE:CB | 15:H:183:ILE:HD11 | 2.27 | 0.65 |
| 18:K:253:MET:O | 18:K:257:VAL:HG23 | 1.96 | 0.65 |
| 21:N:536:ILE:CD1 | 21:N:555:ILE:CG1 | 2.73 | 0.65 |
| 24:Q:61:LEU:HG | 24:Q:65:TYR:CE2 | 2.30 | 0.65 |
| 25:R:70:TYR:CZ | 25:R:76:GLN:HA | 2.32 | 0.65 |
| 28:U:92:TRP:CZ2 | 28:U:120:LEU:HG | 2.32 | 0.65 |
| 31:X:75:TRP:CE2 | 31:X:125:MET:HB2 | 2.24 | 0.65 |
| 33:Z:401:VAL:HG22 | 33:Z:439:TYR:CE2 | 2.31 | 0.65 |
| 2:2:210:THR:HG23 | 3:3:160:GLN:HE21 | 1.61 | 0.65 |
| 21:N:330:THR:CG2 | 21:N:739:PHE:HE1 | 2.01 | 0.65 |
| 22:O:373:TRP:CH2 | 28:U:200:LEU:CD2 | 2.79 | 0.65 |
| 31:X:48:PHE:CZ | 31:X:68:LEU:HD22 | 2.30 | 0.65 |
| 33:Z:884:THR:O | 33:Z:888:LEU:HD11 | 1.96 | 0.65 |
| 3:3:52:THR:HG1 | 4:4:84:ARG:NH2 | 1.94 | 0.65 |
| 19:L:114:GLU:O | 19:L:137:ARG:NE | 2.30 | 0.65 |
| 21:N:909:GLU:HB3 | 21:N:911:LYS:HZ3 | 1.61 | 0.65 |
| 22:O:40:GLN:HB2 | 22:O:58:ARG:NE | 2.11 | 0.65 |
| 23:P:353:ILE:HG23 | 23:P:357:TYR:HD2 | 1.62 | 0.65 |
| 26:S:399:TYR:HB3 | 26:S:402:ILE:HD11 | 1.79 | 0.65 |
| 30:W:19:GLY:O | 30:W:20:ASP:OD1 | 2.15 | 0.65 |
| 5:5:40:PHE:CB | 5:5:73:ARG:NH2 | 2.60 | 0.65 |
| 7:7:152:ASP:OD1 | 7:7:156:ASP:OD2 | 2.15 | 0.65 |
| 9:B:189:ILE:HD11 | 9:B:213:ILE:HG21 | 1.79 | 0.65 |
| 11:D:70:HIS:CE1 | 11:D:97:ARG:HH22 | 2.14 | 0.65 |
| 11:D:92:GLU:OE2 | 11:D:108:TYR:CE2 | 2.45 | 0.65 |
| 12:E:14:THR:CG2 | 12:E:22:PHE:HE2 | 2.10 | 0.65 |
| 12:E:17:PRO:HA | 13:F:24:TYR:CZ | 2.31 | 0.65 |
| 13:F:179:PHE:CZ | 13:F:192:ALA:HB2 | 2.32 | 0.65 |
| 16:I:204:HIS:CB | 16:I:207:LEU:CD1 | 2.68 | 0.65 |
| 18:K:224:LYS:HZ3 | 18:K:236:ARG:HH22 | 1.42 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:88:TYR:CD1 | 20:M:62:ILE:CD1 | 2.78 | 0.65 |
| 21:N:615:ALA:HB3 | 21:N:651:PHE:CZ | 2.29 | 0.65 |
| 24:Q:382:LEU:HD13 | 25:R:263:ARG:NH1 | 2.11 | 0.65 |
| 25:R:410:LEU:CD2 | 28:U:285:ILE:HD13 | 2.26 | 0.65 |
| 26:S:192:GLU:CG | 26:S:239:ARG:HH12 | 2.02 | 0.65 |
| 33:Z:608:TYR:CG | 33:Z:616:LEU:HD11 | 2.32 | 0.65 |
| 10:C:46:LEU:HD21 | 10:C:138:ALA:HB2 | 1.78 | 0.65 |
| 13:F:49:LEU:HD22 | 13:F:201:LEU:HD21 | 1.79 | 0.65 |
| 15:H:53:GLU:HB2 | 33:Z:765:MET:SD | 2.36 | 0.65 |
| 15:H:285:GLY:C | 15:H:287:GLY:N | 2.50 | 0.65 |
| 17:J:249:GLU:HG2 | 17:J:249:GLU:O | 1.97 | 0.65 |
| 19:L:365:THR:HG1 | 19:L:376:PHE:HE1 | 0.67 | 0.65 |
| 21:N:268:GLN:NE2 | 21:N:457:SER:HA | 2.12 | 0.65 |
| 21:N:666:GLN:HG2 | 21:N:875:LEU:HD23 | 1.79 | 0.65 |
| 24:Q:78:ILE:HB | 24:Q:79:PRO:HD3 | 1.78 | 0.65 |
| 25:R:378:ASN:HD22 | 25:R:393:PRO:HA | 1.60 | 0.65 |
| 28:U:65:VAL:HG12 | 30:W:96:LEU:CD1 | 2.26 | 0.65 |
| 33:Z:53:VAL:CG2 | 33:Z:91:PHE:CE2 | 2.78 | 0.65 |
| 33:Z:506:LEU:HB2 | 33:Z:534:PHE:HZ | 1.62 | 0.65 |
| 3:3:37:TYR:HE1 | 3:3:59:ARG:HG3 | 1.58 | 0.65 |
| 8:A:54:ILE:HG22 | 8:A:210:MET:CE | 2.27 | 0.65 |
| 9:B:49:LYS:HE2 | 9:B:210:GLU:HB2 | 1.77 | 0.65 |
| 15:H:172:MET:HB2 | 16:I:129:TYR:CZ | 2.27 | 0.65 |
| 15:H:299:ARG:HH21 | 15:H:344:ASP:HA | 1.61 | 0.65 |
| 17:J:27:ILE:HG21 | 18:K:50:LYS:CE | 2.27 | 0.65 |
| 18:K:212:TYR:HE1 | 18:K:320:ARG:C | 2.00 | 0.65 |
| 28:U:24:ARG:HD3 | 29:V:100:ARG:HG2 | 1.79 | 0.65 |
| 33:Z:160:GLU:O | 33:Z:164:VAL:HG23 | 1.97 | 0.65 |
| 33:Z:415:MET:HB3 | 33:Z:446:GLU:HB3 | 1.78 | 0.65 |
| 9:B:184:GLU:HG2 | 9:B:186:GLU:H | 1.62 | 0.64 |
| 16:I:204:HIS:HD2 | 16:I:207:LEU:HD13 | 1.10 | 0.64 |
| 17:J:39:GLU:OE2 | 17:J:42:ARG:NH2 | 2.29 | 0.64 |
| 18:K:386:ILE:HD13 | 18:K:411:TYR:HD1 | 1.62 | 0.64 |
| 21:N:282:TYR:HE2 | 21:N:286:LEU:HB3 | 1.60 | 0.64 |
| 22:O:228:TYR:CA | 22:O:290:LYS:NZ | 2.57 | 0.64 |
| 24:Q:311:LEU:HD11 | 24:Q:339:TYR:CE1 | 2.32 | 0.64 |
| 1:1:19:ARG:HH22 | 1:1:171:GLY:H | 1.39 | 0.64 |
| 2:2:8:PHE:HE2 | 2:2:10:ASN:HB3 | 1.62 | 0.64 |
| 21:N:162:ARG:CZ | 21:N:165:ILE:HD11 | 2.28 | 0.64 |
| 26:S:461:PHE:CD2 | 28:U:277:TYR:CB | 2.77 | 0.64 |
| 33:Z:813:PHE:CD2 | 33:Z:888:LEU:HD22 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:6:116:PHE:CE2 | 6:6:122:TYR:HB3 | 2.32 | 0.64 |
| 20:M:170:MET:SD | 20:M:244:LEU:HB3 | 2.37 | 0.64 |
| 21:N:596:LEU:HD22 | 21:N:717:LEU:HD13 | 1.73 | 0.64 |
| 33:Z:383:SER:HB3 | 33:Z:849:ARG:HH12 | 1.62 | 0.64 |
| 33:Z:744:ALA:HA | 33:Z:783:VAL:CG2 | 2.27 | 0.64 |
| 5:5:8:PHE:CZ | 5:5:13:ILE:HG12 | 2.33 | 0.64 |
| 8:A:92:ASN:HB2 | 14:G:120:GLN:OE1 | 1.98 | 0.64 |
| 8:A:252:ASP:CB | 23:P:85:LYS:HE3 | 2.25 | 0.64 |
| 10:C:15:PRO:HA | 11:D:22:TYR:CE1 | 2.33 | 0.64 |
| 16:I:210:GLU:OE2 | 33:Z:822:THR:HB | 1.97 | 0.64 |
| 17:J:27:ILE:HG21 | 18:K:50:LYS:HD3 | 1.79 | 0.64 |
| 21:N:324:LYS:HG3 | 21:N:325:PHE:HD2 | 1.62 | 0.64 |
| 24:Q:226:HIS:HA | 24:Q:229:ASP:OD1 | 1.98 | 0.64 |
| 24:Q:429:LYS:HB2 | 29:V:269:ARG:CZ | 2.25 | 0.64 |
| 27:T:139:ASP:HB3 | 27:T:142:LEU:HD12 | 1.80 | 0.64 |
| 33:Z:408:TYR:CZ | 33:Z:411:LYS:NZ | 2.63 | 0.64 |
| 1:1:103:ASP:HB2 | 1:1:106:ASN:OD1 | 1.98 | 0.64 |
| 7:7:7:LYS:HG2 | 7:7:12:VAL:HG12 | 1.80 | 0.64 |
| 15:H:172:MET:HG3 | 16:I:129:TYR:CD2 | 2.30 | 0.64 |
| 16:I:174:ASP:CG | 16:I:177:PRO:HB3 | 2.18 | 0.64 |
| 19:L:164:ASP:OD1 | 20:M:118:VAL:HG11 | 1.96 | 0.64 |
| 22:O:250:TRP:CD1 | 22:O:269:LEU:O | 2.49 | 0.64 |
| 23:P:167:THR:CB | 23:P:168:TYR:CE1 | 2.81 | 0.64 |
| 26:S:159:ASN:HB3 | 26:S:187:ILE:HD11 | 1.80 | 0.64 |
| 29:V:159:ILE:O | 29:V:160:ASP:OD1 | 2.16 | 0.64 |
| 33:Z:439:TYR:O | 33:Z:443:ASP:OD2 | 2.14 | 0.64 |
| 9:B:139:HIS:CD2 | 9:B:234:ARG:CD | 2.80 | 0.64 |
| 10:C:98:TYR:CE1 | 10:C:104:GLU:HG3 | 2.33 | 0.64 |
| 15:H:249:TYR:CZ | 15:H:376:GLU:CA | 2.81 | 0.64 |
| 21:N:36:TRP:CZ3 | 26:S:252:ASP:HB3 | 2.33 | 0.64 |
| 23:P:101:MET:HE2 | 23:P:139:VAL:HG13 | 1.78 | 0.64 |
| 28:U:67:PHE:CZ | 30:W:97:THR:CA | 2.79 | 0.64 |
| 29:V:153:ILE:HG21 | 29:V:203:TYR:OH | 1.96 | 0.64 |
| 33:Z:463:HIS:CE1 | 33:Z:497:PHE:HE1 | 2.16 | 0.64 |
| 1:1:137:TYR:CE1 | 1:1:157:HIS:CD2 | 2.85 | 0.64 |
| 2:2:99:ILE:CG1 | 2:2:127:LEU:HD12 | 2.28 | 0.64 |
| 20:M:289:LYS:HD3 | 20:M:305:MET:CE | 2.27 | 0.64 |
| 24:Q:225:LEU:O | 24:Q:229:ASP:OD1 | 2.16 | 0.64 |
| 26:S:159:ASN:CB | 26:S:187:ILE:HD11 | 2.27 | 0.64 |
| 28:U:16:LEU:HD23 | 28:U:19:LEU:CD1 | 2.23 | 0.64 |
| 30:W:20:ASP:CG | 30:W:25:ARG:HH21 | 2.01 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:884:THR:OG1 | 33:Z:904:LEU:HD21 | 1.98 | 0.64 |
| 1:1:175:MET:HE1 | 1:1:188:PHE:CE1 | 2.33 | 0.64 |
| 10:C:160:TRP:CD2 | 10:C:163:ILE:HD13 | 2.33 | 0.64 |
| 11:D:48:ARG:HH12 | 11:D:57:THR:HB | 1.62 | 0.64 |
| 11:D:193:LYS:CE | 11:D:197:ARG:NH2 | 2.61 | 0.64 |
| 16:I:246:ARG:HD2 | 17:J:278:GLN:HE21 | 1.63 | 0.64 |
| 33:Z:106:TRP:CA | 33:Z:112:LYS:HD3 | 2.23 | 0.64 |
| 33:Z:436:LEU:HD23 | 33:Z:455:ILE:HG12 | 1.80 | 0.64 |
| 33:Z:744:ALA:HA | 33:Z:783:VAL:HG22 | 1.80 | 0.64 |
| 33:Z:957:LEU:HD13 | 33:Z:958:ASN:O | 1.98 | 0.64 |
| 13:F:65:LYS:HB2 | 13:F:222:PHE:CE2 | 2.32 | 0.64 |
| 18:K:241:GLU:OE2 | 19:L:307:GLU:OE1 | 2.16 | 0.64 |
| 20:M:222:GLY:O | 20:M:228:LYS:NZ | 2.24 | 0.64 |
| 22:O:233:LEU:HD13 | 22:O:251:LEU:HD22 | 1.79 | 0.64 |
| 33:Z:106:TRP:HB2 | 33:Z:112:LYS:HZ3 | 1.59 | 0.64 |
| 33:Z:119:LEU:HB3 | 33:Z:137:TYR:CE2 | 2.33 | 0.64 |
| 8:A:128:TYR:CE1 | 8:A:131:ARG:NH1 | 2.66 | 0.64 |
| 17:J:167:PRO:HB3 | 17:J:174:PHE:HE2 | 1.55 | 0.64 |
| 20:M:411:LYS:HE3 | 20:M:413:GLU:HB2 | 1.79 | 0.64 |
| 21:N:492:THR:HA | 21:N:528:ARG:HH11 | 1.63 | 0.64 |
| 23:P:164:GLN:HE22 | 23:P:180:ILE:HA | 1.63 | 0.64 |
| 3:3:109:LYS:HE3 | 3:3:125:LYS:NZ | 2.13 | 0.63 |
| 3:3:140:MET:HE1 | 3:3:144:LEU:HD11 | 1.79 | 0.63 |
| 15:H:367:ARG:HH12 | 20:M:223:PRO:HB3 | 1.62 | 0.63 |
| 20:M:116:ALA:HB1 | 20:M:128:PHE:HE1 | 1.61 | 0.63 |
| 21:N:315:ASN:OD1 | 21:N:318:LYS:NZ | 2.29 | 0.63 |
| 21:N:749:LEU:HG | 21:N:753:PHE:CE1 | 2.33 | 0.63 |
| 27:T:40:LEU:O | 27:T:88:TYR:OH | 2.15 | 0.63 |
| 30:W:172:LEU:HD22 | 30:W:188:SER:HB3 | 1.79 | 0.63 |
| 33:Z:929:VAL:HG22 | 33:Z:957:LEU:HD23 | 1.80 | 0.63 |
| 33:Z:985:LYS:HD2 | 33:Z:991:GLU:H | 1.62 | 0.63 |
| 19:L:95:ILE:HG23 | 20:M:68:LYS:HZ3 | 1.63 | 0.63 |
| 21:N:387:ALA:HA | 21:N:390:LEU:HD12 | 1.79 | 0.63 |
| 21:N:770:LYS:CE | 21:N:917:ILE:HD13 | 2.28 | 0.63 |
| 30:W:44:ASN:HB2 | 30:W:47:ASN:ND2 | 2.09 | 0.63 |
| 33:Z:158:ALA:HB2 | 33:Z:207:ILE:CD1 | 2.28 | 0.63 |
| 33:Z:887:GLY:N | 33:Z:893:PHE:CD2 | 2.67 | 0.63 |
| 1:1:-2:LEU:HD21 | 1:1:46:SER:HA | 1.80 | 0.63 |
| 3:3:54:LEU:HD11 | 3:3:96:VAL:HG11 | 1.79 | 0.63 |
| 18:K:67:TYR:OH | 21:N:609:LEU:CD2 | 2.46 | 0.63 |
| 21:N:117:TYR:OH | 21:N:202:PHE:CA | 2.46 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:383:LYS:HD2 | 21:N:390:LEU:HD13 | 1.81 | 0.63 |
| 22:O:250:TRP:CZ2 | 22:O:271:LYS:HB2 | 2.33 | 0.63 |
| 25:R:209:ARG:CZ | 25:R:243:LEU:CD1 | 2.76 | 0.63 |
| 26:S:311:GLN:HE22 | 26:S:338:MET:H | 1.46 | 0.63 |
| 30:W:6:THR:HG21 | 30:W:40:LYS:NZ | 2.12 | 0.63 |
| 33:Z:130:GLY:O | 33:Z:131:LYS:HG3 | 1.99 | 0.63 |
| 33:Z:327:GLN:HE22 | 33:Z:346:LEU:CD1 | 2.11 | 0.63 |
| 8:A:128:TYR:CE2 | 8:A:134:MET:CE | 2.82 | 0.63 |
| 9:B:239:THR:HG22 | 9:B:241:GLN:N | 2.13 | 0.63 |
| 17:J:221:LYS:HD3 | 18:K:288:SER:CA | 2.28 | 0.63 |
| 21:N:355:TRP:CH2 | 21:N:356:LEU:HD21 | 2.34 | 0.63 |
| 21:N:508:THR:HG22 | 21:N:510:HIS:H | 1.64 | 0.63 |
| 23:P:308:LEU:HD11 | 23:P:349:ASN:HB2 | 0.67 | 0.63 |
| 25:R:354:ALA:HB2 | 25:R:364:LEU:HD23 | 1.80 | 0.63 |
| 33:Z:846:PHE:HE2 | 33:Z:889:VAL:HG11 | 1.63 | 0.63 |
| 5:5:38:ASN:ND2 | 5:5:41:LEU:HD12 | 2.11 | 0.63 |
| 21:N:615:ALA:HB1 | 21:N:651:PHE:CZ | 2.33 | 0.63 |
| 25:R:266:LEU:HG | 25:R:270:VAL:HG23 | 1.80 | 0.63 |
| 6:6:68:PHE:CZ | 13:F:66:CYS:C | 2.72 | 0.63 |
| 7:7:42:VAL:CG2 | 7:7:192:ILE:HD11 | 2.28 | 0.63 |
| 8:A:18:ILE:HB | 9:B:20:GLN:HE22 | 1.64 | 0.63 |
| 10:C:198:SER:CA | 10:C:206:LEU:HD22 | 2.28 | 0.63 |
| 13:F:101:ARG:NH1 | 13:F:103:LEU:CA | 2.48 | 0.63 |
| 13:F:201:LEU:O | 13:F:202:ARG:CG | 2.46 | 0.63 |
| 17:J:76:ILE:HD11 | 17:J:87:LYS:HB2 | 1.79 | 0.63 |
| 21:N:386:MET:HB2 | 21:N:390:LEU:HD11 | 1.81 | 0.63 |
| 21:N:390:LEU:CD2 | 21:N:404:SER:HB3 | 2.28 | 0.63 |
| 21:N:759:ILE:HG23 | 21:N:871:MET:CE | 2.29 | 0.63 |
| 22:O:383:LYS:HD2 | 27:T:257:THR:HG21 | 1.80 | 0.63 |
| 26:S:378:GLN:HB3 | 26:S:382:ARG:HH12 | 1.61 | 0.63 |
| 28:U:277:TYR:OH | 29:V:295:VAL:HG13 | 1.93 | 0.63 |
| 1:1:112:THR:CG2 | 7:7:27:ARG:HH21 | 2.11 | 0.63 |
| 10:C:34:THR:HG22 | 10:C:167:ALA:O | 1.99 | 0.63 |
| 16:I:104:LEU:CG | 16:I:149:LEU:O | 2.47 | 0.63 |
| 16:I:380:LEU:HB3 | 16:I:420:LYS:HE3 | 1.81 | 0.63 |
| 17:J:87:LYS:HG3 | 17:J:93:LYS:HG2 | 1.81 | 0.63 |
| 17:J:250:ILE:HG13 | 17:J:293:ALA:O | 1.99 | 0.63 |
| 20:M:264:ARG:HG2 | 20:M:311:GLN:NE2 | 2.13 | 0.63 |
| 21:N:327:LEU:HD23 | 21:N:743:PHE:CD1 | 2.33 | 0.63 |
| 23:P:119:ILE:CG2 | 23:P:143:LEU:HD22 | 2.28 | 0.63 |
| 23:P:287:ASP:CB | 23:P:297:GLU:OE1 | 2.47 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:P:391:ALA:O | 24:Q:354:PHE:CE1 | 2.51 | 0.63 |
| 25:R:105:LYS:CE | 25:R:109:LYS:HZ1 | 2.10 | 0.63 |
| 33:Z:71:LEU:HD23 | 33:Z:118:VAL:CG1 | 2.29 | 0.63 |
| 33:Z:442:VAL:HG12 | 33:Z:443:ASP:H | 0.56 | 0.63 |
| 2:2:213:LEU:HD13 | 3:3:192:LYS:HD2 | 1.79 | 0.63 |
| 10:C:36:ILE:HG21 | 10:C:197:LEU:HD21 | 1.81 | 0.63 |
| 13:F:206:LEU:CD2 | 13:F:211:LEU:HD11 | 2.27 | 0.63 |
| 21:N:500:ASP:O | 21:N:504:TYR:CD2 | 2.52 | 0.63 |
| 21:N:536:ILE:HG21 | 21:N:555:ILE:HD11 | 1.80 | 0.63 |
| 25:R:338:TYR:CZ | 25:R:368:LEU:CD1 | 2.82 | 0.63 |
| 27:T:157:TYR:HH | 27:T:188:GLU:HG2 | 1.60 | 0.63 |
| 33:Z:501:LYS:HG3 | 33:Z:534:PHE:CE2 | 2.34 | 0.63 |
| 5:5:207:PHE:O | 5:5:208:ASN:OD1 | 2.16 | 0.63 |
| 6:6:7:ALA:HB2 | 6:6:113:VAL:HG23 | 1.80 | 0.63 |
| 8:A:135:ARG:NH2 | 14:G:14:PHE:CD2 | 2.67 | 0.63 |
| 13:F:207:THR:OG1 | 13:F:210:ASN:ND2 | 2.31 | 0.63 |
| 16:I:104:LEU:HG | 16:I:149:LEU:O | 1.99 | 0.63 |
| 19:L:289:ARG:HH11 | 19:L:334:ASP:HA | 1.64 | 0.63 |
| 21:N:771:PHE:CE2 | 21:N:773:MET:HG2 | 2.34 | 0.63 |
| 24:Q:61:LEU:CD1 | 24:Q:65:TYR:CZ | 2.82 | 0.63 |
| 30:W:174:VAL:HG13 | 30:W:184:ASN:HB3 | 1.81 | 0.63 |
| 3:3:26:GLY:HA3 | 3:3:174:TRP:NE1 | 2.14 | 0.62 |
| 3:3:140:MET:CE | 3:3:144:LEU:HD11 | 2.28 | 0.62 |
| 14:G:108:ILE:N | 14:G:109:PRO:HD2 | 2.14 | 0.62 |
| 15:H:299:ARG:CZ | 15:H:345:PRO:HD3 | 2.29 | 0.62 |
| 18:K:72:GLN:O | 18:K:76:LYS:HG3 | 1.98 | 0.62 |
| 19:L:85:GLU:HA | 20:M:58:MET:HE2 | 1.81 | 0.62 |
| 23:P:67:ALA:HA | 23:P:75:LEU:HD22 | 1.81 | 0.62 |
| 25:R:266:LEU:HG | 25:R:270:VAL:CG2 | 2.29 | 0.62 |
| 29:V:92:MET:HA | 29:V:95:LEU:HD12 | 1.81 | 0.62 |
| 11:D:120:TYR:HE2 | 11:D:129:PHE:CZ | 2.16 | 0.62 |
| 13:F:50:LYS:HE3 | 13:F:212:SER:CB | 2.28 | 0.62 |
| 13:F:159:THR:CA | 13:F:169:LYS:NZ | 2.49 | 0.62 |
| 16:I:362:LEU:HD23 | 16:I:377:LEU:HD22 | 1.79 | 0.62 |
| 18:K:242:PHE:C | 18:K:244:HIS:H | 2.02 | 0.62 |
| 20:M:173:ASP:OD2 | 20:M:233:ARG:NH2 | 2.31 | 0.62 |
| 21:N:162:ARG:NE | 21:N:165:ILE:HG12 | 2.14 | 0.62 |
| 23:P:412:LEU:HD22 | 28:U:272:GLU:OE1 | 1.98 | 0.62 |
| 24:Q:311:LEU:CD2 | 24:Q:343:LEU:CD1 | 2.71 | 0.62 |
| 27:T:108:LEU:HD23 | 27:T:174:PHE:CE1 | 2.34 | 0.62 |
| 27:T:226:TRP:CZ3 | 27:T:235:PHE:CE2 | 2.87 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:X:38:ASN:HD21 | 31:X:43:LEU:HG | 1.64 | 0.62 |
| 33:Z:75:ILE:CG2 | 33:Z:75:ILE:O | 2.44 | 0.62 |
| 33:Z:89:LEU:HD22 | 33:Z:125:THR:OG1 | 1.99 | 0.62 |
| 1:1:94:THR:HG22 | 1:1:115:LEU:HD22 | 1.81 | 0.62 |
| 3:3:41:PHE:CD1 | 3:3:181:ILE:HD13 | 2.35 | 0.62 |
| 9:B:75:TYR:CD1 | 9:B:82:TYR:CE1 | 2.86 | 0.62 |
| 11:D:18:PHE:CE1 | 11:D:19:GLN:HB3 | 2.35 | 0.62 |
| 11:D:74:SER:OG | 11:D:134:LEU:HB2 | 1.98 | 0.62 |
| 11:D:217:PRO:O | 11:D:218:ASP:HB2 | 1.98 | 0.62 |
| 12:E:165:TYR:HB2 | 12:E:167:TYR:CZ | 2.34 | 0.62 |
| 13:F:84:LEU:HD11 | 13:F:112:LEU:HD22 | 1.80 | 0.62 |
| 14:G:108:ILE:HG22 | 14:G:148:TYR:CD1 | 2.33 | 0.62 |
| 15:H:49:LEU:HD13 | 33:Z:758:LEU:HB3 | 1.79 | 0.62 |
| 19:L:263:ILE:O | 19:L:267:PHE:CD1 | 2.48 | 0.62 |
| 21:N:223:LEU:CD1 | 21:N:722:THR:HG22 | 2.29 | 0.62 |
| 21:N:602:VAL:O | 21:N:606:VAL:HG22 | 2.00 | 0.62 |
| 25:R:259:PHE:CE1 | 25:R:332:GLU:HB2 | 2.34 | 0.62 |
| 28:U:171:VAL:HG13 | 29:V:213:LEU:HD22 | 1.80 | 0.62 |
| 29:V:188:LEU:C | 29:V:188:LEU:HD13 | 2.20 | 0.62 |
| 3:3:37:TYR:CE1 | 3:3:59:ARG:CG | 2.82 | 0.62 |
| 3:3:79:THR:HG23 | 3:3:115:PHE:HZ | 1.64 | 0.62 |
| 6:6:66:TYR:HE2 | 6:6:73:LYS:C | 2.02 | 0.62 |
| 16:I:263:LEU:HD21 | 17:J:224:GLY:H | 1.64 | 0.62 |
| 23:P:267:PHE:HZ | 23:P:329:PHE:CD2 | 2.16 | 0.62 |
| 23:P:302:LEU:CD1 | 23:P:314:VAL:HG11 | 2.29 | 0.62 |
| 28:U:297:GLN:HE22 | 29:V:277:LYS:HG3 | 1.64 | 0.62 |
| 33:Z:56:LEU:HD11 | 33:Z:71:LEU:HD22 | 1.81 | 0.62 |
| 33:Z:763:HIS:CA | 33:Z:766:HIS:ND1 | 2.62 | 0.62 |
| 15:H:284:VAL:HG12 | 20:M:253:GLN:C | 2.19 | 0.62 |
| 16:I:278:ILE:HG21 | 16:I:325:ILE:HD12 | 1.82 | 0.62 |
| 20:M:195:GLU:HA | 20:M:199:LEU:CD1 | 2.30 | 0.62 |
| 21:N:221:ASP:C | 21:N:894:ARG:HH22 | 2.03 | 0.62 |
| 21:N:749:LEU:CG | 21:N:753:PHE:CZ | 2.82 | 0.62 |
| 24:Q:262:LEU:HD23 | 24:Q:296:ILE:HD13 | 1.81 | 0.62 |
| 26:S:218:LEU:HG | 26:S:256:LYS:HZ1 | 1.64 | 0.62 |
| 27:T:201:PRO:HD2 | 27:T:204:ASN:HD22 | 1.63 | 0.62 |
| 28:U:5:HIS:HE1 | 28:U:158:PRO:HG3 | 1.65 | 0.62 |
| 28:U:104:LEU:O | 28:U:108:GLU:HG3 | 1.99 | 0.62 |
| 33:Z:278:LEU:HD13 | 33:Z:297:VAL:HG13 | 1.81 | 0.62 |
| 4:4:106:TYR:CZ | 4:4:185:LYS:HB3 | 2.34 | 0.62 |
| 10:C:207:THR:HG23 | 10:C:210:ARG:NH2 | 2.13 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:D:10:ILE:HD11 | 12:E:10:ARG:CD | 2.24 | 0.62 |
| 12:E:179:ALA:O | 12:E:183:LEU:HG | 1.98 | 0.62 |
| 13:F:159:THR:CA | 13:F:169:LYS:HZ3 | 2.08 | 0.62 |
| 23:P:307:GLU:OE1 | 23:P:307:GLU:N | 2.33 | 0.62 |
| 26:S:343:LEU:HD11 | 26:S:347:HIS:CE1 | 2.31 | 0.62 |
| 28:U:35:GLY:HA3 | 28:U:93:TYR:CZ | 2.35 | 0.62 |
| 33:Z:865:ASP:OD1 | 33:Z:909:ARG:NE | 2.32 | 0.62 |
| 13:F:91:GLN:CD | 13:F:111:LEU:HD23 | 2.19 | 0.62 |
| 15:H:249:TYR:OH | 15:H:376:GLU:CB | 2.47 | 0.62 |
| 16:I:126:PRO:CG | 16:I:154:MET:HE3 | 2.25 | 0.62 |
| 19:L:348:GLU:HG2 | 19:L:350:PRO:HD3 | 1.82 | 0.62 |
| 22:O:250:TRP:C | 22:O:269:LEU:HD11 | 2.12 | 0.62 |
| 22:O:325:GLU:HB3 | 23:P:364:ARG:HH22 | 1.65 | 0.62 |
| 23:P:306:ASN:ND2 | 23:P:349:ASN:HA | 2.14 | 0.62 |
| 24:Q:191:LEU:O | 24:Q:195:LYS:HG3 | 2.00 | 0.62 |
| 24:Q:353:PRO:O | 24:Q:354:PHE:CD1 | 2.52 | 0.62 |
| 26:S:475:TYR:CE1 | 28:U:291:LEU:O | 2.52 | 0.62 |
| 4:4:65:LEU:CG | 4:4:69:ARG:HE | 2.13 | 0.62 |
| 8:A:148:GLU:CD | 8:A:230:LYS:HE2 | 2.20 | 0.62 |
| 10:C:160:TRP:CG | 10:C:163:ILE:HD13 | 2.35 | 0.62 |
| 13:F:157:TYR:OH | 14:G:59:VAL:CG2 | 2.48 | 0.62 |
| 14:G:10:SER:HA | 14:G:126:ASN:OD1 | 1.99 | 0.62 |
| 14:G:72:HIS:CD2 | 14:G:73:ILE:HG13 | 2.34 | 0.62 |
| 15:H:285:GLY:O | 15:H:288:ALA:N | 2.32 | 0.62 |
| 20:M:216:LYS:NZ | 20:M:321:VAL:HB | 2.15 | 0.62 |
| 22:O:4:ASN:HB2 | 22:O:39:PHE:CZ | 2.34 | 0.62 |
| 24:Q:389:VAL:O | 24:Q:397:LEU:HD12 | 1.99 | 0.62 |
| 25:R:70:TYR:OH | 25:R:76:GLN:N | 2.32 | 0.62 |
| 25:R:239:THR:HG22 | 25:R:246:TYR:H | 1.64 | 0.62 |
| 33:Z:327:GLN:HG2 | 33:Z:349:THR:CB | 2.26 | 0.62 |
| 33:Z:518:LEU:CD1 | 33:Z:562:TRP:CE3 | 2.82 | 0.62 |
| 33:Z:740:VAL:HG11 | 33:Z:764:LEU:HD11 | 1.81 | 0.62 |
| 4:4:65:LEU:HG | 4:4:69:ARG:HE | 1.65 | 0.62 |
| 11:D:19:GLN:HE21 | 11:D:121:THR:HG23 | 1.63 | 0.62 |
| 14:G:51:LYS:HE2 | 14:G:63:ASN:HB2 | 1.82 | 0.62 |
| 15:H:326:ASP:HA | 15:H:329:VAL:HG22 | 1.81 | 0.62 |
| 19:L:74:LEU:HD11 | 20:M:47:GLU:HG3 | 1.80 | 0.62 |
| 20:M:385:GLU:O | 20:M:385:GLU:CD | 2.38 | 0.62 |
| 21:N:302:PHE:CZ | 21:N:757:THR:HB | 2.35 | 0.62 |
| 22:O:280:LEU:HD23 | 22:O:280:LEU:C | 2.20 | 0.62 |
| 23:P:303:PHE:O | 23:P:306:ASN:ND2 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:289:GLU:CD | 24:Q:291:TYR:HE1 | 2.03 | 0.62 |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:HB2 | 1.82 | 0.62 |
| 33:Z:774:ARG:HE | 33:Z:806:GLU:HB3 | 1.64 | 0.62 |
| 16:I:318:ASP:HB3 | 16:I:321:ASP:OD1 | 1.99 | 0.62 |
| 17:J:167:PRO:HD3 | 17:J:174:PHE:CZ | 2.32 | 0.62 |
| 18:K:183:GLU:CG | 18:K:338:ILE:HG12 | 2.30 | 0.62 |
| 22:O:4:ASN:N | 22:O:39:PHE:CE1 | 2.68 | 0.62 |
| 24:Q:146:TYR:CD1 | 24:Q:184:VAL:HG22 | 2.35 | 0.62 |
| 27:T:150:ARG:O | 27:T:154:GLU:HG3 | 2.00 | 0.62 |
| 31:X:38:ASN:ND2 | 31:X:43:LEU:H | 1.98 | 0.62 |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:HD23 | 1.82 | 0.62 |
| 15:H:50:LYS:HZ1 | 33:Z:791:LYS:HA | 1.65 | 0.61 |
| 21:N:21:LYS:O | 21:N:25:LEU:HG | 1.99 | 0.61 |
| 21:N:145:LEU:CB | 21:N:173:LYS:HZ1 | 2.13 | 0.61 |
| 21:N:365:PHE:CE2 | 21:N:402:GLY:C | 2.74 | 0.61 |
| 21:N:424:LYS:HZ2 | 21:N:461:GLU:CB | 2.09 | 0.61 |
| 22:O:233:LEU:CD2 | 22:O:238:ILE:CD1 | 2.78 | 0.61 |
| 23:P:95:TYR:CD2 | 23:P:96:MET:HE2 | 2.34 | 0.61 |
| 26:S:315:LYS:NZ | 26:S:345:TYR:CD1 | 2.60 | 0.61 |
| 2:2:8:PHE:CE1 | 2:2:12:VAL:N | 2.68 | 0.61 |
| 2:2:124:TYR:CE2 | 2:2:139:GLU:HA | 2.35 | 0.61 |
| 15:H:306:ILE:CG2 | 15:H:308:PHE:CZ | 2.83 | 0.61 |
| 17:J:134:VAL:CG1 | 17:J:135:SER:N | 2.34 | 0.61 |
| 18:K:258:PHE:CZ | 18:K:299:LEU:HD12 | 2.35 | 0.61 |
| 22:O:377:VAL:HG12 | 28:U:197:LEU:HD13 | 1.81 | 0.61 |
| 26:S:461:PHE:CE2 | 28:U:274:MET:HA | 2.36 | 0.61 |
| 33:Z:436:LEU:HD21 | 33:Z:455:ILE:HG13 | 1.83 | 0.61 |
| 9:B:160:LYS:HE2 | 10:C:55:THR:O | 2.00 | 0.61 |
| 10:C:66:LEU:HG | 10:C:212:GLU:OE2 | 1.99 | 0.61 |
| 13:F:101:ARG:HH22 | 13:F:103:LEU:CD1 | 2.13 | 0.61 |
| 14:G:200:TYR:HE1 | 14:G:246:ILE:HG21 | 1.62 | 0.61 |
| 16:I:310:LEU:HD13 | 16:I:338:LEU:CA | 2.28 | 0.61 |
| 19:L:298:ASP:OD1 | 19:L:301:ILE:HD12 | 2.00 | 0.61 |
| 20:M:337:LEU:HD22 | 20:M:343:LEU:HD12 | 1.81 | 0.61 |
| 21:N:221:ASP:C | 21:N:894:ARG:NH2 | 2.54 | 0.61 |
| 22:O:159:LYS:HE2 | 22:O:160:LYS:HE3 | 1.82 | 0.61 |
| 23:P:177:ILE:O | 23:P:181:LEU:HG | 2.00 | 0.61 |
| 27:T:53:ASN:O | 27:T:54:ASP:OD1 | 2.18 | 0.61 |
| 30:W:25:ARG:HH11 | 30:W:144:PHE:HE2 | 0.63 | 0.61 |
| 30:W:115:CYS:SG | 30:W:144:PHE:HZ | 2.23 | 0.61 |
| 31:X:38:ASN:HD22 | 31:X:42:GLU:N | 1.98 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:6:61:ASN:O | 6:6:65:TRP:CD1 | 2.53 | 0.61 |
| 6:6:66:TYR:OH | 6:6:73:LYS:CG | 2.48 | 0.61 |
| 14:G:61:GLN:HA | 14:G:64:VAL:CG2 | 2.29 | 0.61 |
| 16:I:380:LEU:HD13 | 16:I:420:LYS:HE3 | 1.83 | 0.61 |
| 19:L:88:TYR:CD1 | 20:M:62:ILE:CG1 | 2.84 | 0.61 |
| 22:O:159:LYS:HG2 | 22:O:160:LYS:HG3 | 1.80 | 0.61 |
| 23:P:220:TYR:O | 23:P:224:LEU:HG | 1.99 | 0.61 |
| 33:Z:71:LEU:O | 33:Z:75:ILE:CG1 | 2.41 | 0.61 |
| 33:Z:546:ILE:HG23 | 33:Z:550:PHE:CE2 | 2.32 | 0.61 |
| 1:1:34:LEU:HD13 | 1:1:176:VAL:HG23 | 1.82 | 0.61 |
| 3:3:96:VAL:O | 3:3:117:LEU:HD23 | 1.99 | 0.61 |
| 5:5:158:LYS:HG2 | 5:5:196:LEU:HD21 | 1.83 | 0.61 |
| 5:5:179:HIS:HB2 | 5:5:188:HIS:CD2 | 2.35 | 0.61 |
| 7:7:92:MET:HA | 7:7:102:LEU:HD12 | 1.82 | 0.61 |
| 8:A:135:ARG:NH2 | 14:G:14:PHE:HD2 | 1.98 | 0.61 |
| 9:B:139:HIS:HD2 | 9:B:234:ARG:CD | 2.14 | 0.61 |
| 19:L:145:ARG:HE | 19:L:162:GLU:CG | 2.11 | 0.61 |
| 21:N:685:VAL:HG13 | 21:N:691:GLN:HG3 | 1.81 | 0.61 |
| 24:Q:331:THR:HG22 | 24:Q:335:PHE:CE2 | 2.36 | 0.61 |
| 26:S:464:ARG:HB2 | 28:U:281:LEU:CD2 | 2.30 | 0.61 |
| 30:W:186:ALA:O | 30:W:192:LEU:HG | 1.99 | 0.61 |
| 3:3:6:MET:CE | 3:3:158:ILE:HA | 2.31 | 0.61 |
| 5:5:135:PHE:HE2 | 5:5:163:ALA:CB | 1.98 | 0.61 |
| 6:6:-5:TYR:HE1 | 6:6:97:TYR:CB | 2.12 | 0.61 |
| 8:A:128:TYR:HE1 | 8:A:131:ARG:NH1 | 1.98 | 0.61 |
| 18:K:280:LYS:HZ2 | 18:K:296:LEU:CD2 | 2.12 | 0.61 |
| 21:N:145:LEU:HB3 | 21:N:173:LYS:NZ | 2.16 | 0.61 |
| 21:N:163:LEU:HB3 | 21:N:209:LYS:HZ1 | 1.66 | 0.61 |
| 21:N:671:LEU:HD13 | 21:N:877:GLN:HG3 | 1.83 | 0.61 |
| 33:Z:574:TYR:OH | 33:Z:584:VAL:HG22 | 2.01 | 0.61 |
| 33:Z:795:THR:CG2 | 33:Z:799:PHE:HE2 | 2.11 | 0.61 |
| 3:3:1:GLY:HA2 | 3:3:17:ASP:OD2 | 2.01 | 0.61 |
| 6:6:31:GLU:OE1 | 7:7:129:TYR:CB | 2.48 | 0.61 |
| 7:7:178:TYR:CE1 | 7:7:210:LYS:HD3 | 2.35 | 0.61 |
| 8:A:29:GLU:OE2 | 18:K:425:ASP:HB2 | 1.99 | 0.61 |
| 10:C:113:ARG:HD3 | 11:D:83:ARG:HD2 | 1.81 | 0.61 |
| 17:J:28:GLN:HG3 | 26:S:225:HIS:NE2 | 2.16 | 0.61 |
| 18:K:67:TYR:OH | 21:N:609:LEU:HD23 | 2.01 | 0.61 |
| 23:P:392:LYS:HG2 | 24:Q:354:PHE:CG | 2.36 | 0.61 |
| 25:R:327:ASP:O | 25:R:331:ARG:HG3 | 2.01 | 0.61 |
| 26:S:315:LYS:CE | 26:S:345:TYR:CE1 | 2.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:V:145:GLN:OE1 | 29:V:148:LYS:NZ | 2.27 | 0.61 |
| 5:5:6:PHE:CE1 | 5:5:13:ILE:HB | 2.35 | 0.61 |
| 6:6:-5:TYR:CE1 | 6:6:97:TYR:HB3 | 2.36 | 0.61 |
| 12:E:17:PRO:HA | 13:F:24:TYR:CD2 | 2.35 | 0.61 |
| 12:E:165:TYR:CB | 12:E:167:TYR:HH | 2.14 | 0.61 |
| 12:E:219:LEU:HB2 | 12:E:236:THR:HG22 | 1.82 | 0.61 |
| 15:H:275:ILE:HG21 | 16:I:308:GLU:OE1 | 2.01 | 0.61 |
| 15:H:358:PRO:HB2 | 15:H:374:LYS:HZ2 | 1.65 | 0.61 |
| 17:J:161:LYS:HG3 | 17:J:165:GLU:OE1 | 2.01 | 0.61 |
| 17:J:236:MET:O | 17:J:240:HIS:CD2 | 2.54 | 0.61 |
| 19:L:178:ILE:CD1 | 19:L:230:LEU:HD22 | 2.29 | 0.61 |
| 21:N:330:THR:O | 21:N:334:VAL:HG23 | 2.01 | 0.61 |
| 22:O:115:ARG:HH21 | 30:W:80:GLN:HE21 | 1.47 | 0.61 |
| 22:O:228:TYR:CG | 22:O:229:ASN:N | 2.63 | 0.61 |
| 23:P:395:ARG:CD | 24:Q:357:VAL:HG12 | 2.30 | 0.61 |
| 25:R:54:ILE:O | 25:R:54:ILE:CG2 | 2.49 | 0.61 |
| 27:T:245:TYR:CD2 | 27:T:246:GLU:N | 2.68 | 0.61 |
| 30:W:7:VAL:HG23 | 30:W:98:LEU:HD21 | 1.83 | 0.61 |
| 3:3:7:THR:HG23 | 3:3:112:ILE:HD11 | 1.83 | 0.61 |
| 14:G:168:ARG:HE | 14:G:172:LYS:HZ2 | 1.42 | 0.61 |
| 16:I:207:LEU:CD2 | 33:Z:930:GLY:CA | 2.77 | 0.61 |
| 17:J:382:PHE:O | 17:J:386:VAL:HG23 | 2.01 | 0.61 |
| 21:N:482:ALA:HB1 | 21:N:517:LEU:HD23 | 1.83 | 0.61 |
| 23:P:210:ASN:HB3 | 23:P:211:PRO:HD2 | 1.82 | 0.61 |
| 30:W:95:GLN:NE2 | 30:W:132:LEU:HA | 2.16 | 0.61 |
| 33:Z:75:ILE:HG21 | 33:Z:121:ILE:HD13 | 1.81 | 0.61 |
| 33:Z:205:LEU:HD23 | 33:Z:236:PHE:HE1 | 1.66 | 0.61 |
| 11:D:96:HIS:NE2 | 11:D:100:LEU:HD22 | 2.15 | 0.61 |
| 16:I:208:TYR:CD1 | 16:I:209:GLU:N | 2.69 | 0.61 |
| 16:I:221:LEU:HD23 | 16:I:348:ILE:HB | 1.83 | 0.61 |
| 23:P:154:ASP:CG | 23:P:190:LYS:NZ | 2.54 | 0.61 |
| 24:Q:165:PHE:CE1 | 24:Q:173:SER:OG | 2.49 | 0.61 |
| 29:V:135:ARG:CD | 29:V:157:ARG:NH2 | 2.39 | 0.61 |
| 33:Z:232:LYS:HB3 | 33:Z:236:PHE:CE2 | 2.36 | 0.61 |
| 2:2:97:TYR:CZ | 2:2:115:ALA:HB3 | 2.36 | 0.60 |
| 4:4:44:SER:OG | 4:4:102:LEU:HB2 | 2.01 | 0.60 |
| 6:6:73:LYS:HD2 | 12:E:108:ASN:ND2 | 2.16 | 0.60 |
| 8:A:53:VAL:HG11 | 8:A:82:VAL:HG21 | 1.83 | 0.60 |
| 15:H:285:GLY:H | 15:H:331:ARG:HH12 | 1.49 | 0.60 |
| 21:N:593:PHE:CZ | 21:N:734:VAL:CG2 | 2.80 | 0.60 |
| 33:Z:763:HIS:ND1 | 33:Z:766:HIS:CE1 | 2.69 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:880:SER:HB2 | 33:Z:906:ALA:HB3 | 1.82 | 0.60 |
| 3:3:129:VAL:HG22 | 3:3:138:PHE:HE1 | 1.54 | 0.60 |
| 8:A:24:ARG:NH1 | 18:K:426:PHE:CE2 | 2.70 | 0.60 |
| 12:E:153:TYR:OH | 12:E:223:THR:HA | 2.01 | 0.60 |
| 13:F:72:LEU:HD22 | 13:F:132:LEU:HD13 | 1.83 | 0.60 |
| 16:I:395:MET:CE | 16:I:420:LYS:CE | 2.78 | 0.60 |
| 18:K:159:SER:HB3 | 18:K:244:HIS:NE2 | 2.15 | 0.60 |
| 21:N:602:VAL:HB | 21:N:603:PRO:HD3 | 1.83 | 0.60 |
| 21:N:770:LYS:CE | 21:N:917:ILE:HG21 | 2.28 | 0.60 |
| 23:P:422:LEU:HD12 | 28:U:262:GLN:NE2 | 2.17 | 0.60 |
| 27:T:245:TYR:O | 27:T:246:GLU:HB2 | 2.01 | 0.60 |
| 30:W:186:ALA:CA | 30:W:191:ILE:HG21 | 1.99 | 0.60 |
| 33:Z:224:LEU:CD2 | 33:Z:236:PHE:HE2 | 2.14 | 0.60 |
| 33:Z:546:ILE:CG2 | 33:Z:550:PHE:HE2 | 2.09 | 0.60 |
| 5:5:81:LYS:HD3 | 5:5:121:ARG:NE | 2.16 | 0.60 |
| 6:6:34:VAL:HG12 | 6:6:196:LEU:HD12 | 1.82 | 0.60 |
| 6:6:89:TYR:CE1 | 6:6:92:ARG:NE | 2.69 | 0.60 |
| 12:E:20:ARG:CD | 20:M:432:PHE:CZ | 2.77 | 0.60 |
| 17:J:329:ARG:NH1 | 17:J:333:ARG:NH1 | 2.50 | 0.60 |
| 17:J:340:GLY:HA3 | 25:R:238:PHE:HE1 | 1.65 | 0.60 |
| 21:N:361:ASN:HB3 | 21:N:399:PHE:CE2 | 2.36 | 0.60 |
| 21:N:596:LEU:HD21 | 21:N:627:ILE:HG22 | 1.83 | 0.60 |
| 22:O:237:PRO:HB2 | 22:O:241:THR:HG23 | 1.83 | 0.60 |
| 22:O:250:TRP:CB | 22:O:269:LEU:CD2 | 2.73 | 0.60 |
| 25:R:50:VAL:HG13 | 25:R:54:ILE:HD11 | 1.81 | 0.60 |
| 26:S:401:LYS:CE | 26:S:444:GLU:OE2 | 2.36 | 0.60 |
| 31:X:25:THR:OG1 | 31:X:82:LYS:NZ | 2.28 | 0.60 |
| 33:Z:250:VAL:CG2 | 33:Z:272:TYR:OH | 2.48 | 0.60 |
| 2:2:36:ARG:HB2 | 2:2:42:TRP:CZ3 | 2.37 | 0.60 |
| 2:2:59:ILE:HG13 | 2:2:83:LEU:HD23 | 1.83 | 0.60 |
| 4:4:55:PHE:HZ | 4:4:83:VAL:HG13 | 1.65 | 0.60 |
| 7:7:186:ASN:OD1 | 7:7:205:GLN:HG2 | 2.01 | 0.60 |
| 20:M:290:ARG:HD3 | 20:M:294:GLU:HB2 | 1.83 | 0.60 |
| 27:T:157:TYR:CZ | 27:T:188:GLU:HG2 | 2.36 | 0.60 |
| 33:Z:295:ARG:NE | 33:Z:325:GLY:O | 2.34 | 0.60 |
| 33:Z:821:GLY:CA | 33:Z:863:THR:HG22 | 2.20 | 0.60 |
| 1:1:-2:LEU:HD12 | 1:1:-1:GLY:N | 2.16 | 0.60 |
| 10:C:177:GLN:NE2 | 11:D:52:LEU:HB3 | 2.16 | 0.60 |
| 16:I:200:LEU:CB | 33:Z:931:GLN:HG2 | 2.29 | 0.60 |
| 17:J:27:ILE:HG21 | 18:K:50:LYS:CD | 2.32 | 0.60 |
| 18:K:205:PRO:HD2 | 18:K:207:ARG:HH22 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:K:423:LYS:HE3 | 18:K:424:PHE:HE2 | 1.64 | 0.60 |
| 21:N:67:LYS:CG | 21:N:97:PHE:CE1 | 2.85 | 0.60 |
| 21:N:331:ALA:HB2 | 21:N:697:PHE:HD1 | 1.67 | 0.60 |
| 22:O:15:ARG:CA | 30:W:20:ASP:OD1 | 2.49 | 0.60 |
| 24:Q:322:GLU:HG3 | 24:Q:326:MET:HE2 | 1.82 | 0.60 |
| 26:S:425:ARG:NH1 | 27:T:155:GLY:N | 2.49 | 0.60 |
| 33:Z:64:TYR:CE2 | 33:Z:111:LEU:HB3 | 2.36 | 0.60 |
| 2:2:124:TYR:CZ | 2:2:139:GLU:HA | 2.37 | 0.60 |
| 13:F:160:ALA:N | 13:F:169:LYS:HD3 | 2.16 | 0.60 |
| 13:F:203:ASP:OD1 | 13:F:204:GLU:HG3 | 2.01 | 0.60 |
| 15:H:295:PHE:HZ | 15:H:336:LEU:HD12 | 1.62 | 0.60 |
| 16:I:290:LYS:HE3 | 16:I:336:PRO:HD3 | 1.84 | 0.60 |
| 17:J:219:VAL:CB | 18:K:281:ARG:HD2 | 2.27 | 0.60 |
| 18:K:161:MET:CE | 18:K:237:VAL:HG13 | 2.31 | 0.60 |
| 23:P:308:LEU:CD2 | 23:P:369:LEU:HD23 | 2.20 | 0.60 |
| 27:T:144:TYR:HB2 | 27:T:145:PRO:HD3 | 1.83 | 0.60 |
| 28:U:92:TRP:CZ2 | 28:U:120:LEU:CG | 2.84 | 0.60 |
| 2:2:8:PHE:CE2 | 2:2:10:ASN:HB3 | 2.36 | 0.60 |
| 9:B:174:PHE:HB3 | 9:B:178:ARG:CZ | 2.31 | 0.60 |
| 14:G:168:ARG:O | 14:G:172:LYS:HG3 | 2.01 | 0.60 |
| 16:I:263:LEU:HD21 | 17:J:224:GLY:N | 2.16 | 0.60 |
| 17:J:363:THR:HA | 18:K:203:ILE:HD13 | 1.83 | 0.60 |
| 31:X:91:PHE:H | 31:X:96:ARG:CG | 2.03 | 0.60 |
| 33:Z:306:MET:HE3 | 33:Z:310:LEU:HD21 | 1.84 | 0.60 |
| 33:Z:931:GLN:HB2 | 33:Z:955:VAL:HG21 | 1.82 | 0.60 |
| 1:1:57:ASP:HB3 | 8:A:106:TYR:CZ | 2.35 | 0.60 |
| 10:C:193:ALA:O | 10:C:197:LEU:HG | 2.00 | 0.60 |
| 11:D:193:LYS:HE3 | 11:D:197:ARG:CZ | 2.32 | 0.60 |
| 17:J:224:GLY:C | 17:J:225:GLU:C | 2.60 | 0.60 |
| 17:J:328:LEU:HD23 | 17:J:343:LEU:HD22 | 1.82 | 0.60 |
| 21:N:405:LEU:HD22 | 21:N:423:LEU:CD2 | 2.31 | 0.60 |
| 23:P:193:TYR:HE1 | 23:P:230:HIS:HD1 | 1.50 | 0.60 |
| 24:Q:309:ARG:CZ | 24:Q:345:SER:CB | 2.54 | 0.60 |
| 27:T:229:VAL:HG12 | 27:T:230:ASN:N | 2.17 | 0.60 |
| 28:U:16:LEU:HD12 | 29:V:35:LEU:CD1 | 2.32 | 0.60 |
| 29:V:159:ILE:HB | 29:V:194:ARG:H | 1.66 | 0.60 |
| 33:Z:99:LEU:O | 33:Z:102:ILE:HG22 | 2.02 | 0.60 |
| 33:Z:884:THR:HG21 | 33:Z:904:LEU:CG | 2.31 | 0.60 |
| 4:4:37:LEU:HD22 | 4:4:43:MET:SD | 2.41 | 0.60 |
| 4:4:103:ILE:CD1 | 4:4:118:ILE:HD12 | 2.32 | 0.60 |
| 4:4:129:TYR:CD1 | 4:4:143:LEU:HD13 | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:232:LYS:CD | 8:A:234:PHE:HE1 | 2.15 | 0.60 |
| 13:F:105:VAL:CG2 | 13:F:145:LEU:CD1 | 2.65 | 0.60 |
| 15:H:249:TYR:CE2 | 15:H:374:LYS:HG2 | 2.37 | 0.60 |
| 15:H:451:ILE:O | 15:H:455:LYS:HG3 | 2.01 | 0.60 |
| 18:K:386:ILE:HA | 18:K:414:GLN:NE2 | 2.12 | 0.60 |
| 20:M:81:ASN:ND2 | 20:M:143:ASN:H | 2.00 | 0.60 |
| 21:N:329:HIS:CG | 29:V:182:LYS:HZ2 | 2.18 | 0.60 |
| 21:N:405:LEU:HD13 | 21:N:446:ALA:HB2 | 1.83 | 0.60 |
| 21:N:539:MET:HE2 | 21:N:551:GLY:CA | 2.32 | 0.60 |
| 21:N:601:THR:O | 21:N:605:ILE:HG12 | 2.01 | 0.60 |
| 24:Q:11:ALA:HB1 | 24:Q:27:TYR:CE1 | 2.37 | 0.60 |
| 24:Q:88:PHE:CD2 | 24:Q:89:ALA:N | 2.69 | 0.60 |
| 24:Q:383:ASP:OD1 | 25:R:267:LYS:NZ | 2.35 | 0.60 |
| 25:R:258:LEU:HD12 | 25:R:288:SER:HB2 | 1.83 | 0.60 |
| 33:Z:608:TYR:CD2 | 33:Z:616:LEU:HD11 | 2.36 | 0.60 |
| 1:1:174:ARG:HH11 | 1:1:185:ARG:HH21 | 1.42 | 0.60 |
| 5:5:135:PHE:HB2 | 5:5:167:ARG:CZ | 2.32 | 0.60 |
| 18:K:192:LEU:HD21 | 18:K:266:PRO:HB3 | 1.84 | 0.60 |
| 18:K:258:PHE:CD2 | 18:K:302:GLN:HB3 | 2.37 | 0.60 |
| 21:N:109:TYR:HE1 | 21:N:129:ILE:HD12 | 1.67 | 0.60 |
| 21:N:330:THR:CG2 | 21:N:739:PHE:CE1 | 2.76 | 0.60 |
| 21:N:596:LEU:CD1 | 21:N:717:LEU:HD13 | 2.29 | 0.60 |
| 24:Q:275:ILE:CD1 | 24:Q:306:TYR:CD2 | 2.74 | 0.60 |
| 26:S:242:LEU:HD21 | 26:S:279:ILE:HG13 | 1.83 | 0.60 |
| 27:T:126:LEU:HD22 | 27:T:136:LEU:HD22 | 1.80 | 0.60 |
| 33:Z:518:LEU:HG | 33:Z:524:ALA:HB3 | 1.84 | 0.60 |
| 5:5:93:ALA:HB1 | 6:6:93:PHE:HE1 | 1.67 | 0.59 |
| 13:F:5:ASN:HB3 | 14:G:9:LEU:HD11 | 1.84 | 0.59 |
| 16:I:220:ILE:CD1 | 16:I:344:ILE:HG21 | 2.32 | 0.59 |
| 21:N:376:LYS:HE2 | 21:N:750:SER:O | 2.02 | 0.59 |
| 22:O:131:SER:HB3 | 22:O:135:ARG:NH1 | 2.16 | 0.59 |
| 25:R:222:ARG:HA | 25:R:224:PHE:CE2 | 2.37 | 0.59 |
| 25:R:338:TYR:CE2 | 25:R:368:LEU:HD13 | 2.36 | 0.59 |
| 26:S:425:ARG:HH11 | 27:T:155:GLY:CA | 2.15 | 0.59 |
| 28:U:57:GLU:HG2 | 30:W:96:LEU:HD22 | 1.84 | 0.59 |
| 28:U:92:TRP:HZ2 | 28:U:120:LEU:CD1 | 1.93 | 0.59 |
| 33:Z:64:TYR:CD2 | 33:Z:68:LEU:HD11 | 2.37 | 0.59 |
| 13:F:201:LEU:HD22 | 13:F:204:GLU:HB2 | 1.84 | 0.59 |
| 17:J:27:ILE:CG2 | 18:K:50:LYS:HE2 | 2.32 | 0.59 |
| 17:J:59:LYS:HE2 | 17:J:63:ARG:HH12 | 1.67 | 0.59 |
| 20:M:345:ARG:HG3 | 20:M:347:ILE:HG13 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:306:ASN:O | 21:N:308:ASN:ND2 | 2.36 | 0.59 |
| 22:O:83:LEU:HD12 | 22:O:128:LEU:CD2 | 2.32 | 0.59 |
| 23:P:241:LEU:HD11 | 23:P:260:VAL:HG13 | 1.84 | 0.59 |
| 23:P:395:ARG:HD2 | 24:Q:357:VAL:CG1 | 2.31 | 0.59 |
| 25:R:422:ARG:NH1 | 26:S:474:GLU:HG3 | 2.17 | 0.59 |
| 30:W:21:PHE:HZ | 30:W:144:PHE:HD2 | 1.39 | 0.59 |
| 9:B:179:TRP:CD1 | 9:B:183:LEU:HD12 | 2.36 | 0.59 |
| 11:D:53:LYS:NZ | 11:D:209:ASN:OD1 | 2.32 | 0.59 |
| 12:E:46:VAL:HG11 | 12:E:145:ALA:HB1 | 1.84 | 0.59 |
| 14:G:183:PRO:O | 14:G:184:GLU:CG | 2.49 | 0.59 |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:HG21 | 1.85 | 0.59 |
| 17:J:211:ILE:HD12 | 17:J:243:SER:OG | 2.02 | 0.59 |
| 20:M:218:ALA:HB3 | 20:M:324:LEU:HD23 | 1.84 | 0.59 |
| 23:P:137:ALA:HB1 | 23:P:179:PHE:CE2 | 2.38 | 0.59 |
| 29:V:186:GLN:O | 29:V:190:HIS:HD2 | 1.85 | 0.59 |
| 33:Z:327:GLN:NE2 | 33:Z:346:LEU:HD12 | 2.16 | 0.59 |
| 33:Z:383:SER:O | 33:Z:386:VAL:HG12 | 2.03 | 0.59 |
| 33:Z:931:GLN:HG3 | 33:Z:931:GLN:O | 2.01 | 0.59 |
| 5:5:38:ASN:HB2 | 5:5:39:PRO:HD2 | 1.84 | 0.59 |
| 14:G:203:HIS:CE1 | 14:G:211:PHE:HD1 | 2.21 | 0.59 |
| 19:L:149:ASP:OD2 | 19:L:152:THR:N | 2.24 | 0.59 |
| 19:L:290:ARG:HH11 | 19:L:293:GLU:CA | 2.13 | 0.59 |
| 21:N:83:LEU:HD22 | 21:N:132:LYS:HB3 | 1.85 | 0.59 |
| 21:N:490:LEU:HD23 | 21:N:491:GLY:N | 2.17 | 0.59 |
| 21:N:599:TYR:HD1 | 21:N:634:LEU:HD22 | 1.66 | 0.59 |
| 33:Z:190:THR:O | 33:Z:190:THR:HG22 | 2.02 | 0.59 |
| 33:Z:217:GLU:OE1 | 33:Z:244:ARG:NE | 2.31 | 0.59 |
| 9:B:174:PHE:HB3 | 9:B:178:ARG:NH2 | 2.17 | 0.59 |
| 10:C:70:ASN:ND2 | 10:C:95:ALA:HB1 | 2.18 | 0.59 |
| 13:F:22:VAL:O | 13:F:26:LEU:HG | 2.02 | 0.59 |
| 13:F:34:VAL:HG21 | 13:F:200:SER:OG | 2.02 | 0.59 |
| 17:J:224:GLY:C | 17:J:226:GLY:N | 2.56 | 0.59 |
| 19:L:102:GLY:HA3 | 20:M:153:TYR:HD2 | 1.67 | 0.59 |
| 19:L:264:ARG:HA | 19:L:311:GLN:HE22 | 1.66 | 0.59 |
| 28:U:66:TRP:CZ3 | 28:U:68:LEU:HB3 | 2.37 | 0.59 |
| 33:Z:64:TYR:CD2 | 33:Z:111:LEU:CG | 2.81 | 0.59 |
| 33:Z:278:LEU:CD1 | 33:Z:297:VAL:HG13 | 2.32 | 0.59 |
| 33:Z:279:THR:HG21 | 33:Z:977:ILE:HD13 | 1.83 | 0.59 |
| 1:1:-4:VAL:HG11 | 1:1:49:ALA:HB3 | 1.83 | 0.59 |
| 2:2:210:THR:OG1 | 3:3:160:GLN:NE2 | 2.35 | 0.59 |
| 11:D:11:PHE:CE2 | 12:E:26:TYR:HB2 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:F:12:THR:CG2 | 13:F:19:LEU:HD13 | 2.06 | 0.59 |
| 18:K:177:LEU:HB2 | 18:K:181:LYS:HE3 | 1.85 | 0.59 |
| 20:M:253:GLN:HG3 | 20:M:258:GLU:CB | 2.32 | 0.59 |
| 21:N:43:LEU:HD21 | 21:N:69:TYR:HE1 | 1.66 | 0.59 |
| 22:O:44:SER:OG | 22:O:73:ILE:HG13 | 2.01 | 0.59 |
| 22:O:59:LEU:CD2 | 22:O:85:SER:CB | 2.76 | 0.59 |
| 23:P:332:GLU:N | 23:P:337:HIS:NE2 | 2.50 | 0.59 |
| 23:P:391:ALA:O | 24:Q:354:PHE:CD1 | 2.55 | 0.59 |
| 28:U:67:PHE:CE1 | 30:W:97:THR:CB | 2.85 | 0.59 |
| 6:6:70:HIS:CD2 | 12:E:111:SER:HB2 | 2.38 | 0.59 |
| 8:A:117:LEU:HD23 | 8:A:143:PHE:CD1 | 2.37 | 0.59 |
| 15:H:284:VAL:HG11 | 20:M:254:MET:N | 2.11 | 0.59 |
| 17:J:329:ARG:HH12 | 17:J:333:ARG:NH1 | 2.01 | 0.59 |
| 19:L:360:ILE:HG23 | 19:L:391:ILE:HG21 | 1.84 | 0.59 |
| 22:O:266:PHE:CE1 | 22:O:280:LEU:HD21 | 2.38 | 0.59 |
| 23:P:79:LEU:HD13 | 23:P:100:VAL:HG21 | 1.83 | 0.59 |
| 24:Q:179:LEU:HD13 | 24:Q:218:LEU:HD23 | 1.83 | 0.59 |
| 24:Q:190:ASN:ND2 | 24:Q:193:LYS:HD2 | 2.18 | 0.59 |
| 25:R:70:TYR:O | 25:R:70:TYR:CD2 | 2.55 | 0.59 |
| 28:U:37:ILE:HG23 | 28:U:93:TYR:HD2 | 1.66 | 0.59 |
| 7:7:163:GLN:O | 7:7:167:GLU:HG3 | 2.03 | 0.59 |
| 10:C:162:ALA:HB1 | 10:C:176:LEU:HD21 | 1.83 | 0.59 |
| 12:E:165:TYR:HB3 | 12:E:167:TYR:CZ | 2.38 | 0.59 |
| 21:N:302:PHE:CE2 | 21:N:757:THR:HB | 2.37 | 0.59 |
| 21:N:371:LEU:O | 21:N:375:HIS:ND1 | 2.18 | 0.59 |
| 21:N:406:TYR:HD1 | 21:N:448:LEU:HB2 | 1.66 | 0.59 |
| 24:Q:83:GLU:HA | 24:Q:86:MET:CG | 2.33 | 0.59 |
| 33:Z:74:SER:HB2 | 33:Z:79:THR:CG2 | 2.25 | 0.59 |
| 33:Z:748:LEU:CG | 33:Z:783:VAL:HA | 2.33 | 0.59 |
| 1:1:193:TYR:CD1 | 1:1:194:GLU:N | 2.71 | 0.59 |
| 2:2:8:PHE:CZ | 2:2:11:GLY:N | 2.68 | 0.59 |
| 4:4:34:THR:CG2 | 4:4:181:LYS:HZ1 | 2.16 | 0.59 |
| 10:C:42:ASP:HA | 10:C:218:LYS:NZ | 2.17 | 0.59 |
| 21:N:394:ARG:HG2 | 21:N:395:ALA:O | 2.03 | 0.59 |
| 25:R:65:TYR:O | 25:R:69:GLU:HG2 | 2.03 | 0.59 |
| 25:R:73:ASN:H | 25:R:76:GLN:HE21 | 1.50 | 0.59 |
| 28:U:100:ARG:N | 28:U:103:ASP:OD2 | 2.35 | 0.59 |
| 29:V:127:LYS:HE3 | 29:V:194:ARG:CD | 2.32 | 0.59 |
| 33:Z:823:ASN:CG | 33:Z:856:HIS:HD1 | 2.06 | 0.59 |
| 1:1:14:LEU:CG | 1:1:100:ALA:CB | 2.80 | 0.59 |
| 1:1:174:ARG:HH12 | 1:1:185:ARG:NH2 | 1.98 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:13:ASP:OD1 | 8:A:14:ARG:HG3 | 2.02 | 0.59 |
| 8:A:64:LEU:HD13 | 14:G:157:TRP:HD1 | 1.66 | 0.59 |
| 15:H:334:LEU:HD13 | 20:M:285:ALA:HB2 | 1.84 | 0.59 |
| 16:I:76:VAL:HG12 | 33:Z:621:LEU:HD13 | 1.85 | 0.59 |
| 16:I:205:PRO:O | 16:I:208:TYR:CD2 | 2.56 | 0.59 |
| 17:J:214:SER:CB | 17:J:217:GLU:OE1 | 2.51 | 0.59 |
| 18:K:239:GLY:HA2 | 18:K:242:PHE:CE2 | 2.38 | 0.59 |
| 21:N:490:LEU:HD21 | 21:N:526:TYR:CG | 2.37 | 0.59 |
| 21:N:656:ALA:O | 21:N:660:LEU:HG | 2.02 | 0.59 |
| 22:O:199:LEU:HD11 | 22:O:204:SER:O | 2.03 | 0.59 |
| 23:P:425:HIS:HA | 28:U:228:LYS:NZ | 2.18 | 0.59 |
| 25:R:170:VAL:CG1 | 25:R:194:VAL:CG2 | 2.80 | 0.59 |
| 26:S:461:PHE:CE2 | 28:U:274:MET:CA | 2.78 | 0.59 |
| 31:X:47:ASP:OD1 | 31:X:67:ILE:HG22 | 2.02 | 0.59 |
| 31:X:79:LYS:HE2 | 31:X:98:PHE:CZ | 2.28 | 0.59 |
| 33:Z:50:GLU:OE2 | 33:Z:55:ARG:CZ | 2.48 | 0.59 |
| 33:Z:138:ARG:NH2 | 33:Z:157:LEU:CG | 2.63 | 0.59 |
| 5:5:40:PHE:CB | 5:5:73:ARG:HH21 | 2.13 | 0.58 |
| 5:5:185:TRP:HZ3 | 5:5:187:TYR:HB3 | 1.68 | 0.58 |
| 10:C:66:LEU:HG | 10:C:212:GLU:CD | 2.22 | 0.58 |
| 12:E:221:CYS:N | 12:E:231:TYR:CE1 | 2.71 | 0.58 |
| 13:F:91:GLN:NE2 | 13:F:108:ALA:HA | 2.18 | 0.58 |
| 21:N:315:ASN:HA | 21:N:318:LYS:HZ2 | 1.68 | 0.58 |
| 26:S:242:LEU:HD21 | 26:S:279:ILE:CG1 | 2.33 | 0.58 |
| 11:D:96:HIS:CD2 | 11:D:100:LEU:HD22 | 2.38 | 0.58 |
| 12:E:165:TYR:HB3 | 12:E:167:TYR:CE1 | 2.36 | 0.58 |
| 13:F:84:LEU:CD1 | 13:F:112:LEU:HD22 | 2.33 | 0.58 |
| 19:L:145:ARG:HH21 | 19:L:163:THR:C | 2.05 | 0.58 |
| 25:R:154:LEU:CD1 | 25:R:173:THR:OG1 | 2.52 | 0.58 |
| 25:R:167:LYS:NZ | 25:R:199:GLU:HG2 | 2.17 | 0.58 |
| 33:Z:241:THR:HG22 | 33:Z:244:ARG:H | 1.69 | 0.58 |
| 3:3:-2:ASN:HD21 | 3:3:48:ALA:H | 1.49 | 0.58 |
| 15:H:217:GLN:HE21 | 15:H:248:LEU:HD13 | 1.68 | 0.58 |
| 16:I:214:LYS:HZ2 | 16:I:318:ASP:CA | 2.16 | 0.58 |
| 27:T:63:GLU:OE2 | 27:T:89:TYR:OH | 2.19 | 0.58 |
| 33:Z:923:ILE:CD1 | 33:Z:985:LYS:HE2 | 2.25 | 0.58 |
| 4:4:102:LEU:HD21 | 4:4:132:HIS:NE2 | 2.19 | 0.58 |
| 5:5:8:PHE:HE1 | 5:5:12:ILE:C | 2.07 | 0.58 |
| 11:D:193:LYS:HE3 | 11:D:197:ARG:NH2 | 2.17 | 0.58 |
| 11:D:193:LYS:CG | 11:D:197:ARG:NH1 | 2.63 | 0.58 |
| 15:H:284:VAL:CA | 20:M:254:MET:HB3 | 2.32 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:I:96:LEU:O | 16:I:100:ARG:HG3 | 2.03 | 0.58 |
| 18:K:227:ALA:CB | 18:K:268:ILE:HD12 | 2.34 | 0.58 |
| 18:K:280:LYS:HE3 | 18:K:296:LEU:HD22 | 1.86 | 0.58 |
| 19:L:163:THR:HG21 | 19:L:264:ARG:HH22 | 1.68 | 0.58 |
| 19:L:389:ALA:HB2 | 20:M:339:ARG:HH21 | 1.69 | 0.58 |
| 22:O:325:GLU:HB3 | 23:P:364:ARG:NH2 | 2.19 | 0.58 |
| 33:Z:188:ALA:CA | 33:Z:201:LEU:HD11 | 2.33 | 0.58 |
| 33:Z:286:VAL:O | 33:Z:287:ARG:HB2 | 2.01 | 0.58 |
| 33:Z:522:THR:HG23 | 33:Z:559:LYS:NZ | 2.19 | 0.58 |
| 5:5:159:ARG:NH1 | 5:5:200:VAL:HA | 2.13 | 0.58 |
| 6:6:-5:TYR:CE1 | 6:6:97:TYR:CG | 2.92 | 0.58 |
| 6:6:66:TYR:CD2 | 6:6:73:LYS:O | 2.56 | 0.58 |
| 8:A:148:GLU:OE1 | 8:A:230:LYS:HE2 | 2.03 | 0.58 |
| 12:E:138:PHE:HB3 | 12:E:140:VAL:HG12 | 1.86 | 0.58 |
| 14:G:168:ARG:CG | 14:G:172:LYS:HE3 | 2.33 | 0.58 |
| 22:O:250:TRP:HZ2 | 22:O:271:LYS:CB | 2.17 | 0.58 |
| 23:P:263:HIS:HE1 | 23:P:325:ASP:HA | 1.67 | 0.58 |
| 25:R:167:LYS:NZ | 25:R:198:ILE:HB | 2.18 | 0.58 |
| 1:1:3:ILE:HG13 | 1:1:98:ILE:HD12 | 1.85 | 0.58 |
| 9:B:159:TRP:CZ2 | 10:C:57:LEU:HD13 | 2.39 | 0.58 |
| 9:B:159:TRP:HZ3 | 10:C:54:SER:HB2 | 1.69 | 0.58 |
| 12:E:198:LEU:CD1 | 12:E:243:LEU:HD13 | 2.33 | 0.58 |
| 12:E:198:LEU:HD11 | 12:E:243:LEU:HD13 | 1.85 | 0.58 |
| 13:F:145:LEU:HD21 | 13:F:153:VAL:HG13 | 1.84 | 0.58 |
| 14:G:215:ILE:HG22 | 14:G:235:LEU:HD13 | 1.85 | 0.58 |
| 16:I:126:PRO:HB2 | 16:I:128:TYR:HE2 | 1.54 | 0.58 |
| 24:Q:179:LEU:HD21 | 24:Q:217:GLU:HB3 | 1.84 | 0.58 |
| 24:Q:343:LEU:HD11 | 24:Q:368:LEU:CD1 | 2.30 | 0.58 |
| 25:R:258:LEU:CD1 | 25:R:288:SER:HB2 | 2.32 | 0.58 |
| 26:S:188:TYR:HE2 | 26:S:239:ARG:NH1 | 1.94 | 0.58 |
| 28:U:280:ASN:HB2 | 29:V:291:ASN:OD1 | 2.03 | 0.58 |
| 31:X:10:PHE:HE2 | 31:X:101:LEU:CD1 | 2.17 | 0.58 |
| 33:Z:522:THR:HG23 | 33:Z:559:LYS:HZ3 | 1.69 | 0.58 |
| 8:A:34:ALA:O | 8:A:35:THR:HG23 | 2.04 | 0.58 |
| 10:C:98:TYR:HE1 | 10:C:104:GLU:HG3 | 1.68 | 0.58 |
| 14:G:53:ILE:CD1 | 14:G:212:GLU:HB2 | 2.29 | 0.58 |
| 15:H:105:ILE:HD12 | 15:H:169:GLU:OE2 | 2.03 | 0.58 |
| 18:K:272:ASP:HB3 | 19:L:306:MET:HE1 | 0.67 | 0.58 |
| 24:Q:299:MET:HE1 | 24:Q:335:PHE:CE1 | 2.38 | 0.58 |
| 26:S:322:LEU:HD21 | 26:S:349:THR:HG23 | 1.85 | 0.58 |
| 28:U:293:GLU:HG2 | 29:V:277:LYS:NZ | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:177:VAL:HG12 | 3:3:190:TYR:CE1 | 2.38 | 0.58 |
| 6:6:141:LEU:HD12 | 6:6:145:VAL:CG2 | 2.34 | 0.58 |
| 7:7:129:TYR:CE1 | 7:7:134:LEU:CD2 | 2.69 | 0.58 |
| 20:M:289:LYS:HD3 | 20:M:305:MET:HE1 | 1.86 | 0.58 |
| 21:N:353:LEU:H | 21:N:354:PRO:CD | 2.17 | 0.58 |
| 21:N:492:THR:C | 21:N:528:ARG:NH1 | 2.57 | 0.58 |
| 23:P:366:ASN:ND2 | 23:P:373:GLU:CA | 2.60 | 0.58 |
| 24:Q:146:TYR:CD1 | 24:Q:184:VAL:HA | 2.33 | 0.58 |
| 30:W:87:MET:HE1 | 30:W:114:VAL:HG22 | 1.86 | 0.58 |
| 31:X:79:LYS:CD | 31:X:98:PHE:HE2 | 2.16 | 0.58 |
| 33:Z:278:LEU:CG | 33:Z:297:VAL:HG13 | 2.34 | 0.58 |
| 12:E:207:VAL:CA | 15:H:409:ARG:HH12 | 2.17 | 0.58 |
| 13:F:51:ARG:HD3 | 13:F:204:GLU:OE1 | 2.03 | 0.58 |
| 15:H:102:CYS:HB3 | 15:H:105:ILE:HD13 | 1.86 | 0.58 |
| 15:H:105:ILE:HG23 | 15:H:169:GLU:OE2 | 2.04 | 0.58 |
| 22:O:250:TRP:HZ2 | 22:O:271:LYS:HB2 | 1.68 | 0.58 |
| 25:R:283:THR:O | 25:R:289:ILE:HD11 | 2.03 | 0.58 |
| 28:U:50:ASN:HD22 | 28:U:87:GLU:CD | 2.08 | 0.58 |
| 11:D:203:VAL:O | 11:D:204:GLN:HB2 | 2.03 | 0.58 |
| 12:E:31:ILE:CD1 | 12:E:141:ALA:HB2 | 2.34 | 0.58 |
| 12:E:207:VAL:HB | 15:H:409:ARG:NH1 | 2.18 | 0.58 |
| 13:F:18:ARG:NH1 | 13:F:23:GLU:HB2 | 2.18 | 0.58 |
| 14:G:122:HIS:CE1 | 14:G:128:VAL:CG1 | 2.87 | 0.58 |
| 15:H:74:THR:HG22 | 15:H:74:THR:O | 2.04 | 0.58 |
| 16:I:103:PRO:HG3 | 17:J:120:TYR:OH | 2.03 | 0.58 |
| 17:J:39:GLU:CD | 17:J:42:ARG:HH21 | 2.06 | 0.58 |
| 19:L:145:ARG:NH2 | 19:L:163:THR:HA | 2.18 | 0.58 |
| 20:M:203:ARG:HD3 | 20:M:206:LYS:CD | 2.33 | 0.58 |
| 20:M:203:ARG:HD3 | 20:M:206:LYS:NZ | 2.19 | 0.58 |
| 25:R:73:ASN:H | 25:R:76:GLN:NE2 | 2.01 | 0.58 |
| 25:R:107:GLU:CG | 25:R:111:LYS:HE2 | 2.19 | 0.58 |
| 26:S:234:ILE:O | 26:S:238:LEU:HG | 2.04 | 0.58 |
| 26:S:416:GLU:O | 26:S:417:GLN:NE2 | 2.37 | 0.58 |
| 30:W:140:ASP:OD2 | 30:W:190:ILE:HD12 | 2.04 | 0.58 |
| 31:X:67:ILE:HD12 | 31:X:69:ILE:CD1 | 2.29 | 0.58 |
| 33:Z:242:PHE:CB | 33:Z:275:GLN:HG3 | 2.34 | 0.58 |
| 2:2:27:ALA:O | 2:2:28:ASP:OD1 | 2.22 | 0.57 |
| 4:4:66:TYR:CD2 | 10:C:102:TYR:OH | 2.56 | 0.57 |
| 6:6:68:PHE:HZ | 13:F:67:ASP:HA | 1.69 | 0.57 |
| 15:H:206:VAL:HG23 | 15:H:261:ARG:HH21 | 1.69 | 0.57 |
| 15:H:396:MET:CE | 15:H:438:ALA:HB2 | 1.76 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:I:340:ARG:HH12 | 16:I:343:ARG:HG2 | 1.67 | 0.57 |
| 17:J:212:ARG:CZ | 17:J:246:PHE:CE2 | 2.88 | 0.57 |
| 17:J:374:ARG:NH2 | 17:J:381:ASP:OD2 | 2.36 | 0.57 |
| 20:M:119:VAL:HG11 | 20:M:155:ILE:CD1 | 2.31 | 0.57 |
| 22:O:269:LEU:HD23 | 22:O:269:LEU:C | 2.24 | 0.57 |
| 23:P:234:TYR:CE1 | 23:P:270:LEU:HD13 | 2.38 | 0.57 |
| 23:P:264:ILE:CG2 | 23:P:280:LEU:HD11 | 2.34 | 0.57 |
| 27:T:119:THR:CG2 | 27:T:123:HIS:HE1 | 2.12 | 0.57 |
| 1:1:19:ARG:NH2 | 1:1:170:GLY:C | 2.53 | 0.57 |
| 10:C:62:SER:OG | 10:C:231:LYS:HD3 | 2.04 | 0.57 |
| 13:F:50:LYS:HE3 | 13:F:212:SER:HB3 | 1.86 | 0.57 |
| 14:G:11:ASN:HB2 | 14:G:126:ASN:HA | 1.86 | 0.57 |
| 15:H:357:ARG:CZ | 15:H:359:ASN:HD22 | 2.17 | 0.57 |
| 27:T:161:TRP:CE3 | 27:T:162:ASP:OD1 | 2.56 | 0.57 |
| 33:Z:64:TYR:O | 33:Z:68:LEU:HG | 2.04 | 0.57 |
| 33:Z:312:TYR:OH | 33:Z:348:LEU:HD21 | 2.04 | 0.57 |
| 33:Z:497:PHE:CB | 33:Z:533:VAL:HG22 | 2.34 | 0.57 |
| 2:2:50:ALA:CB | 3:3:118:ILE:HG21 | 2.30 | 0.57 |
| 2:2:59:ILE:HD11 | 2:2:86:HIS:CE1 | 2.40 | 0.57 |
| 8:A:72:ILE:HG12 | 8:A:82:VAL:HG22 | 1.87 | 0.57 |
| 10:C:123:THR:CG2 | 10:C:130:PRO:HB3 | 2.34 | 0.57 |
| 16:I:136:VAL:HG11 | 16:I:159:VAL:HG12 | 1.86 | 0.57 |
| 17:J:277:ASN:ND2 | 17:J:309:ARG:CZ | 2.59 | 0.57 |
| 19:L:117:TYR:HE1 | 19:L:131:VAL:HG11 | 1.68 | 0.57 |
| 21:N:328:PHE:CZ | 21:N:693:GLY:HA2 | 2.35 | 0.57 |
| 22:O:4:ASN:HB2 | 22:O:39:PHE:CE1 | 2.39 | 0.57 |
| 23:P:203:ILE:HG21 | 23:P:220:TYR:CZ | 2.39 | 0.57 |
| 27:T:164:LEU:HD21 | 27:T:178:THR:HA | 1.86 | 0.57 |
| 33:Z:321:PHE:CE1 | 33:Z:349:THR:HA | 2.39 | 0.57 |
| 33:Z:553:ARG:NH1 | 33:Z:595:MET:CE | 2.66 | 0.57 |
| 8:A:52:VAL:HG11 | 8:A:203:VAL:HG22 | 1.87 | 0.57 |
| 9:B:245:ASP:HA | 24:Q:95:LYS:HD3 | 1.85 | 0.57 |
| 16:I:102:ASN:HD21 | 17:J:97:ASP:H | 1.52 | 0.57 |
| 16:I:170:VAL:H | 17:J:227:SER:HB3 | 1.70 | 0.57 |
| 16:I:395:MET:CE | 16:I:420:LYS:HE2 | 2.34 | 0.57 |
| 17:J:59:LYS:HG2 | 17:J:63:ARG:NH1 | 2.19 | 0.57 |
| 17:J:115:LEU:HD13 | 17:J:122:LEU:HD23 | 1.86 | 0.57 |
| 17:J:277:ASN:HD21 | 17:J:309:ARG:NH2 | 2.03 | 0.57 |
| 17:J:316:PHE:CG | 17:J:317:PRO:HD2 | 2.39 | 0.57 |
| 27:T:151:TRP:HD1 | 27:T:154:GLU:OE2 | 1.88 | 0.57 |
| 28:U:67:PHE:CZ | 30:W:97:THR:CG2 | 2.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:99:LEU:CB | 33:Z:119:LEU:HD21 | 2.34 | 0.57 |
| 33:Z:748:LEU:CD1 | 33:Z:783:VAL:HA | 2.34 | 0.57 |
| 33:Z:900:LEU:HD22 | 33:Z:903:MET:HE2 | 1.87 | 0.57 |
| 3:3:109:LYS:HE3 | 3:3:125:LYS:HZ3 | 1.69 | 0.57 |
| 13:F:43:HIS:CD2 | 13:F:217:GLY:HA3 | 2.39 | 0.57 |
| 17:J:369:ALA:HB1 | 17:J:374:ARG:HG3 | 1.86 | 0.57 |
| 18:K:211:LEU:HD23 | 18:K:338:ILE:HB | 1.85 | 0.57 |
| 21:N:355:TRP:CH2 | 21:N:356:LEU:CD2 | 2.87 | 0.57 |
| 24:Q:74:LEU:CD2 | 24:Q:104:PHE:HD1 | 2.15 | 0.57 |
| 28:U:54:LEU:HD23 | 28:U:72:TYR:CE2 | 2.39 | 0.57 |
| 28:U:89:LEU:HD23 | 28:U:113:TYR:O | 2.05 | 0.57 |
| 6:6:39:ASP:O | 6:6:40:ASN:CB | 2.50 | 0.57 |
| 9:B:158:PRO:O | 10:C:57:LEU:HD12 | 2.05 | 0.57 |
| 10:C:59:GLN:O | 10:C:232:PRO:HG2 | 2.05 | 0.57 |
| 11:D:120:TYR:CE2 | 11:D:129:PHE:CZ | 2.93 | 0.57 |
| 13:F:12:THR:HG21 | 13:F:19:LEU:HD11 | 1.85 | 0.57 |
| 13:F:65:LYS:HE2 | 13:F:222:PHE:CD2 | 2.37 | 0.57 |
| 15:H:244:LYS:HE3 | 15:H:340:LEU:O | 2.04 | 0.57 |
| 16:I:104:LEU:HD23 | 16:I:149:LEU:O | 2.01 | 0.57 |
| 18:K:216:GLY:HA3 | 19:L:342:ARG:HH21 | 1.68 | 0.57 |
| 18:K:393:ARG:NH2 | 19:L:345:ARG:HH12 | 2.03 | 0.57 |
| 19:L:401:PHE:HD1 | 19:L:404:ARG:CZ | 2.16 | 0.57 |
| 22:O:30:GLU:HB3 | 22:O:58:ARG:NH1 | 2.20 | 0.57 |
| 22:O:228:TYR:HA | 22:O:290:LYS:HZ3 | 1.67 | 0.57 |
| 23:P:272:PRO:C | 23:P:273:TYR:CD1 | 2.77 | 0.57 |
| 24:Q:6:SER:O | 24:Q:10:GLU:HG3 | 2.04 | 0.57 |
| 24:Q:88:PHE:CG | 24:Q:89:ALA:N | 2.73 | 0.57 |
| 25:R:140:TYR:HD2 | 25:R:141:TYR:CD1 | 2.22 | 0.57 |
| 26:S:151:GLU:OE1 | 26:S:154:GLN:HB2 | 2.04 | 0.57 |
| 33:Z:233:LEU:C | 33:Z:271:ILE:HD11 | 2.24 | 0.57 |
| 1:1:83:LYS:HZ3 | 1:1:118:SER:HA | 0.77 | 0.57 |
| 2:2:196:ARG:HH21 | 2:2:199:LYS:HD3 | 1.69 | 0.57 |
| 3:3:42:LEU:HD21 | 3:3:44:ILE:HD11 | 1.86 | 0.57 |
| 5:5:40:PHE:CG | 5:5:73:ARG:NH2 | 2.73 | 0.57 |
| 9:B:48:GLU:HG2 | 9:B:196:LEU:HD11 | 1.87 | 0.57 |
| 10:C:50:ARG:NH2 | 10:C:209:ASP:HA | 2.19 | 0.57 |
| 13:F:65:LYS:CB | 13:F:222:PHE:CE2 | 2.87 | 0.57 |
| 25:R:70:TYR:OH | 25:R:76:GLN:CA | 2.52 | 0.57 |
| 1:1:30:VAL:CG2 | 1:1:172:VAL:HG21 | 2.35 | 0.57 |
| 3:3:68:LYS:HG2 | 10:C:92:ARG:HH11 | 1.70 | 0.57 |
| 5:5:162:LEU:CD2 | 5:5:200:VAL:HG21 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:41:ASN:OD1 | 8:A:173:PRO:HD2 | 2.05 | 0.57 |
| 8:A:163:TYR:O | 8:A:164:VAL:HG13 | 2.04 | 0.57 |
| 19:L:165:PRO:HA | 19:L:265:GLU:OE2 | 2.04 | 0.57 |
| 21:N:331:ALA:HB2 | 21:N:697:PHE:CD1 | 2.39 | 0.57 |
| 24:Q:148:LYS:O | 24:Q:149:LYS:HB2 | 2.04 | 0.57 |
| 24:Q:268:SER:O | 24:Q:272:LEU:HG | 2.04 | 0.57 |
| 25:R:107:GLU:HG2 | 25:R:111:LYS:CE | 2.21 | 0.57 |
| 25:R:203:ASP:OD1 | 25:R:204:TRP:N | 2.38 | 0.57 |
| 28:U:21:HIS:CE1 | 28:U:93:TYR:CZ | 2.92 | 0.57 |
| 28:U:67:PHE:CE2 | 30:W:100:HIS:CE1 | 2.92 | 0.57 |
| 31:X:90:VAL:HB | 31:X:96:ARG:HD3 | 1.86 | 0.57 |
| 33:Z:71:LEU:HD23 | 33:Z:118:VAL:HG11 | 1.85 | 0.57 |
| 33:Z:321:PHE:CZ | 33:Z:349:THR:HA | 2.40 | 0.57 |
| 1:1:75:THR:HG22 | 1:1:111:TYR:HD1 | 1.69 | 0.57 |
| 10:C:140:TYR:HD1 | 10:C:146:TYR:CE1 | 2.23 | 0.57 |
| 17:J:218:LEU:HD12 | 17:J:229:MET:HB3 | 1.86 | 0.57 |
| 20:M:56:ASN:O | 20:M:60:GLU:HG2 | 2.04 | 0.57 |
| 21:N:31:VAL:CG2 | 21:N:35:LEU:HD12 | 2.34 | 0.57 |
| 21:N:114:SER:HA | 21:N:161:TYR:CE2 | 2.40 | 0.57 |
| 21:N:593:PHE:HA | 21:N:596:LEU:HG | 1.86 | 0.57 |
| 30:W:186:ALA:HB1 | 30:W:191:ILE:HG23 | 1.85 | 0.57 |
| 31:X:14:VAL:HG13 | 31:X:50:TRP:CE2 | 2.39 | 0.57 |
| 33:Z:75:ILE:CG2 | 33:Z:121:ILE:CG2 | 2.56 | 0.57 |
| 7:7:131:SER:OG | 7:7:132:PRO:HD2 | 2.04 | 0.57 |
| 14:G:200:TYR:CZ | 14:G:246:ILE:HG22 | 2.39 | 0.57 |
| 18:K:393:ARG:HH21 | 19:L:345:ARG:HH12 | 1.51 | 0.57 |
| 21:N:657:MET:HB3 | 21:N:682:PHE:CE1 | 2.40 | 0.57 |
| 21:N:717:LEU:O | 21:N:725:LEU:HD22 | 2.04 | 0.57 |
| 22:O:250:TRP:HA | 22:O:269:LEU:HG | 1.86 | 0.57 |
| 25:R:50:VAL:HG12 | 25:R:54:ILE:HD12 | 1.84 | 0.57 |
| 27:T:11:LEU:HD22 | 27:T:30:ILE:CD1 | 2.30 | 0.57 |
| 1:1:-4:VAL:HG12 | 1:1:49:ALA:CB | 2.35 | 0.56 |
| 3:3:37:TYR:CZ | 3:3:59:ARG:CB | 2.88 | 0.56 |
| 6:6:29:ARG:HA | 6:6:191:ASP:OD2 | 2.04 | 0.56 |
| 6:6:85:GLN:HG3 | 6:6:122:TYR:CD1 | 2.35 | 0.56 |
| 16:I:246:ARG:HH21 | 17:J:274:GLU:HG2 | 1.70 | 0.56 |
| 19:L:365:THR:OG1 | 19:L:376:PHE:CZ | 2.57 | 0.56 |
| 20:M:167:VAL:HG23 | 20:M:269:LEU:HD12 | 1.86 | 0.56 |
| 20:M:203:ARG:NH1 | 20:M:206:LYS:NZ | 2.53 | 0.56 |
| 21:N:162:ARG:HE | 21:N:164:ASP:HB3 | 1.70 | 0.56 |
| 21:N:353:LEU:H | 21:N:354:PRO:HD3 | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:O:250:TRP:CG | 22:O:269:LEU:CD2 | 2.88 | 0.56 |
| 25:R:335:ARG:HD3 | 25:R:376:GLN:HB3 | 1.84 | 0.56 |
| 27:T:119:THR:HG23 | 27:T:123:HIS:CE1 | 2.38 | 0.56 |
| 28:U:5:HIS:ND1 | 28:U:6:GLU:O | 2.37 | 0.56 |
| 33:Z:354:PRO:O | 33:Z:357:ILE:HG12 | 2.05 | 0.56 |
| 33:Z:612:GLY:N | 33:Z:746:ILE:HG23 | 2.20 | 0.56 |
| 1:1:5:ALA:HB2 | 1:1:14:LEU:HG | 1.87 | 0.56 |
| 1:1:12:VAL:HG22 | 1:1:14:LEU:HD12 | 1.86 | 0.56 |
| 1:1:83:LYS:NZ | 1:1:117:GLY:O | 2.38 | 0.56 |
| 1:1:173:ILE:HD12 | 1:1:193:TYR:CB | 2.35 | 0.56 |
| 15:H:97:LEU:HB2 | 15:H:173:ARG:HD3 | 1.86 | 0.56 |
| 17:J:25:GLN:NE2 | 21:N:99:GLU:HB3 | 2.20 | 0.56 |
| 20:M:290:ARG:CD | 20:M:294:GLU:HB3 | 2.31 | 0.56 |
| 22:O:260:VAL:HG11 | 22:O:262:ASP:OD2 | 2.05 | 0.56 |
| 23:P:288:ASN:O | 23:P:289:ASN:HB2 | 2.06 | 0.56 |
| 25:R:170:VAL:HG11 | 25:R:194:VAL:CG2 | 2.35 | 0.56 |
| 28:U:83:ILE:HD11 | 29:V:87:PHE:HZ | 1.69 | 0.56 |
| 33:Z:269:TYR:OH | 33:Z:293:MET:HB3 | 2.04 | 0.56 |
| 1:1:10:ASP:O | 1:1:102:TYR:HE1 | 1.87 | 0.56 |
| 1:1:11:GLY:HA3 | 1:1:102:TYR:CD1 | 2.41 | 0.56 |
| 1:1:13:ILE:HD12 | 1:1:151:THR:CG2 | 2.35 | 0.56 |
| 1:1:82:PHE:CB | 1:1:113:ILE:HD13 | 2.36 | 0.56 |
| 1:1:83:LYS:CD | 1:1:119:VAL:CG2 | 2.69 | 0.56 |
| 3:3:53:THR:O | 3:3:57:MET:HG2 | 2.06 | 0.56 |
| 5:5:7:ARG:HE | 5:5:110:PRO:HG2 | 1.69 | 0.56 |
| 11:D:67:ILE:HD13 | 11:D:109:LEU:HD21 | 1.86 | 0.56 |
| 12:E:14:THR:HG21 | 12:E:22:PHE:HE2 | 1.69 | 0.56 |
| 13:F:3:ARG:HE | 15:H:359:ASN:CG | 2.08 | 0.56 |
| 13:F:87:TYR:HE2 | 13:F:128:TYR:OH | 1.88 | 0.56 |
| 14:G:111:PHE:HA | 14:G:114:ARG:CZ | 2.36 | 0.56 |
| 15:H:62:ARG:HB2 | 16:I:134:SER:HB2 | 1.86 | 0.56 |
| 16:I:257:LEU:HD12 | 16:I:258:GLY:N | 2.21 | 0.56 |
| 17:J:367:MET:O | 17:J:371:ARG:HG3 | 2.05 | 0.56 |
| 19:L:82:ARG:HG2 | 19:L:86:LYS:HE3 | 1.86 | 0.56 |
| 21:N:602:VAL:CG1 | 21:N:625:LEU:HD23 | 2.36 | 0.56 |
| 22:O:131:SER:O | 22:O:135:ARG:HG3 | 2.05 | 0.56 |
| 22:O:222:LEU:HB3 | 22:O:280:LEU:HD11 | 1.87 | 0.56 |
| 24:Q:100:LEU:HD23 | 24:Q:103:LYS:HD2 | 1.87 | 0.56 |
| 25:R:134:TRP:CZ3 | 25:R:156:LYS:NZ | 2.70 | 0.56 |
| 25:R:137:LEU:CB | 25:R:141:TYR:CE2 | 2.80 | 0.56 |
| 25:R:167:LYS:HZ1 | 25:R:198:ILE:HB | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:S:267:SER:OG | 26:S:305:LYS:HE3 | 2.05 | 0.56 |
| 27:T:28:PRO:HB2 | 27:T:29:PRO:HD3 | 1.88 | 0.56 |
| 28:U:50:ASN:ND2 | 28:U:87:GLU:OE2 | 2.37 | 0.56 |
| 29:V:53:MET:CG | 29:V:108:TYR:HD1 | 2.19 | 0.56 |
| 33:Z:64:TYR:CE1 | 33:Z:68:LEU:HD11 | 2.40 | 0.56 |
| 33:Z:221:VAL:CG2 | 33:Z:245:VAL:HG13 | 2.34 | 0.56 |
| 33:Z:320:SER:O | 33:Z:326:VAL:HG11 | 2.05 | 0.56 |
| 33:Z:912:PHE:CE2 | 33:Z:980:VAL:HG23 | 2.39 | 0.56 |
| 33:Z:929:VAL:CG2 | 33:Z:957:LEU:HD23 | 2.35 | 0.56 |
| 10:C:140:TYR:HD1 | 10:C:146:TYR:CD1 | 2.23 | 0.56 |
| 10:C:177:GLN:HE22 | 11:D:52:LEU:HD22 | 1.70 | 0.56 |
| 18:K:67:TYR:HD1 | 21:N:572:LEU:HB3 | 1.70 | 0.56 |
| 20:M:170:MET:SD | 20:M:244:LEU:HD22 | 2.45 | 0.56 |
| 24:Q:61:LEU:HD11 | 24:Q:65:TYR:OH | 2.06 | 0.56 |
| 27:T:27:LEU:O | 27:T:31:LYS:HG3 | 2.04 | 0.56 |
| 27:T:62:LEU:HB2 | 27:T:85:LEU:HD13 | 1.87 | 0.56 |
| 4:4:117:GLN:HE22 | 4:4:130:GLY:HA3 | 1.69 | 0.56 |
| 5:5:144:TYR:O | 5:5:145:LYS:HB2 | 2.05 | 0.56 |
| 7:7:178:TYR:HD2 | 7:7:179:ARG:HG3 | 1.70 | 0.56 |
| 8:A:128:TYR:CD2 | 8:A:134:MET:HE2 | 2.41 | 0.56 |
| 8:A:162:TYR:CZ | 8:A:164:VAL:CG1 | 2.88 | 0.56 |
| 13:F:157:TYR:HH | 14:G:59:VAL:HG23 | 1.70 | 0.56 |
| 13:F:159:THR:CA | 13:F:169:LYS:HZ2 | 2.16 | 0.56 |
| 15:H:308:PHE:CD1 | 15:H:351:VAL:HG13 | 2.40 | 0.56 |
| 15:H:428:MET:HG3 | 16:I:346:ARG:HH21 | 1.70 | 0.56 |
| 19:L:386:PHE:HD1 | 19:L:390:ASP:HB3 | 1.70 | 0.56 |
| 20:M:424:ALA:O | 20:M:425:ARG:HB2 | 2.05 | 0.56 |
| 24:Q:74:LEU:HD21 | 24:Q:104:PHE:HD1 | 1.69 | 0.56 |
| 24:Q:81:SER:HA | 24:Q:84:TYR:CD2 | 2.41 | 0.56 |
| 24:Q:343:LEU:HD12 | 24:Q:366:ILE:HD11 | 1.88 | 0.56 |
| 33:Z:763:HIS:C | 33:Z:766:HIS:CE1 | 2.79 | 0.56 |
| 3:3:1:GLY:HA3 | 3:3:33:LYS:NZ | 2.20 | 0.56 |
| 5:5:8:PHE:CZ | 5:5:13:ILE:CG1 | 2.88 | 0.56 |
| 10:C:140:TYR:CD1 | 10:C:146:TYR:CE1 | 2.93 | 0.56 |
| 13:F:87:TYR:CE2 | 13:F:128:TYR:OH | 2.59 | 0.56 |
| 15:H:50:LYS:NZ | 33:Z:791:LYS:HG2 | 2.21 | 0.56 |
| 15:H:249:TYR:HE2 | 15:H:374:LYS:HG2 | 1.70 | 0.56 |
| 17:J:77:LYS:HG2 | 17:J:78:ILE:O | 2.06 | 0.56 |
| 17:J:96:VAL:HG11 | 17:J:115:LEU:HD21 | 1.87 | 0.56 |
| 19:L:163:THR:CG2 | 19:L:264:ARG:HH22 | 2.19 | 0.56 |
| 22:O:41:LEU:H | 22:O:58:ARG:HD2 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:P:431:HIS:CE1 | 28:U:137:TYR:HE1 | 2.24 | 0.56 |
| 24:Q:220:LEU:HD12 | 24:Q:239:PHE:HE1 | 1.69 | 0.56 |
| 25:R:137:LEU:HD22 | 25:R:141:TYR:CE2 | 2.41 | 0.56 |
| 26:S:294:ILE:CG1 | 26:S:317:HIS:HE1 | 2.18 | 0.56 |
| 33:Z:371:SER:O | 33:Z:372:ALA:HB2 | 2.05 | 0.56 |
| 5:5:158:LYS:HB2 | 5:5:177:LEU:HD11 | 1.87 | 0.56 |
| 6:6:66:TYR:OH | 6:6:73:LYS:CD | 2.54 | 0.56 |
| 12:E:85:ALA:HB2 | 12:E:140:VAL:HG21 | 1.88 | 0.56 |
| 14:G:168:ARG:HG3 | 14:G:172:LYS:HE3 | 1.88 | 0.56 |
| 16:I:81:ILE:HG12 | 33:Z:766:HIS:CE1 | 2.39 | 0.56 |
| 20:M:82:VAL:HG21 | 20:M:140:LEU:HD22 | 1.87 | 0.56 |
| 20:M:203:ARG:CZ | 20:M:206:LYS:NZ | 2.69 | 0.56 |
| 21:N:214:LEU:HD23 | 21:N:217:MET:HE2 | 1.86 | 0.56 |
| 21:N:749:LEU:HD23 | 21:N:753:PHE:HZ | 1.70 | 0.56 |
| 24:Q:355:GLU:HG2 | 24:Q:397:LEU:HG | 1.87 | 0.56 |
| 27:T:185:ILE:HG22 | 27:T:189:ILE:CD1 | 2.35 | 0.56 |
| 30:W:186:ALA:HA | 30:W:191:ILE:HG22 | 0.65 | 0.56 |
| 31:X:94:ASN:O | 31:X:95:GLU:HB2 | 2.05 | 0.56 |
| 2:2:6:VAL:HG21 | 2:2:154:LEU:HD23 | 1.87 | 0.56 |
| 3:3:150:GLU:HB3 | 3:3:151:PRO:HD2 | 1.88 | 0.56 |
| 4:4:166:GLU:HB3 | 4:4:170:ARG:NH2 | 2.15 | 0.56 |
| 8:A:75:ILE:HD13 | 8:A:117:LEU:CD2 | 2.36 | 0.56 |
| 15:H:173:ARG:NH2 | 16:I:119:ILE:HG21 | 2.21 | 0.56 |
| 15:H:295:PHE:HZ | 15:H:336:LEU:CD1 | 2.17 | 0.56 |
| 16:I:326:MET:SD | 16:I:344:ILE:HD11 | 2.46 | 0.56 |
| 17:J:337:LEU:CD2 | 17:J:382:PHE:CZ | 2.47 | 0.56 |
| 18:K:161:MET:CE | 18:K:257:VAL:HG21 | 2.36 | 0.56 |
| 18:K:184:ILE:HD12 | 18:K:222:LEU:HD13 | 1.86 | 0.56 |
| 22:O:217:LEU:CD1 | 22:O:238:ILE:HG21 | 2.35 | 0.56 |
| 23:P:130:ILE:HG22 | 23:P:136:ARG:NH2 | 2.21 | 0.56 |
| 23:P:131:PHE:CB | 23:P:136:ARG:HH11 | 2.18 | 0.56 |
| 23:P:269:VAL:O | 23:P:344:ARG:HG3 | 2.06 | 0.56 |
| 24:Q:9:GLU:HG2 | 24:Q:13:ARG:HH12 | 1.70 | 0.56 |
| 27:T:253:GLU:O | 27:T:254:ASP:CB | 2.54 | 0.56 |
| 30:W:12:ASN:H | 30:W:55:ALA:HB3 | 1.70 | 0.56 |
| 33:Z:317:GLN:HE22 | 33:Z:874:ASN:HA | 1.71 | 0.56 |
| 4:4:143:LEU:HD23 | 4:4:159:LEU:HD21 | 1.85 | 0.56 |
| 8:A:83:VAL:HG22 | 8:A:141:LEU:HD22 | 1.87 | 0.56 |
| 10:C:152:ASN:HB2 | 10:C:153:PRO:HD2 | 1.88 | 0.56 |
| 13:F:105:VAL:CG2 | 13:F:145:LEU:HD13 | 2.21 | 0.56 |
| 21:N:220:CYS:SG | 21:N:225:LEU:HD11 | 2.46 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:U:62:ASN:ND2 | 28:U:65:VAL:HG23 | 2.21 | 0.56 |
| 1:1:31:THR:HG21 | 1:1:33:LYS:HE2 | 1.87 | 0.56 |
| 11:D:111:ARG:HG2 | 11:D:156:TYR:OH | 2.06 | 0.56 |
| 11:D:193:LYS:NZ | 11:D:236:ILE:HG13 | 2.21 | 0.56 |
| 14:G:183:PRO:C | 14:G:184:GLU:HG2 | 2.25 | 0.56 |
| 15:H:328:GLU:HA | 15:H:331:ARG:NH2 | 2.21 | 0.56 |
| 17:J:316:PHE:CD1 | 17:J:317:PRO:HD2 | 2.41 | 0.56 |
| 18:K:137:VAL:HB | 18:K:146:LEU:HD13 | 1.87 | 0.56 |
| 18:K:326:PRO:O | 18:K:330:ARG:HG3 | 2.06 | 0.56 |
| 20:M:62:ILE:HG13 | 20:M:66:LYS:HE3 | 1.87 | 0.56 |
| 20:M:81:ASN:HB2 | 20:M:163:PHE:CD1 | 2.41 | 0.56 |
| 21:N:768:ILE:HD13 | 21:N:871:MET:HE3 | 1.87 | 0.56 |
| 22:O:102:LEU:C | 22:O:103:LYS:HG2 | 2.27 | 0.56 |
| 22:O:179:PHE:HB3 | 22:O:188:PHE:HB2 | 1.86 | 0.56 |
| 24:Q:385:ILE:HG22 | 24:Q:386:PHE:CE1 | 2.40 | 0.56 |
| 25:R:252:TYR:CE1 | 25:R:319:CYS:SG | 2.96 | 0.56 |
| 27:T:86:LYS:CE | 27:T:128:TYR:CD2 | 2.81 | 0.56 |
| 27:T:194:GLU:HB2 | 27:T:226:TRP:HZ2 | 1.71 | 0.56 |
| 1:1:-8:LYS:HZ3 | 2:2:117:GLY:CA | 2.08 | 0.55 |
| 1:1:193:TYR:CD1 | 1:1:193:TYR:C | 2.79 | 0.55 |
| 16:I:117:HIS:HB3 | 16:I:129:TYR:O | 2.06 | 0.55 |
| 16:I:222:TYR:OH | 16:I:349:LEU:CB | 2.43 | 0.55 |
| 21:N:338:PHE:CZ | 21:N:749:LEU:HD23 | 2.41 | 0.55 |
| 21:N:777:ALA:HA | 21:N:878:GLN:HE21 | 1.71 | 0.55 |
| 22:O:15:ARG:HB3 | 30:W:20:ASP:OD1 | 2.07 | 0.55 |
| 24:Q:264:TYR:CZ | 24:Q:330:LEU:HD23 | 2.41 | 0.55 |
| 26:S:257:LEU:CD2 | 26:S:272:TYR:CE1 | 2.89 | 0.55 |
| 26:S:258:GLU:O | 26:S:259:TYR:CD1 | 2.59 | 0.55 |
| 26:S:452:TYR:HA | 26:S:456:ASP:OD2 | 2.05 | 0.55 |
| 27:T:185:ILE:HG22 | 27:T:189:ILE:HD12 | 1.88 | 0.55 |
| 29:V:71:MET:CE | 29:V:83:VAL:HG13 | 2.35 | 0.55 |
| 3:3:89:ARG:HB3 | 3:3:94:TYR:CD1 | 2.41 | 0.55 |
| 3:3:109:LYS:HG2 | 3:3:110:PRO:O | 2.07 | 0.55 |
| 4:4:17:SER:HB3 | 4:4:33:LYS:CE | 2.37 | 0.55 |
| 6:6:-5:TYR:HE1 | 6:6:97:TYR:HB3 | 1.71 | 0.55 |
| 8:A:19:PHE:HA | 8:A:25:LEU:CD2 | 2.34 | 0.55 |
| 13:F:101:ARG:CZ | 13:F:103:LEU:HA | 2.32 | 0.55 |
| 15:H:340:LEU:HD13 | 15:H:370:ARG:CG | 2.25 | 0.55 |
| 19:L:389:ALA:HB1 | 20:M:339:ARG:HE | 1.72 | 0.55 |
| 22:O:69:PHE:CE2 | 22:O:73:ILE:O | 2.60 | 0.55 |
| 24:Q:86:MET:SD | 24:Q:93:THR:HG21 | 2.46 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:425:GLN:HB3 | 29:V:269:ARG:HG2 | 1.86 | 0.55 |
| 25:R:137:LEU:O | 25:R:141:TYR:HD2 | 1.85 | 0.55 |
| 26:S:286:TYR:CE1 | 26:S:323:LEU:HD13 | 2.39 | 0.55 |
| 33:Z:168:GLN:OE1 | 33:Z:195:PHE:CE1 | 2.59 | 0.55 |
| 6:6:141:LEU:CD1 | 6:6:145:VAL:HG21 | 2.37 | 0.55 |
| 8:A:75:ILE:HD13 | 8:A:117:LEU:HD21 | 1.87 | 0.55 |
| 8:A:163:TYR:O | 8:A:164:VAL:CG1 | 2.54 | 0.55 |
| 9:B:39:ALA:C | 9:B:40:THR:HG23 | 2.26 | 0.55 |
| 10:C:65:LYS:HA | 10:C:67:TYR:HE1 | 1.71 | 0.55 |
| 11:D:146:LYS:HE2 | 11:D:148:TYR:HE2 | 1.71 | 0.55 |
| 15:H:365:LEU:HD22 | 15:H:370:ARG:HH22 | 1.70 | 0.55 |
| 17:J:331:HIS:CE1 | 17:J:359:LYS:HE2 | 2.41 | 0.55 |
| 21:N:308:ASN:HB2 | 21:N:711:ARG:HD2 | 1.88 | 0.55 |
| 25:R:266:LEU:C | 25:R:266:LEU:HD23 | 2.27 | 0.55 |
| 31:X:66:LEU:CD2 | 31:X:97:TYR:CD1 | 2.89 | 0.55 |
| 33:Z:149:TRP:CD1 | 33:Z:214:HIS:CE1 | 2.95 | 0.55 |
| 33:Z:973:TYR:HA | 33:Z:984:LYS:HD3 | 1.88 | 0.55 |
| 4:4:37:LEU:CD1 | 4:4:60:GLN:HA | 2.37 | 0.55 |
| 10:C:3:SER:CB | 11:D:6:ARG:HH21 | 2.18 | 0.55 |
| 12:E:15:PHE:HE1 | 13:F:126:ARG:HE | 1.54 | 0.55 |
| 13:F:117:GLN:HG3 | 13:F:121:GLN:NE2 | 2.21 | 0.55 |
| 15:H:343:PHE:HZ | 20:M:233:ARG:NH2 | 2.04 | 0.55 |
| 17:J:62:LEU:CD1 | 18:K:89:ILE:HG13 | 2.27 | 0.55 |
| 17:J:219:VAL:HB | 18:K:281:ARG:CG | 2.36 | 0.55 |
| 18:K:258:PHE:HB2 | 18:K:302:GLN:OE1 | 2.06 | 0.55 |
| 23:P:416:SER:OG | 29:V:245:VAL:HG22 | 2.07 | 0.55 |
| 24:Q:426:LEU:CD2 | 28:U:293:GLU:OE1 | 2.53 | 0.55 |
| 28:U:65:VAL:HG12 | 30:W:96:LEU:HD11 | 1.86 | 0.55 |
| 4:4:17:SER:HB3 | 4:4:33:LYS:HE2 | 1.89 | 0.55 |
| 11:D:193:LYS:HZ3 | 11:D:235:GLN:HB2 | 1.71 | 0.55 |
| 16:I:377:LEU:O | 16:I:381:VAL:HG23 | 2.06 | 0.55 |
| 21:N:406:TYR:OH | 21:N:748:PHE:HE1 | 1.76 | 0.55 |
| 22:O:157:LEU:HD22 | 22:O:171:PHE:CG | 2.41 | 0.55 |
| 24:Q:167:LYS:O | 24:Q:168:LEU:HD23 | 2.06 | 0.55 |
| 25:R:354:ALA:HA | 25:R:364:LEU:HD22 | 1.88 | 0.55 |
| 26:S:323:LEU:CD2 | 26:S:383:LEU:HD23 | 2.37 | 0.55 |
| 27:T:186:ARG:NH1 | 27:T:220:PHE:HE2 | 2.00 | 0.55 |
| 30:W:25:ARG:NH1 | 30:W:144:PHE:CD2 | 2.61 | 0.55 |
| 33:Z:205:LEU:HA | 33:Z:236:PHE:CZ | 2.41 | 0.55 |
| 1:1:82:PHE:HB3 | 1:1:113:ILE:HD13 | 1.88 | 0.55 |
| 7:7:8:TYR:CZ | 7:7:11:GLY:HA3 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:7:92:MET:CE | 7:7:122:VAL:HG22 | 2.37 | 0.55 |
| 9:B:75:TYR:CD1 | 9:B:82:TYR:CD1 | 2.94 | 0.55 |
| 10:C:136:ILE:HD11 | 10:C:165:VAL:CG2 | 2.36 | 0.55 |
| 13:F:206:LEU:HD21 | 13:F:211:LEU:HD11 | 1.88 | 0.55 |
| 18:K:258:PHE:HZ | 18:K:299:LEU:CD1 | 2.19 | 0.55 |
| 19:L:178:ILE:HD13 | 19:L:230:LEU:HD23 | 1.87 | 0.55 |
| 21:N:43:LEU:HD11 | 21:N:69:TYR:CE1 | 2.42 | 0.55 |
| 21:N:588:VAL:CG1 | 21:N:621:THR:CG2 | 2.57 | 0.55 |
| 24:Q:74:LEU:HD21 | 24:Q:104:PHE:CD1 | 2.42 | 0.55 |
| 33:Z:92:LEU:HD23 | 33:Z:122:LEU:HD13 | 1.88 | 0.55 |
| 1:1:17:ASP:HB3 | 1:1:163:ILE:HD11 | 1.89 | 0.55 |
| 2:2:99:ILE:HG12 | 2:2:127:LEU:HD12 | 1.88 | 0.55 |
| 2:2:223:ILE:HG12 | 10:C:222:ASP:OD2 | 2.06 | 0.55 |
| 3:3:6:MET:HE1 | 3:3:158:ILE:HA | 1.87 | 0.55 |
| 6:6:91:LYS:CB | 6:6:96:TYR:HE1 | 2.00 | 0.55 |
| 11:D:17:ILE:CG2 | 11:D:19:GLN:HG2 | 2.36 | 0.55 |
| 13:F:145:LEU:HD23 | 13:F:146:GLU:C | 2.26 | 0.55 |
| 17:J:27:ILE:HG21 | 18:K:50:LYS:HE2 | 1.87 | 0.55 |
| 17:J:223:ILE:O | 17:J:225:GLU:N | 2.40 | 0.55 |
| 19:L:117:TYR:HE1 | 19:L:131:VAL:CG1 | 2.19 | 0.55 |
| 19:L:145:ARG:NH2 | 19:L:163:THR:CA | 2.68 | 0.55 |
| 20:M:431:SER:O | 20:M:432:PHE:CD1 | 2.59 | 0.55 |
| 21:N:325:PHE:H | 29:V:185:ILE:HG21 | 1.72 | 0.55 |
| 21:N:749:LEU:CD2 | 21:N:753:PHE:HZ | 2.19 | 0.55 |
| 23:P:425:HIS:HA | 28:U:228:LYS:HZ1 | 1.71 | 0.55 |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:HD21 | 1.71 | 0.55 |
| 26:S:286:TYR:HB3 | 26:S:324:MET:HB3 | 1.89 | 0.55 |
| 27:T:103:SER:HB3 | 27:T:141:LEU:HD12 | 1.89 | 0.55 |
| 28:U:104:LEU:HD11 | 28:U:152:LYS:HD2 | 1.88 | 0.55 |
| 29:V:127:LYS:HE3 | 29:V:194:ARG:CZ | 2.37 | 0.55 |
| 8:A:30:TYR:C | 14:G:14:PHE:CE1 | 2.80 | 0.55 |
| 12:E:68:VAL:HG12 | 12:E:93:ARG:HH21 | 1.71 | 0.55 |
| 12:E:109:VAL:HG11 | 12:E:156:PHE:CD1 | 2.42 | 0.55 |
| 13:F:47:VAL:HG21 | 13:F:193:GLY:HA3 | 1.89 | 0.55 |
| 14:G:233:ASP:O | 14:G:237:GLU:HG3 | 2.06 | 0.55 |
| 15:H:345:PRO:HD2 | 15:H:349:ILE:HD12 | 1.87 | 0.55 |
| 18:K:395:VAL:HG13 | 19:L:206:ILE:HG22 | 1.88 | 0.55 |
| 21:N:355:TRP:CZ3 | 21:N:356:LEU:HD23 | 2.41 | 0.55 |
| 22:O:250:TRP:CZ2 | 22:O:271:LYS:HG3 | 2.41 | 0.55 |
| 25:R:170:VAL:HG11 | 25:R:194:VAL:HG22 | 1.89 | 0.55 |
| 28:U:83:ILE:HG22 | 28:U:84:ASN:ND2 | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:U:92:TRP:CE2 | 28:U:120:LEU:HG | 2.41 | 0.55 |
| 33:Z:56:LEU:CD2 | 33:Z:68:LEU:CD2 | 2.79 | 0.55 |
| 4:4:84:ARG:HD2 | 4:4:124:LYS:HB3 | 1.89 | 0.55 |
| 8:A:83:VAL:HG22 | 8:A:141:LEU:HD23 | 1.89 | 0.55 |
| 15:H:326:ASP:HA | 15:H:329:VAL:CG2 | 2.37 | 0.55 |
| 16:I:208:TYR:CD1 | 16:I:208:TYR:C | 2.80 | 0.55 |
| 20:M:385:GLU:O | 20:M:385:GLU:OE1 | 2.25 | 0.55 |
| 21:N:358:LYS:HD2 | 29:V:183:ALA:HA | 1.88 | 0.55 |
| 23:P:95:TYR:CD2 | 23:P:96:MET:HE3 | 2.28 | 0.55 |
| 23:P:271:SER:O | 23:P:344:ARG:CD | 2.55 | 0.55 |
| 23:P:425:HIS:CB | 28:U:228:LYS:HZ1 | 2.20 | 0.55 |
| 25:R:167:LYS:HZ3 | 25:R:199:GLU:HG2 | 1.71 | 0.55 |
| 25:R:251:THR:O | 25:R:255:VAL:HG23 | 2.06 | 0.55 |
| 28:U:83:ILE:HD11 | 29:V:87:PHE:CZ | 2.41 | 0.55 |
| 30:W:180:LEU:HD13 | 30:W:182:TYR:HE1 | 1.72 | 0.55 |
| 33:Z:497:PHE:CZ | 33:Z:505:VAL:HG12 | 2.41 | 0.55 |
| 33:Z:549:ASN:HD22 | 33:Z:562:TRP:HH2 | 1.53 | 0.55 |
| 33:Z:604:GLY:O | 33:Z:608:TYR:CD2 | 2.57 | 0.55 |
| 1:1:75:THR:CG2 | 1:1:111:TYR:HD1 | 2.20 | 0.55 |
| 8:A:128:TYR:CE1 | 8:A:134:MET:CE | 2.90 | 0.55 |
| 9:B:43:VAL:CG1 | 9:B:137:ALA:HB1 | 2.36 | 0.55 |
| 10:C:13:PHE:HA | 10:C:19:LEU:HD23 | 1.88 | 0.55 |
| 16:I:340:ARG:HH12 | 16:I:343:ARG:CG | 2.19 | 0.55 |
| 17:J:33:LYS:O | 17:J:37:LYS:HG2 | 2.07 | 0.55 |
| 18:K:389:GLU:HB3 | 18:K:414:GLN:NE2 | 2.22 | 0.55 |
| 19:L:115:GLU:HG2 | 19:L:137:ARG:NH2 | 2.21 | 0.55 |
| 19:L:170:MET:HE1 | 19:L:266:MET:N | 2.22 | 0.55 |
| 19:L:289:ARG:HD3 | 19:L:334:ASP:OD1 | 2.06 | 0.55 |
| 21:N:302:PHE:CD1 | 21:N:306:ASN:ND2 | 2.75 | 0.55 |
| 22:O:217:LEU:HD12 | 22:O:238:ILE:HG21 | 1.89 | 0.55 |
| 27:T:112:ASN:HA | 27:T:177:PHE:CE1 | 2.42 | 0.55 |
| 33:Z:79:THR:O | 33:Z:80:SER:CB | 2.55 | 0.55 |
| 33:Z:851:ALA:O | 33:Z:855:LEU:HG | 2.06 | 0.55 |
| 15:H:69:VAL:HG21 | 16:I:133:LEU:HG | 1.87 | 0.54 |
| 15:H:172:MET:CG | 16:I:129:TYR:HD2 | 2.06 | 0.54 |
| 16:I:214:LYS:NZ | 16:I:318:ASP:CA | 2.70 | 0.54 |
| 21:N:130:ASP:HB3 | 21:N:133:LEU:HD12 | 1.89 | 0.54 |
| 21:N:717:LEU:HD21 | 21:N:733:LEU:HD13 | 1.88 | 0.54 |
| 22:O:165:LEU:HD12 | 22:O:202:SER:HB3 | 1.90 | 0.54 |
| 28:U:14:VAL:HG21 | 28:U:48:VAL:HG12 | 1.88 | 0.54 |
| 33:Z:303:ASP:C | 33:Z:307:HIS:CD2 | 2.80 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:887:GLY:H | 33:Z:893:PHE:HD2 | 1.55 | 0.54 |
| 2:2:124:TYR:CZ | 2:2:139:GLU:CB | 2.87 | 0.54 |
| 8:A:81:MET:SD | 8:A:143:PHE:HE1 | 2.29 | 0.54 |
| 9:B:151:ASP:HB3 | 9:B:152:PRO:HD2 | 1.88 | 0.54 |
| 11:D:6:ARG:HA | 12:E:125:GLU:OE1 | 2.08 | 0.54 |
| 14:G:217:TRP:NE1 | 14:G:228:LYS:HB2 | 2.19 | 0.54 |
| 15:H:208:TYR:CD1 | 15:H:211:VAL:CG1 | 2.90 | 0.54 |
| 16:I:220:ILE:CG1 | 16:I:344:ILE:HG21 | 2.38 | 0.54 |
| 17:J:156:GLN:HE22 | 17:J:314:ILE:HG21 | 1.72 | 0.54 |
| 19:L:149:ASP:CG | 19:L:152:THR:HB | 2.28 | 0.54 |
| 19:L:226:THR:HA | 19:L:389:ALA:HB2 | 1.88 | 0.54 |
| 20:M:253:GLN:CG | 20:M:258:GLU:HB2 | 2.37 | 0.54 |
| 21:N:16:ASN:O | 21:N:17:GLN:CG | 2.55 | 0.54 |
| 22:O:117:ASN:ND2 | 22:O:167:ILE:HA | 2.22 | 0.54 |
| 22:O:250:TRP:CA | 22:O:269:LEU:HD21 | 2.37 | 0.54 |
| 23:P:105:LYS:HB2 | 23:P:115:ARG:NH1 | 2.22 | 0.54 |
| 25:R:62:TYR:CE2 | 25:R:180:PHE:HB3 | 2.42 | 0.54 |
| 28:U:52:PHE:CD2 | 28:U:72:TYR:CE2 | 2.88 | 0.54 |
| 29:V:121:VAL:HG13 | 29:V:122:ASP:N | 2.23 | 0.54 |
| 33:Z:493:LEU:HD21 | 33:Z:497:PHE:CE2 | 2.42 | 0.54 |
| 33:Z:550:PHE:CE1 | 33:Z:566:LEU:HB2 | 2.42 | 0.54 |
| 33:Z:867:PHE:O | 33:Z:909:ARG:NH2 | 2.40 | 0.54 |
| 1:1:75:THR:CG2 | 1:1:111:TYR:CD1 | 2.91 | 0.54 |
| 4:4:106:TYR:CZ | 4:4:185:LYS:CB | 2.90 | 0.54 |
| 5:5:8:PHE:HZ | 5:5:13:ILE:HD11 | 1.70 | 0.54 |
| 10:C:2:GLY:N | 14:G:126:ASN:HD21 | 2.06 | 0.54 |
| 14:G:199:ILE:HD13 | 14:G:213:LEU:HG | 1.90 | 0.54 |
| 17:J:212:ARG:CZ | 17:J:246:PHE:HE2 | 2.19 | 0.54 |
| 18:K:209:VAL:HG22 | 18:K:336:ARG:HB2 | 1.88 | 0.54 |
| 21:N:529:GLN:NE2 | 21:N:559:TYR:HA | 2.21 | 0.54 |
| 27:T:270:ILE:HD11 | 29:V:288:LEU:HD21 | 1.88 | 0.54 |
| 33:Z:102:ILE:CG2 | 33:Z:115:LEU:HD13 | 2.38 | 0.54 |
| 4:4:13:ILE:HG12 | 4:4:182:ILE:HG12 | 1.88 | 0.54 |
| 7:7:41:THR:HG21 | 7:7:84:ILE:HD12 | 1.90 | 0.54 |
| 7:7:48:ASP:OD1 | 7:7:50:SER:HB2 | 2.08 | 0.54 |
| 8:A:197:GLU:O | 8:A:198:SER:OG | 2.23 | 0.54 |
| 13:F:101:ARG:HH22 | 13:F:103:LEU:HD13 | 1.72 | 0.54 |
| 16:I:220:ILE:HD11 | 16:I:344:ILE:HD13 | 1.90 | 0.54 |
| 17:J:186:ILE:HD11 | 17:J:300:LEU:HD11 | 1.89 | 0.54 |
| 17:J:305:LEU:HB3 | 17:J:313:LYS:HE2 | 1.87 | 0.54 |
| 21:N:158:LEU:HD12 | 21:N:202:PHE:CE2 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:649:VAL:HG11 | 21:N:651:PHE:CE2 | 2.42 | 0.54 |
| 21:N:919:THR:CG2 | 21:N:921:ARG:HG2 | 2.36 | 0.54 |
| 22:O:167:ILE:HG23 | 22:O:168:THR:N | 2.22 | 0.54 |
| 29:V:71:MET:HA | 29:V:87:PHE:CE2 | 2.42 | 0.54 |
| 33:Z:562:TRP:CD2 | 33:Z:566:LEU:CD1 | 2.87 | 0.54 |
| 33:Z:812:ILE:HD11 | 33:Z:834:LEU:HD22 | 1.89 | 0.54 |
| 1:1:57:ASP:CB | 8:A:106:TYR:HE1 | 2.17 | 0.54 |
| 3:3:19:ARG:NH2 | 3:3:171:LEU:HD23 | 2.22 | 0.54 |
| 8:A:75:ILE:HD11 | 8:A:81:MET:HB2 | 1.89 | 0.54 |
| 9:B:174:PHE:HB3 | 9:B:178:ARG:HH22 | 1.71 | 0.54 |
| 11:D:138:PHE:HE1 | 11:D:215:VAL:HG12 | 1.72 | 0.54 |
| 14:G:122:HIS:CE1 | 14:G:128:VAL:HG11 | 2.42 | 0.54 |
| 19:L:95:ILE:CG2 | 20:M:68:LYS:HZ2 | 2.18 | 0.54 |
| 19:L:336:ALA:CA | 19:L:342:ARG:HH11 | 2.20 | 0.54 |
| 21:N:736:PHE:CD1 | 21:N:749:LEU:HB2 | 2.43 | 0.54 |
| 22:O:40:GLN:NE2 | 22:O:55:THR:O | 2.41 | 0.54 |
| 33:Z:509:LEU:HD13 | 33:Z:530:LEU:HD23 | 1.88 | 0.54 |
| 33:Z:557:GLU:OE1 | 33:Z:562:TRP:HZ3 | 1.86 | 0.54 |
| 4:4:8:VAL:CG2 | 4:4:11:SER:OG | 2.55 | 0.54 |
| 5:5:76:VAL:HG21 | 5:5:103:GLY:HA3 | 1.90 | 0.54 |
| 8:A:128:TYR:CE1 | 8:A:134:MET:HE1 | 2.42 | 0.54 |
| 8:A:163:TYR:C | 8:A:164:VAL:HG13 | 2.28 | 0.54 |
| 11:D:17:ILE:HG22 | 11:D:19:GLN:HG2 | 1.90 | 0.54 |
| 11:D:82:SER:OG | 11:D:131:VAL:HG11 | 2.08 | 0.54 |
| 12:E:165:TYR:HB2 | 12:E:167:TYR:HH | 1.70 | 0.54 |
| 18:K:84:GLU:O | 18:K:88:ARG:HG3 | 2.08 | 0.54 |
| 19:L:113:SER:OG | 19:L:116:LYS:HB2 | 2.08 | 0.54 |
| 21:N:654:GLN:HG3 | 21:N:698:GLY:CA | 2.37 | 0.54 |
| 31:X:29:VAL:HG21 | 31:X:59:ARG:HH12 | 1.72 | 0.54 |
| 33:Z:385:PHE:HE2 | 33:Z:389:PHE:HE2 | 1.48 | 0.54 |
| 1:1:89:ASN:HB3 | 1:1:92:ASN:OD1 | 2.07 | 0.54 |
| 3:3:59:ARG:HH21 | 10:C:100:LYS:HA | 1.71 | 0.54 |
| 3:3:63:ASN:CB | 10:C:96:GLN:HE22 | 2.20 | 0.54 |
| 5:5:6:PHE:CZ | 5:5:13:ILE:CB | 2.89 | 0.54 |
| 5:5:174:SER:CB | 5:5:190:ASN:HD21 | 2.21 | 0.54 |
| 6:6:68:PHE:CZ | 13:F:66:CYS:O | 2.61 | 0.54 |
| 7:7:103:TRP:CE3 | 7:7:124:LEU:HD22 | 2.43 | 0.54 |
| 8:A:57:LYS:NZ | 8:A:66:PRO:HB2 | 2.23 | 0.54 |
| 11:D:37:LYS:CE | 11:D:160:SER:HA | 2.38 | 0.54 |
| 11:D:159:TRP:CZ2 | 12:E:59:LEU:CD1 | 2.89 | 0.54 |
| 16:I:253:ILE:CD1 | 16:I:287:ILE:HA | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:J:338:THR:HA | 17:J:376:HIS:NE2 | 2.22 | 0.54 |
| 21:N:77:SER:O | 21:N:81:TYR:CD1 | 2.52 | 0.54 |
| 21:N:363:ALA:HB2 | 29:V:182:LYS:NZ | 2.23 | 0.54 |
| 21:N:641:LEU:CD1 | 21:N:660:LEU:HD23 | 2.36 | 0.54 |
| 22:O:384:MET:CE | 28:U:190:LEU:N | 2.70 | 0.54 |
| 25:R:259:PHE:HE1 | 25:R:332:GLU:HB2 | 1.72 | 0.54 |
| 27:T:50:ILE:HD13 | 27:T:96:LEU:HB3 | 1.88 | 0.54 |
| 32:Y:82:ASP:O | 32:Y:86:ARG:HG3 | 2.07 | 0.54 |
| 33:Z:223:LEU:O | 33:Z:227:ILE:HG23 | 2.08 | 0.54 |
| 33:Z:318:LYS:HB2 | 33:Z:874:ASN:HD21 | 1.72 | 0.54 |
| 33:Z:774:ARG:O | 33:Z:777:PRO:HD2 | 2.07 | 0.54 |
| 1:1:70:TYR:CD1 | 14:G:110:ALA:CB | 2.88 | 0.54 |
| 4:4:32:ASP:CB | 4:4:35:ARG:HH12 | 2.18 | 0.54 |
| 14:G:111:PHE:CB | 14:G:114:ARG:NH2 | 2.71 | 0.54 |
| 14:G:192:VAL:HG13 | 14:G:215:ILE:CD1 | 2.33 | 0.54 |
| 15:H:306:ILE:HG21 | 15:H:308:PHE:CE1 | 2.39 | 0.54 |
| 23:P:130:ILE:O | 23:P:136:ARG:CZ | 2.55 | 0.54 |
| 24:Q:50:ARG:NH2 | 24:Q:53:GLU:OE1 | 2.41 | 0.54 |
| 24:Q:419:LEU:HD22 | 28:U:289:ASP:OD2 | 2.08 | 0.54 |
| 25:R:276:LEU:O | 25:R:280:ILE:HG23 | 2.07 | 0.54 |
| 26:S:256:LYS:O | 26:S:259:TYR:CD1 | 2.61 | 0.54 |
| 27:T:126:LEU:CD2 | 27:T:136:LEU:CD2 | 2.79 | 0.54 |
| 33:Z:119:LEU:HD13 | 33:Z:137:TYR:CE2 | 2.43 | 0.54 |
| 33:Z:286:VAL:HG11 | 33:Z:317:GLN:HG2 | 1.89 | 0.54 |
| 33:Z:601:VAL:HB | 33:Z:620:LEU:HD23 | 1.90 | 0.54 |
| 2:2:59:ILE:HD12 | 2:2:82:MET:CB | 2.37 | 0.54 |
| 2:2:109:HIS:HB3 | 2:2:111:PHE:CE2 | 2.43 | 0.54 |
| 2:2:124:TYR:CZ | 2:2:139:GLU:CA | 2.90 | 0.54 |
| 11:D:10:ILE:CD1 | 12:E:10:ARG:HB3 | 2.38 | 0.54 |
| 12:E:20:ARG:CG | 20:M:432:PHE:HZ | 2.20 | 0.54 |
| 15:H:344:ASP:OD1 | 15:H:345:PRO:HD2 | 2.08 | 0.54 |
| 17:J:363:THR:OG1 | 18:K:203:ILE:HD11 | 2.08 | 0.54 |
| 17:J:377:VAL:HG12 | 17:J:378:THR:N | 2.23 | 0.54 |
| 18:K:126:LEU:HD22 | 18:K:149:ILE:HD12 | 1.90 | 0.54 |
| 22:O:215:TYR:CZ | 22:O:219:ILE:HD11 | 2.43 | 0.54 |
| 23:P:72:TRP:CZ2 | 23:P:103:TYR:HB3 | 2.38 | 0.54 |
| 23:P:163:LEU:O | 23:P:167:THR:HG23 | 2.08 | 0.54 |
| 2:2:126:SER:OG | 2:2:135:MET:HB3 | 2.07 | 0.54 |
| 3:3:41:PHE:CE1 | 3:3:181:ILE:HD13 | 2.42 | 0.54 |
| 6:6:61:ASN:O | 6:6:65:TRP:HD1 | 1.91 | 0.54 |
| 7:7:145:PRO:HA | 7:7:148:ARG:NE | 2.12 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:K:161:MET:HE3 | 18:K:237:VAL:HG13 | 1.90 | 0.54 |
| 20:M:72:ASN:CB | 20:M:156:LEU:CD2 | 2.86 | 0.54 |
| 21:N:909:GLU:HB3 | 21:N:911:LYS:HZ1 | 1.72 | 0.54 |
| 22:O:217:LEU:HD12 | 22:O:238:ILE:CG2 | 2.38 | 0.54 |
| 22:O:250:TRP:CG | 22:O:269:LEU:HD21 | 2.40 | 0.54 |
| 25:R:211:LYS:HZ1 | 25:R:234:SER:HA | 1.73 | 0.54 |
| 25:R:262:GLU:HA | 25:R:336:LYS:NZ | 2.23 | 0.54 |
| 27:T:112:ASN:CB | 27:T:177:PHE:CZ | 2.90 | 0.54 |
| 33:Z:149:TRP:CG | 33:Z:214:HIS:CE1 | 2.96 | 0.54 |
| 33:Z:316:ALA:HB1 | 33:Z:868:ASN:OD1 | 2.08 | 0.54 |
| 1:1:120:HIS:HB2 | 7:7:28:PHE:CE1 | 2.44 | 0.53 |
| 3:3:37:TYR:CE1 | 3:3:59:ARG:CB | 2.92 | 0.53 |
| 4:4:32:ASP:HB3 | 4:4:35:ARG:NH1 | 2.21 | 0.53 |
| 4:4:129:TYR:CG | 4:4:143:LEU:HD13 | 2.43 | 0.53 |
| 5:5:135:PHE:CB | 5:5:167:ARG:NH2 | 2.65 | 0.53 |
| 7:7:145:PRO:HG3 | 7:7:148:ARG:NH2 | 2.23 | 0.53 |
| 8:A:84:ASN:HD22 | 8:A:171:THR:HG23 | 1.74 | 0.53 |
| 18:K:374:ARG:HH12 | 18:K:408:GLU:HG2 | 1.73 | 0.53 |
| 20:M:216:LYS:HE3 | 20:M:267:PHE:HE1 | 1.73 | 0.53 |
| 21:N:585:ARG:HH21 | 21:N:623:PHE:HE2 | 1.43 | 0.53 |
| 23:P:241:LEU:HD23 | 23:P:264:ILE:CG1 | 2.37 | 0.53 |
| 24:Q:158:ILE:HG23 | 24:Q:177:VAL:CG1 | 2.38 | 0.53 |
| 28:U:16:LEU:HA | 28:U:19:LEU:HD12 | 1.90 | 0.53 |
| 33:Z:582:ASP:HA | 33:Z:585:LEU:HD12 | 1.90 | 0.53 |
| 2:2:99:ILE:HG13 | 2:2:127:LEU:HD12 | 1.90 | 0.53 |
| 4:4:34:THR:HG21 | 4:4:181:LYS:NZ | 2.23 | 0.53 |
| 4:4:84:ARG:HD2 | 4:4:124:LYS:CB | 2.38 | 0.53 |
| 4:4:161:LYS:HE2 | 4:4:165:GLN:HE21 | 1.72 | 0.53 |
| 7:7:118:PHE:CE2 | 7:7:120:ARG:CD | 2.89 | 0.53 |
| 8:A:189:SER:OG | 8:A:191:ILE:HG12 | 2.08 | 0.53 |
| 8:A:252:ASP:C | 23:P:44:LYS:HZ3 | 2.04 | 0.53 |
| 16:I:148:LEU:HD23 | 16:I:160:LEU:HD22 | 1.90 | 0.53 |
| 17:J:61:GLU:O | 17:J:65:LEU:HG | 2.08 | 0.53 |
| 18:K:132:LYS:HB2 | 18:K:135:MET:CG | 2.36 | 0.53 |
| 18:K:183:GLU:HG2 | 18:K:338:ILE:HG12 | 1.89 | 0.53 |
| 21:N:340:HIS:CB | 21:N:374:ILE:HG12 | 2.38 | 0.53 |
| 27:T:59:LYS:HG3 | 27:T:85:LEU:HD11 | 1.90 | 0.53 |
| 31:X:38:ASN:ND2 | 31:X:43:LEU:HG | 2.23 | 0.53 |
| 2:2:72:ARG:NH1 | 8:A:113:PRO:HB3 | 2.23 | 0.53 |
| 2:2:112:SER:HB2 | 2:2:127:LEU:HD11 | 1.89 | 0.53 |
| 3:3:83:SER:HB2 | 3:3:121:ILE:HD11 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:129:VAL:CG2 | 3:3:138:PHE:CZ | 2.91 | 0.53 |
| 5:5:3:THR:HG23 | 5:5:16:VAL:HG12 | 1.89 | 0.53 |
| 10:C:40:ALA:CA | 10:C:184:MET:SD | 2.84 | 0.53 |
| 11:D:10:ILE:HG22 | 11:D:18:PHE:CE2 | 2.43 | 0.53 |
| 12:E:17:PRO:CA | 13:F:24:TYR:CE2 | 2.89 | 0.53 |
| 17:J:370:LEU:HD23 | 17:J:370:LEU:C | 2.29 | 0.53 |
| 23:P:97:ILE:O | 23:P:101:MET:HG2 | 2.08 | 0.53 |
| 23:P:144:VAL:HG12 | 23:P:148:LYS:HE3 | 1.90 | 0.53 |
| 24:Q:4:PRO:HB3 | 24:Q:50:ARG:NH1 | 2.23 | 0.53 |
| 25:R:179:PHE:HE1 | 25:R:321:TYR:HH | 1.56 | 0.53 |
| 27:T:266:TYR:C | 27:T:266:TYR:CD1 | 2.82 | 0.53 |
| 33:Z:106:TRP:HB2 | 33:Z:112:LYS:HZ2 | 1.73 | 0.53 |
| 33:Z:126:TYR:O | 33:Z:127:SER:HB2 | 2.08 | 0.53 |
| 33:Z:497:PHE:CD2 | 33:Z:505:VAL:HB | 2.43 | 0.53 |
| 4:4:81:SER:CA | 4:4:124:LYS:NZ | 2.68 | 0.53 |
| 11:D:18:PHE:CG | 11:D:19:GLN:N | 2.76 | 0.53 |
| 11:D:157:SER:HG | 11:D:159:TRP:HE1 | 1.55 | 0.53 |
| 12:E:207:VAL:CB | 15:H:409:ARG:NH1 | 2.71 | 0.53 |
| 17:J:153:LEU:O | 17:J:157:ILE:HG13 | 2.08 | 0.53 |
| 21:N:145:LEU:HD22 | 21:N:173:LYS:NZ | 2.21 | 0.53 |
| 21:N:362:TRP:CH2 | 29:V:23:THR:HB | 2.44 | 0.53 |
| 22:O:80:LYS:HE2 | 22:O:81:TYR:HE1 | 1.74 | 0.53 |
| 25:R:301:TYR:CZ | 25:R:305:PHE:CZ | 2.94 | 0.53 |
| 27:T:249:MET:O | 27:T:250:MET:CB | 2.56 | 0.53 |
| 30:W:186:ALA:HB1 | 30:W:191:ILE:HG21 | 1.76 | 0.53 |
| 1:1:5:ALA:CB | 1:1:14:LEU:HG | 2.39 | 0.53 |
| 1:1:14:LEU:CD1 | 1:1:100:ALA:HB1 | 2.32 | 0.53 |
| 4:4:66:TYR:CZ | 10:C:102:TYR:OH | 2.61 | 0.53 |
| 8:A:54:ILE:CG2 | 8:A:210:MET:CE | 2.86 | 0.53 |
| 10:C:209:ASP:OD1 | 10:C:210:ARG:HG3 | 2.09 | 0.53 |
| 13:F:101:ARG:HH12 | 13:F:103:LEU:HA | 1.67 | 0.53 |
| 15:H:365:LEU:HD23 | 15:H:370:ARG:CZ | 2.38 | 0.53 |
| 18:K:105:GLN:O | 18:K:106:ASN:HB2 | 2.09 | 0.53 |
| 20:M:197:ILE:HG13 | 20:M:198:VAL:N | 2.24 | 0.53 |
| 21:N:117:TYR:CZ | 21:N:202:PHE:HB2 | 2.43 | 0.53 |
| 23:P:426:ILE:HA | 23:P:429:ILE:HD12 | 1.89 | 0.53 |
| 24:Q:50:ARG:CZ | 24:Q:53:GLU:OE1 | 2.57 | 0.53 |
| 24:Q:99:THR:CG2 | 24:Q:103:LYS:HE3 | 2.37 | 0.53 |
| 24:Q:249:LEU:C | 24:Q:250:THR:HG22 | 2.25 | 0.53 |
| 25:R:31:PHE:CZ | 25:R:320:LYS:HA | 2.43 | 0.53 |
| 25:R:70:TYR:OH | 25:R:76:GLN:HA | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:493:LEU:CD1 | 33:Z:497:PHE:CE2 | 2.88 | 0.53 |
| 33:Z:915:ALA:HB1 | 33:Z:983:LEU:CD1 | 2.38 | 0.53 |
| 6:6:70:HIS:CD2 | 12:E:111:SER:CB | 2.92 | 0.53 |
| 9:B:40:THR:HG21 | 9:B:182:GLU:HG2 | 1.91 | 0.53 |
| 14:G:136:ILE:HG12 | 14:G:149:MET:CG | 2.39 | 0.53 |
| 14:G:136:ILE:HG12 | 14:G:149:MET:HG3 | 1.90 | 0.53 |
| 16:I:384:LYS:HZ3 | 16:I:420:LYS:HZ2 | 0.63 | 0.53 |
| 17:J:234:PHE:HZ | 17:J:279:LEU:HD21 | 1.74 | 0.53 |
| 17:J:338:THR:O | 17:J:341:ILE:HG22 | 2.08 | 0.53 |
| 19:L:167:VAL:HG23 | 20:M:142:PRO:CG | 2.33 | 0.53 |
| 21:N:130:ASP:OD2 | 21:N:132:LYS:HB2 | 2.09 | 0.53 |
| 25:R:237:THR:C | 25:R:246:TYR:CE1 | 2.82 | 0.53 |
| 26:S:436:ILE:HG23 | 27:T:197:TYR:CE2 | 2.43 | 0.53 |
| 33:Z:57:LYS:HE2 | 33:Z:98:ASP:OD2 | 2.08 | 0.53 |
| 33:Z:246:CYS:O | 33:Z:250:VAL:HG23 | 2.08 | 0.53 |
| 33:Z:394:TYR:HB3 | 33:Z:859:LYS:HE3 | 1.90 | 0.53 |
| 33:Z:550:PHE:HZ | 33:Z:566:LEU:CB | 2.13 | 0.53 |
| 8:A:91:ARG:HH21 | 14:G:113:ASP:CG | 2.11 | 0.53 |
| 9:B:219:PRO:CA | 9:B:222:LEU:HD12 | 2.32 | 0.53 |
| 12:E:68:VAL:CG1 | 12:E:93:ARG:NH2 | 2.71 | 0.53 |
| 15:H:157:VAL:HG12 | 15:H:159:LEU:H | 1.74 | 0.53 |
| 16:I:354:ASP:OD1 | 16:I:357:THR:HG23 | 2.08 | 0.53 |
| 17:J:370:LEU:HD23 | 17:J:370:LEU:O | 2.07 | 0.53 |
| 19:L:386:PHE:CD1 | 19:L:390:ASP:HB3 | 2.43 | 0.53 |
| 21:N:223:LEU:CD2 | 21:N:897:LYS:HB2 | 2.39 | 0.53 |
| 21:N:719:ASN:N | 21:N:726:ASP:OD2 | 2.41 | 0.53 |
| 23:P:202:LYS:HE2 | 23:P:206:LYS:HZ2 | 1.72 | 0.53 |
| 23:P:431:HIS:CE1 | 28:U:156:HIS:H | 2.27 | 0.53 |
| 24:Q:201:ALA:HB1 | 24:Q:218:LEU:HD21 | 1.89 | 0.53 |
| 27:T:26:LEU:O | 27:T:29:PRO:HD2 | 2.08 | 0.53 |
| 27:T:119:THR:HG22 | 27:T:123:HIS:CE1 | 2.44 | 0.53 |
| 30:W:131:THR:HG23 | 30:W:134:LYS:HD2 | 1.89 | 0.53 |
| 33:Z:249:MET:CE | 33:Z:268:ALA:HB2 | 2.38 | 0.53 |
| 33:Z:385:PHE:HZ | 33:Z:389:PHE:CZ | 2.20 | 0.53 |
| 33:Z:397:ASP:OD1 | 33:Z:425:ILE:HD12 | 2.09 | 0.53 |
| 33:Z:846:PHE:CE2 | 33:Z:901:PHE:HE2 | 2.27 | 0.53 |
| 1:1:59:VAL:HG21 | 1:1:82:PHE:CE1 | 2.44 | 0.53 |
| 1:1:66:TYR:CE2 | 1:1:73:PRO:CB | 2.89 | 0.53 |
| 3:3:54:LEU:CD1 | 3:3:96:VAL:HG11 | 2.38 | 0.53 |
| 10:C:120:GLN:OE1 | 11:D:80:ALA:HB1 | 2.09 | 0.53 |
| 12:E:219:LEU:HB2 | 12:E:236:THR:CG2 | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:200:VAL:HG13 | 15:H:270:THR:CG2 | 2.38 | 0.53 |
| 15:H:224:VAL:O | 15:H:228:PRO:HG3 | 2.07 | 0.53 |
| 15:H:358:PRO:HB2 | 15:H:374:LYS:NZ | 2.23 | 0.53 |
| 20:M:75:LEU:HD23 | 20:M:77:TYR:HB2 | 1.89 | 0.53 |
| 21:N:221:ASP:HA | 21:N:894:ARG:HH12 | 1.74 | 0.53 |
| 21:N:919:THR:HG23 | 21:N:921:ARG:HG2 | 1.89 | 0.53 |
| 23:P:425:HIS:O | 23:P:429:ILE:HG13 | 2.09 | 0.53 |
| 26:S:339:GLN:HA | 26:S:342:LEU:HD12 | 1.91 | 0.53 |
| 33:Z:609:THR:HG21 | 33:Z:878:LEU:HD13 | 1.91 | 0.53 |
| 33:Z:809:MET:HG2 | 33:Z:847:ILE:CD1 | 2.38 | 0.53 |
| 1:1:120:HIS:CE1 | 7:7:31:VAL:HG22 | 2.44 | 0.53 |
| 2:2:36:ARG:NH2 | 2:2:39:PRO:CD | 2.72 | 0.53 |
| 5:5:32:LYS:O | 5:5:33:ARG:NH1 | 2.36 | 0.53 |
| 15:H:99:VAL:O | 15:H:173:ARG:HD3 | 2.08 | 0.53 |
| 16:I:193:GLU:O | 16:I:346:ARG:NH1 | 2.42 | 0.53 |
| 18:K:393:ARG:HH21 | 19:L:345:ARG:NH1 | 2.06 | 0.53 |
| 20:M:264:ARG:HG2 | 20:M:311:GLN:HE21 | 1.74 | 0.53 |
| 21:N:619:CYS:SG | 21:N:655:ALA:HB2 | 2.49 | 0.53 |
| 21:N:649:VAL:CG1 | 21:N:651:PHE:CE2 | 2.91 | 0.53 |
| 22:O:15:ARG:CB | 30:W:20:ASP:OD1 | 2.57 | 0.53 |
| 22:O:26:PHE:HZ | 22:O:64:ASN:ND2 | 2.05 | 0.53 |
| 22:O:384:MET:HE3 | 28:U:190:LEU:HA | 1.90 | 0.53 |
| 29:V:140:VAL:CG1 | 29:V:156:PHE:HE2 | 2.22 | 0.53 |
| 30:W:179:ARG:NE | 30:W:184:ASN:OD1 | 2.37 | 0.53 |
| 33:Z:51:LEU:HB3 | 33:Z:91:PHE:CZ | 2.34 | 0.53 |
| 33:Z:298:PHE:HZ | 33:Z:314:LEU:HD22 | 1.74 | 0.53 |
| 33:Z:322:GLU:HG2 | 33:Z:464:ASP:CG | 2.29 | 0.53 |
| 33:Z:383:SER:HA | 33:Z:849:ARG:HH11 | 1.74 | 0.53 |
| 33:Z:463:HIS:NE2 | 33:Z:497:PHE:CE1 | 2.77 | 0.53 |
| 4:4:7:ARG:HH11 | 4:4:114:GLU:HA | 1.74 | 0.53 |
| 4:4:45:PHE:HB3 | 4:4:99:VAL:HG11 | 1.92 | 0.53 |
| 8:A:46:ARG:HD2 | 8:A:152:PRO:HB2 | 1.90 | 0.53 |
| 10:C:41:SER:HB3 | 10:C:184:MET:CE | 2.38 | 0.53 |
| 10:C:98:TYR:CE1 | 10:C:105:ASP:O | 2.62 | 0.53 |
| 15:H:379:LEU:HD21 | 15:H:415:THR:HG22 | 1.89 | 0.53 |
| 15:H:385:ARG:HB3 | 15:H:389:PHE:CE2 | 2.44 | 0.53 |
| 18:K:423:LYS:HG3 | 18:K:424:PHE:CD2 | 2.43 | 0.53 |
| 19:L:228:LYS:HB2 | 19:L:349:ILE:HD11 | 1.90 | 0.53 |
| 22:O:188:PHE:CD2 | 22:O:220:SER:HB3 | 2.44 | 0.53 |
| 24:Q:104:PHE:HE2 | 24:Q:114:GLN:HA | 1.74 | 0.53 |
| 25:R:70:TYR:HE2 | 25:R:77:SER:H | 1.57 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:R:110:ILE:HD11 | 25:R:140:TYR:OH | 2.09 | 0.53 |
| 26:S:378:GLN:CB | 26:S:382:ARG:HH12 | 2.21 | 0.53 |
| 27:T:8:THR:HG23 | 27:T:61:ILE:CG1 | 2.38 | 0.53 |
| 30:W:6:THR:HG23 | 30:W:111:VAL:HG23 | 1.90 | 0.53 |
| 33:Z:263:ALA:O | 33:Z:267:THR:HG23 | 2.08 | 0.53 |
| 33:Z:419:VAL:HG21 | 33:Z:447:VAL:HA | 1.91 | 0.53 |
| 33:Z:553:ARG:HH12 | 33:Z:595:MET:HE3 | 1.74 | 0.53 |
| 33:Z:773:ARG:O | 33:Z:776:VAL:HG12 | 2.09 | 0.53 |
| 3:3:16:CYS:SG | 3:3:34:ILE:HD12 | 2.49 | 0.52 |
| 5:5:111:THR:HG21 | 5:5:113:TYR:OH | 2.07 | 0.52 |
| 8:A:88:PRO:O | 14:G:120:GLN:NE2 | 2.42 | 0.52 |
| 12:E:207:VAL:CB | 15:H:409:ARG:HH12 | 2.22 | 0.52 |
| 15:H:308:PHE:HE1 | 15:H:351:VAL:HG13 | 1.73 | 0.52 |
| 17:J:62:LEU:HD13 | 18:K:86:VAL:HA | 1.90 | 0.52 |
| 17:J:206:THR:O | 17:J:207:ASP:HB2 | 2.09 | 0.52 |
| 18:K:168:ASP:OD1 | 19:L:315:PHE:CE1 | 2.62 | 0.52 |
| 18:K:239:GLY:HA2 | 18:K:242:PHE:CD2 | 2.44 | 0.52 |
| 21:N:762:ARG:HB2 | 21:N:769:PRO:HG3 | 1.90 | 0.52 |
| 22:O:245:ASP:HA | 22:O:249:ASP:OD1 | 2.09 | 0.52 |
| 24:Q:331:THR:CG2 | 24:Q:335:PHE:CE2 | 2.92 | 0.52 |
| 25:R:222:ARG:HA | 25:R:224:PHE:CZ | 2.45 | 0.52 |
| 26:S:145:PHE:HD2 | 26:S:152:LEU:CD2 | 2.21 | 0.52 |
| 33:Z:65:GLU:CA | 33:Z:111:LEU:HD21 | 2.38 | 0.52 |
| 5:5:55:TRP:HE1 | 6:6:89:TYR:HH | 0.55 | 0.52 |
| 14:G:161:GLY:HA3 | 14:G:175:LEU:HD21 | 1.90 | 0.52 |
| 15:H:284:VAL:N | 20:M:254:MET:HB3 | 2.25 | 0.52 |
| 17:J:236:MET:O | 17:J:240:HIS:HD2 | 1.91 | 0.52 |
| 19:L:178:ILE:HD12 | 19:L:183:ILE:HG21 | 1.91 | 0.52 |
| 19:L:247:PRO:HB3 | 20:M:303:ARG:NH2 | 2.24 | 0.52 |
| 19:L:312:MET:SD | 19:L:342:ARG:HA | 2.48 | 0.52 |
| 22:O:301:PHE:CZ | 28:U:234:ASN:HA | 2.43 | 0.52 |
| 27:T:236:ASN:OD1 | 27:T:238:GLN:HB2 | 2.10 | 0.52 |
| 31:X:14:VAL:HG13 | 31:X:50:TRP:CZ2 | 2.44 | 0.52 |
| 31:X:75:TRP:NE1 | 31:X:125:MET:CB | 2.63 | 0.52 |
| 33:Z:138:ARG:HH12 | 33:Z:160:GLU:HB3 | 1.73 | 0.52 |
| 1:1:18:SER:HB3 | 1:1:31:THR:HG22 | 1.91 | 0.52 |
| 2:2:25:ILE:HG21 | 3:3:138:PHE:HB3 | 1.92 | 0.52 |
| 7:7:-7:GLN:CG | 7:7:101:PRO:HD2 | 2.35 | 0.52 |
| 10:C:26:LEU:HD23 | 10:C:153:PRO:CG | 2.39 | 0.52 |
| 12:E:207:VAL:CA | 15:H:409:ARG:NH1 | 2.70 | 0.52 |
| 19:L:170:MET:HG2 | 19:L:266:MET:CE | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:257:GLY:HA2 | 19:L:303:ARG:NH2 | 2.24 | 0.52 |
| 26:S:188:TYR:OH | 26:S:240:ASP:HB2 | 2.09 | 0.52 |
| 26:S:250:ALA:CB | 26:S:279:ILE:HD13 | 2.39 | 0.52 |
| 30:W:172:LEU:CD1 | 30:W:190:ILE:HB | 2.37 | 0.52 |
| 33:Z:53:VAL:HG23 | 33:Z:91:PHE:CD2 | 2.44 | 0.52 |
| 33:Z:474:LEU:HD23 | 33:Z:493:LEU:HD23 | 1.68 | 0.52 |
| 33:Z:805:LEU:HD22 | 33:Z:841:GLU:CG | 2.39 | 0.52 |
| 3:3:169:ASP:HB2 | 3:3:172:SER:OG | 2.09 | 0.52 |
| 7:7:138:PHE:CZ | 7:7:142:MET:HG3 | 2.45 | 0.52 |
| 7:7:187:PHE:HE1 | 7:7:205:GLN:C | 2.12 | 0.52 |
| 15:H:174:VAL:HG13 | 15:H:183:ILE:CG2 | 2.24 | 0.52 |
| 16:I:106:ILE:HD13 | 16:I:160:LEU:HD21 | 1.89 | 0.52 |
| 16:I:278:ILE:CG2 | 16:I:325:ILE:HD12 | 2.39 | 0.52 |
| 18:K:170:THR:HG23 | 18:K:172:ALA:H | 1.74 | 0.52 |
| 20:M:129:LEU:HD13 | 20:M:130:PRO:O | 2.09 | 0.52 |
| 20:M:167:VAL:CG2 | 20:M:269:LEU:HD12 | 2.39 | 0.52 |
| 21:N:232:LEU:HD12 | 21:N:237:LEU:CD1 | 2.40 | 0.52 |
| 22:O:4:ASN:HB2 | 22:O:39:PHE:CE2 | 2.44 | 0.52 |
| 22:O:117:ASN:HD22 | 22:O:167:ILE:HD12 | 1.74 | 0.52 |
| 22:O:228:TYR:HE2 | 22:O:231:GLY:H | 1.57 | 0.52 |
| 23:P:319:GLU:HB3 | 23:P:323:ASN:OD1 | 2.09 | 0.52 |
| 23:P:440:HIS:ND1 | 28:U:209:GLU:HB3 | 2.24 | 0.52 |
| 24:Q:122:ILE:HG22 | 24:Q:126:LYS:HE3 | 1.90 | 0.52 |
| 24:Q:395:GLY:O | 24:Q:396:TRP:HD1 | 1.93 | 0.52 |
| 25:R:179:PHE:CE1 | 25:R:321:TYR:OH | 2.62 | 0.52 |
| 27:T:202:LEU:O | 27:T:205:ILE:HG22 | 2.08 | 0.52 |
| 28:U:37:ILE:CG2 | 28:U:93:TYR:HD2 | 2.23 | 0.52 |
| 29:V:52:LEU:HD12 | 29:V:69:PHE:CZ | 2.45 | 0.52 |
| 29:V:180:LEU:O | 29:V:181:ASN:HB2 | 2.10 | 0.52 |
| 33:Z:809:MET:HG2 | 33:Z:847:ILE:HD12 | 1.91 | 0.52 |
| 8:A:156:LYS:HB3 | 8:A:166:TYR:CZ | 2.43 | 0.52 |
| 15:H:284:VAL:HG13 | 20:M:252:VAL:HG12 | 1.91 | 0.52 |
| 16:I:222:TYR:CD1 | 16:I:348:ILE:O | 2.63 | 0.52 |
| 19:L:88:TYR:CE1 | 20:M:62:ILE:HG21 | 2.45 | 0.52 |
| 19:L:88:TYR:CE1 | 20:M:62:ILE:CG2 | 2.92 | 0.52 |
| 20:M:197:ILE:CB | 20:M:322:LYS:HD3 | 2.32 | 0.52 |
| 21:N:150:LEU:HD21 | 21:N:173:LYS:HG3 | 1.90 | 0.52 |
| 21:N:363:ALA:HB2 | 29:V:182:LYS:HZ3 | 1.72 | 0.52 |
| 21:N:645:THR:HG21 | 21:N:660:LEU:HD11 | 1.90 | 0.52 |
| 21:N:745:LEU:O | 21:N:748:PHE:HD1 | 1.92 | 0.52 |
| 23:P:333:ALA:HB3 | 23:P:336:HIS:HB2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:250:THR:HG23 | 24:Q:251:THR:H | 1.72 | 0.52 |
| 26:S:237:ILE:HG21 | 26:S:253:PHE:CZ | 2.45 | 0.52 |
| 27:T:89:TYR:CG | 27:T:102:LYS:CD | 2.92 | 0.52 |
| 33:Z:81:SER:O | 33:Z:82:MET:CB | 2.57 | 0.52 |
| 33:Z:392:LEU:HD11 | 33:Z:427:GLN:HB3 | 1.90 | 0.52 |
| 33:Z:886:VAL:CA | 33:Z:893:PHE:CE2 | 2.82 | 0.52 |
| 4:4:145:HIS:CD2 | 4:4:146:HIS:CE1 | 2.96 | 0.52 |
| 6:6:-5:TYR:CD1 | 6:6:97:TYR:CG | 2.97 | 0.52 |
| 9:B:139:HIS:CE1 | 9:B:145:PHE:CZ | 2.98 | 0.52 |
| 11:D:34:VAL:HG12 | 11:D:163:THR:OG1 | 2.08 | 0.52 |
| 13:F:11:VAL:HA | 14:G:129:ARG:HG2 | 1.91 | 0.52 |
| 15:H:215:LYS:O | 15:H:219:GLU:HG3 | 2.09 | 0.52 |
| 15:H:295:PHE:CD1 | 15:H:339:GLN:HG3 | 2.44 | 0.52 |
| 15:H:302:LYS:HD2 | 15:H:348:ASN:HD22 | 1.73 | 0.52 |
| 15:H:389:PHE:HZ | 15:H:419:LEU:CD2 | 2.18 | 0.52 |
| 16:I:217:LYS:HD3 | 16:I:343:ARG:HD2 | 1.91 | 0.52 |
| 17:J:219:VAL:CG1 | 18:K:281:ARG:HD2 | 2.39 | 0.52 |
| 18:K:242:PHE:C | 18:K:243:VAL:HA | 2.30 | 0.52 |
| 20:M:218:ALA:HB3 | 20:M:324:LEU:HD22 | 1.92 | 0.52 |
| 24:Q:222:SER:O | 24:Q:226:HIS:ND1 | 2.30 | 0.52 |
| 26:S:230:LYS:NZ | 26:S:256:LYS:O | 2.37 | 0.52 |
| 28:U:54:LEU:CD2 | 28:U:72:TYR:HD2 | 2.22 | 0.52 |
| 29:V:135:ARG:NE | 29:V:157:ARG:NH1 | 2.08 | 0.52 |
| 33:Z:272:TYR:CE2 | 33:Z:284:LEU:HD11 | 2.39 | 0.52 |
| 1:1:14:LEU:CD1 | 1:1:100:ALA:CB | 2.87 | 0.52 |
| 3:3:26:GLY:HA3 | 3:3:174:TRP:CE2 | 2.44 | 0.52 |
| 6:6:66:TYR:OH | 6:6:73:LYS:HE2 | 2.10 | 0.52 |
| 6:6:136:LEU:HD21 | 6:6:185:ARG:HD2 | 1.90 | 0.52 |
| 12:E:98:THR:HG22 | 12:E:102:TYR:CD2 | 2.45 | 0.52 |
| 17:J:166:LEU:C | 17:J:174:PHE:CE1 | 2.83 | 0.52 |
| 18:K:395:VAL:HG11 | 19:L:207:PHE:CD1 | 2.44 | 0.52 |
| 21:N:602:VAL:HG12 | 21:N:625:LEU:HD23 | 1.92 | 0.52 |
| 23:P:287:ASP:HB3 | 23:P:297:GLU:OE1 | 2.09 | 0.52 |
| 25:R:266:LEU:HA | 25:R:270:VAL:HG21 | 1.80 | 0.52 |
| 26:S:257:LEU:HD23 | 26:S:272:TYR:CZ | 2.44 | 0.52 |
| 26:S:311:GLN:NE2 | 26:S:338:MET:H | 2.08 | 0.52 |
| 26:S:315:LYS:HD3 | 26:S:345:TYR:HE1 | 1.58 | 0.52 |
| 27:T:24:GLU:HA | 27:T:27:LEU:HD12 | 1.92 | 0.52 |
| 31:X:87:PHE:HE2 | 31:X:121:ILE:HG21 | 1.75 | 0.52 |
| 33:Z:518:LEU:HD23 | 33:Z:523:ALA:O | 2.09 | 0.52 |
| 33:Z:531:ALA:HA | 33:Z:573:LEU:HD21 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:612:GLY:CA | 33:Z:746:ILE:HG21 | 2.37 | 0.52 |
| 33:Z:821:GLY:O | 33:Z:962:ARG:NH2 | 2.42 | 0.52 |
| 5:5:111:THR:CG2 | 5:5:113:TYR:CE1 | 2.92 | 0.52 |
| 10:C:29:ILE:CD1 | 10:C:153:PRO:HD3 | 2.40 | 0.52 |
| 12:E:109:VAL:CG1 | 12:E:156:PHE:CE1 | 2.93 | 0.52 |
| 15:H:324:GLY:HA2 | 20:M:290:ARG:NH2 | 2.09 | 0.52 |
| 15:H:330:GLN:O | 15:H:334:LEU:HG | 2.09 | 0.52 |
| 16:I:104:LEU:HD21 | 16:I:149:LEU:C | 2.29 | 0.52 |
| 17:J:218:LEU:HD11 | 17:J:229:MET:C | 2.30 | 0.52 |
| 17:J:345:LYS:O | 17:J:349:LYS:HG3 | 2.10 | 0.52 |
| 21:N:269:LEU:O | 21:N:273:LEU:HG | 2.10 | 0.52 |
| 21:N:318:LYS:HA | 29:V:180:LEU:CD1 | 2.40 | 0.52 |
| 21:N:654:GLN:HG3 | 21:N:698:GLY:HA3 | 1.90 | 0.52 |
| 22:O:150:LEU:HD22 | 22:O:175:ASN:OD1 | 2.09 | 0.52 |
| 24:Q:220:LEU:HD12 | 24:Q:239:PHE:CE1 | 2.45 | 0.52 |
| 27:T:104:LYS:N | 27:T:141:LEU:HD13 | 2.25 | 0.52 |
| 28:U:54:LEU:HD22 | 28:U:72:TYR:HD2 | 1.74 | 0.52 |
| 33:Z:601:VAL:HB | 33:Z:620:LEU:CD2 | 2.40 | 0.52 |
| 2:2:8:PHE:CE1 | 2:2:11:GLY:CA | 2.92 | 0.52 |
| 6:6:58:ARG:CD | 6:6:87:LEU:HD22 | 2.39 | 0.52 |
| 7:7:49:ILE:HG23 | 7:7:52:MET:HE3 | 1.91 | 0.52 |
| 8:A:135:ARG:HH21 | 14:G:14:PHE:HD2 | 1.56 | 0.52 |
| 15:H:412:PRO:HG2 | 15:H:451:ILE:HG13 | 1.91 | 0.52 |
| 16:I:204:HIS:CD2 | 16:I:207:LEU:HD11 | 2.13 | 0.52 |
| 18:K:209:VAL:HG11 | 18:K:338:ILE:HD12 | 1.91 | 0.52 |
| 18:K:281:ARG:HD3 | 18:K:286:THR:HB | 1.92 | 0.52 |
| 20:M:354:GLU:HG2 | 20:M:357:ARG:NH2 | 2.25 | 0.52 |
| 21:N:759:ILE:HG12 | 21:N:871:MET:SD | 2.50 | 0.52 |
| 22:O:30:GLU:CD | 22:O:58:ARG:NH1 | 2.63 | 0.52 |
| 26:S:425:ARG:NH1 | 27:T:155:GLY:CA | 2.72 | 0.52 |
| 33:Z:327:GLN:HG3 | 33:Z:349:THR:O | 2.10 | 0.52 |
| 4:4:26:VAL:CG1 | 4:4:29:ASP:HB3 | 2.31 | 0.52 |
| 7:7:131:SER:HB3 | 7:7:134:LEU:HD21 | 1.91 | 0.52 |
| 10:C:177:GLN:CG | 11:D:54:LEU:HD21 | 2.27 | 0.52 |
| 11:D:146:LYS:HB3 | 11:D:148:TYR:HE2 | 1.75 | 0.52 |
| 13:F:81:ALA:HB2 | 13:F:130:VAL:HG21 | 1.92 | 0.52 |
| 16:I:380:LEU:HD13 | 16:I:420:LYS:CE | 2.40 | 0.52 |
| 17:J:329:ARG:HH11 | 17:J:333:ARG:NH2 | 2.07 | 0.52 |
| 22:O:59:LEU:CD2 | 22:O:85:SER:HB3 | 2.32 | 0.52 |
| 22:O:102:LEU:O | 22:O:103:LYS:HG2 | 2.09 | 0.52 |
| 23:P:104:LEU:HD13 | 23:P:115:ARG:HG2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:S:141:LEU:O | 26:S:145:PHE:CE1 | 2.62 | 0.52 |
| 28:U:54:LEU:HD23 | 28:U:72:TYR:CD2 | 2.45 | 0.52 |
| 29:V:57:PHE:HE2 | 29:V:59:ASP:O | 1.92 | 0.52 |
| 33:Z:419:VAL:O | 33:Z:422:ILE:CG1 | 2.34 | 0.52 |
| 1:1:36:ARG:HB2 | 1:1:42:TRP:CZ3 | 2.45 | 0.51 |
| 2:2:103:VAL:O | 2:2:104:ASP:OD1 | 2.28 | 0.51 |
| 2:2:160:GLN:O | 2:2:164:TRP:CD1 | 2.63 | 0.51 |
| 2:2:210:THR:CG2 | 3:3:160:GLN:HE21 | 2.22 | 0.51 |
| 4:4:45:PHE:HB3 | 4:4:99:VAL:CG1 | 2.41 | 0.51 |
| 6:6:13:VAL:HG12 | 6:6:197:ILE:HG23 | 1.92 | 0.51 |
| 8:A:252:ASP:HB2 | 23:P:85:LYS:HE3 | 1.92 | 0.51 |
| 9:B:94:HIS:HA | 9:B:98:LYS:HE2 | 1.92 | 0.51 |
| 10:C:15:PRO:HB2 | 16:I:332:GLU:OE1 | 2.10 | 0.51 |
| 12:E:157:HIS:ND1 | 12:E:170:LYS:HE2 | 2.25 | 0.51 |
| 14:G:111:PHE:HA | 14:G:114:ARG:NH2 | 2.25 | 0.51 |
| 14:G:122:HIS:NE2 | 14:G:128:VAL:CG1 | 2.63 | 0.51 |
| 17:J:167:PRO:N | 17:J:174:PHE:CE1 | 2.77 | 0.51 |
| 18:K:421:VAL:O | 18:K:422:ASP:HB2 | 2.09 | 0.51 |
| 21:N:273:LEU:O | 21:N:277:LEU:CG | 2.50 | 0.51 |
| 21:N:654:GLN:HE21 | 21:N:697:PHE:HD2 | 1.55 | 0.51 |
| 21:N:717:LEU:HD22 | 21:N:733:LEU:HD12 | 1.92 | 0.51 |
| 23:P:218:LEU:HD22 | 23:P:256:LYS:NZ | 2.25 | 0.51 |
| 24:Q:146:TYR:CD1 | 24:Q:151:TYR:CE1 | 2.97 | 0.51 |
| 24:Q:302:VAL:HG13 | 24:Q:314:PHE:CE1 | 2.45 | 0.51 |
| 25:R:335:ARG:HA | 25:R:371:PHE:CE2 | 2.45 | 0.51 |
| 26:S:151:GLU:OE1 | 26:S:154:GLN:N | 2.39 | 0.51 |
| 28:U:39:GLY:HA2 | 28:U:49:THR:OG1 | 2.10 | 0.51 |
| 28:U:283:ARG:CD | 29:V:287:THR:HG22 | 2.39 | 0.51 |
| 30:W:6:THR:HG21 | 30:W:40:LYS:HZ2 | 1.75 | 0.51 |
| 33:Z:495:ILE:HD11 | 33:Z:903:MET:HG2 | 1.92 | 0.51 |
| 33:Z:957:LEU:CD1 | 33:Z:958:ASN:O | 2.59 | 0.51 |
| 4:4:102:LEU:CD2 | 4:4:117:GLN:HG2 | 2.36 | 0.51 |
| 6:6:-2:ASN:OD1 | 6:6:48:PHE:CD1 | 2.64 | 0.51 |
| 7:7:6:MET:CE | 7:7:150:VAL:HG11 | 2.40 | 0.51 |
| 9:B:160:LYS:HE2 | 10:C:56:LEU:HA | 1.92 | 0.51 |
| 10:C:41:SER:HB3 | 10:C:184:MET:HE1 | 1.92 | 0.51 |
| 12:E:154:GLN:HE22 | 12:E:166:ARG:HH21 | 1.57 | 0.51 |
| 15:H:331:ARG:CD | 20:M:252:VAL:HG11 | 2.40 | 0.51 |
| 16:I:397:THR:HG22 | 17:J:312:ARG:HH22 | 1.75 | 0.51 |
| 16:I:433:GLU:OE1 | 16:I:433:GLU:N | 2.40 | 0.51 |
| 18:K:160:VAL:HG12 | 18:K:238:ASN:ND2 | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:M:394:VAL:HA | 20:M:423:GLN:NE2 | 2.19 | 0.51 |
| 21:N:94:LYS:HE2 | 21:N:143:LYS:HZ1 | 1.72 | 0.51 |
| 22:O:23:HIS:CE1 | 22:O:24:PRO:HD2 | 2.43 | 0.51 |
| 22:O:189:TYR:CZ | 22:O:193:LEU:HD11 | 2.44 | 0.51 |
| 23:P:333:ALA:O | 23:P:337:HIS:CD2 | 2.64 | 0.51 |
| 24:Q:114:GLN:HG3 | 24:Q:144:LEU:HD11 | 1.92 | 0.51 |
| 27:T:111:LEU:HG | 27:T:145:PRO:HG3 | 1.90 | 0.51 |
| 33:Z:86:PRO:HG2 | 33:Z:87:LYS:HG3 | 1.92 | 0.51 |
| 33:Z:99:LEU:HB3 | 33:Z:119:LEU:HD21 | 1.92 | 0.51 |
| 33:Z:443:ASP:CB | 33:Z:447:VAL:CB | 2.84 | 0.51 |
| 33:Z:955:VAL:HG12 | 33:Z:956:LEU:HG | 1.92 | 0.51 |
| 1:1:6:VAL:HG13 | 1:1:142:PHE:CE1 | 2.46 | 0.51 |
| 2:2:75:ARG:HB3 | 2:2:77:VAL:HG22 | 1.91 | 0.51 |
| 5:5:58:TRP:CH2 | 5:5:62:GLN:NE2 | 2.78 | 0.51 |
| 12:E:165:TYR:CB | 12:E:167:TYR:OH | 2.58 | 0.51 |
| 12:E:196:ALA:O | 12:E:200:VAL:HG23 | 2.11 | 0.51 |
| 16:I:317:ASP:HB3 | 16:I:343:ARG:CZ | 2.40 | 0.51 |
| 21:N:749:LEU:HD12 | 21:N:752:SER:OG | 2.10 | 0.51 |
| 23:P:241:LEU:CD2 | 23:P:264:ILE:HG13 | 2.41 | 0.51 |
| 25:R:121:GLU:HG2 | 25:R:130:GLN:HE22 | 1.76 | 0.51 |
| 29:V:53:MET:HE1 | 29:V:65:VAL:HG21 | 1.93 | 0.51 |
| 33:Z:278:LEU:HB3 | 33:Z:297:VAL:HG11 | 1.93 | 0.51 |
| 33:Z:463:HIS:HA | 33:Z:466:GLU:CD | 2.31 | 0.51 |
| 33:Z:550:PHE:HE1 | 33:Z:566:LEU:HB2 | 1.76 | 0.51 |
| 1:1:11:GLY:CA | 1:1:102:TYR:CE1 | 2.93 | 0.51 |
| 5:5:158:LYS:HE3 | 5:5:196:LEU:CD1 | 2.40 | 0.51 |
| 9:B:239:THR:HG22 | 9:B:240:SER:N | 2.25 | 0.51 |
| 12:E:121:LEU:HD22 | 13:F:79:PRO:CB | 2.41 | 0.51 |
| 13:F:65:LYS:HA | 13:F:222:PHE:CE2 | 2.45 | 0.51 |
| 15:H:59:ILE:HD11 | 16:I:92:GLU:OE1 | 2.06 | 0.51 |
| 21:N:308:ASN:CB | 21:N:711:ARG:HD2 | 2.41 | 0.51 |
| 21:N:315:ASN:CG | 21:N:318:LYS:HZ2 | 2.11 | 0.51 |
| 22:O:79:VAL:HB | 22:O:83:LEU:HD12 | 1.92 | 0.51 |
| 22:O:250:TRP:CZ2 | 22:O:271:LYS:CB | 2.94 | 0.51 |
| 22:O:280:LEU:HD23 | 22:O:280:LEU:O | 2.11 | 0.51 |
| 23:P:154:ASP:OD2 | 23:P:190:LYS:NZ | 2.43 | 0.51 |
| 23:P:344:ARG:NH2 | 23:P:347:GLU:CD | 2.61 | 0.51 |
| 30:W:95:GLN:HA | 30:W:98:LEU:HD12 | 1.91 | 0.51 |
| 33:Z:363:ASP:O | 33:Z:366:LYS:HD3 | 2.10 | 0.51 |
| 33:Z:821:GLY:HA2 | 33:Z:863:THR:CG2 | 2.24 | 0.51 |
| 4:4:65:LEU:CD1 | 4:4:69:ARG:HE | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:232:LYS:CG | 8:A:234:PHE:HE1 | 2.23 | 0.51 |
| 13:F:7:ASP:CB | 13:F:21:GLN:NE2 | 2.74 | 0.51 |
| 14:G:200:TYR:CD1 | 14:G:246:ILE:HG21 | 2.46 | 0.51 |
| 15:H:49:LEU:HD21 | 33:Z:759:ARG:HA | 1.93 | 0.51 |
| 16:I:220:ILE:HG13 | 16:I:344:ILE:CG2 | 2.38 | 0.51 |
| 17:J:218:LEU:CD2 | 17:J:230:VAL:HG22 | 2.40 | 0.51 |
| 19:L:214:PRO:HD2 | 19:L:216:LYS:NZ | 2.24 | 0.51 |
| 19:L:290:ARG:NH1 | 19:L:293:GLU:HA | 2.24 | 0.51 |
| 21:N:83:LEU:HD11 | 21:N:133:LEU:CD2 | 2.41 | 0.51 |
| 21:N:508:THR:HG22 | 21:N:510:HIS:N | 2.25 | 0.51 |
| 23:P:130:ILE:CG2 | 23:P:136:ARG:NH2 | 2.73 | 0.51 |
| 24:Q:88:PHE:CE2 | 24:Q:89:ALA:HB2 | 2.46 | 0.51 |
| 26:S:218:LEU:C | 26:S:256:LYS:HZ1 | 2.14 | 0.51 |
| 26:S:388:ILE:HG21 | 26:S:422:MET:CE | 2.40 | 0.51 |
| 30:W:21:PHE:CD1 | 30:W:25:ARG:HG3 | 2.44 | 0.51 |
| 33:Z:138:ARG:HH21 | 33:Z:157:LEU:HD11 | 1.69 | 0.51 |
| 33:Z:338:HIS:CD2 | 33:Z:339:PHE:CZ | 2.94 | 0.51 |
| 1:1:55:ILE:HG23 | 1:1:85:LEU:HD13 | 1.93 | 0.51 |
| 2:2:36:ARG:CZ | 2:2:38:SER:CA | 2.88 | 0.51 |
| 3:3:28:SER:CB | 4:4:127:LEU:HD21 | 2.40 | 0.51 |
| 5:5:179:HIS:HB3 | 5:5:188:HIS:NE2 | 2.26 | 0.51 |
| 8:A:54:ILE:HD13 | 8:A:207:ILE:HG13 | 1.92 | 0.51 |
| 12:E:15:PHE:HD1 | 12:E:21:LEU:CD1 | 2.18 | 0.51 |
| 19:L:196:VAL:HG11 | 19:L:345:ARG:HE | 1.75 | 0.51 |
| 19:L:264:ARG:HA | 19:L:311:GLN:NE2 | 2.26 | 0.51 |
| 22:O:15:ARG:HH11 | 22:O:72:LYS:HG2 | 1.76 | 0.51 |
| 22:O:41:LEU:HG | 22:O:58:ARG:HG3 | 1.91 | 0.51 |
| 24:Q:146:TYR:CZ | 24:Q:183:LYS:O | 2.64 | 0.51 |
| 26:S:315:LYS:HB2 | 26:S:345:TYR:OH | 2.11 | 0.51 |
| 26:S:399:TYR:CD2 | 26:S:401:LYS:O | 2.50 | 0.51 |
| 30:W:76:LEU:O | 30:W:79:THR:HG23 | 2.10 | 0.51 |
| 33:Z:71:LEU:CD2 | 33:Z:118:VAL:CG1 | 2.89 | 0.51 |
| 33:Z:497:PHE:CD2 | 33:Z:505:VAL:HG11 | 2.45 | 0.51 |
| 33:Z:866:VAL:HB | 33:Z:873:LEU:CG | 2.36 | 0.51 |
| 6:6:141:LEU:HD11 | 6:6:145:VAL:HG21 | 1.93 | 0.51 |
| 8:A:54:ILE:HD12 | 8:A:206:ALA:CB | 2.41 | 0.51 |
| 9:B:184:GLU:HG2 | 9:B:185:LEU:N | 2.26 | 0.51 |
| 18:K:244:HIS:CD2 | 19:L:256:ILE:HG23 | 2.46 | 0.51 |
| 19:L:281:ASP:OD2 | 19:L:282:GLU:HG2 | 2.11 | 0.51 |
| 21:N:349:ILE:O | 21:N:353:LEU:HD23 | 2.11 | 0.51 |
| 26:S:157:GLU:HG2 | 26:S:161:LYS:HE3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:T:151:TRP:CZ3 | 27:T:159:LYS:HB3 | 2.45 | 0.51 |
| 28:U:83:ILE:HG21 | 29:V:70:ALA:HB3 | 1.93 | 0.51 |
| 29:V:168:LEU:CD1 | 29:V:188:LEU:HG | 2.41 | 0.51 |
| 33:Z:138:ARG:CZ | 33:Z:157:LEU:CD1 | 2.86 | 0.51 |
| 33:Z:208:VAL:HG11 | 33:Z:236:PHE:CG | 2.44 | 0.51 |
| 33:Z:306:MET:HE2 | 33:Z:310:LEU:HD21 | 1.93 | 0.51 |
| 33:Z:515:SER:O | 33:Z:516:THR:OG1 | 2.10 | 0.51 |
| 4:4:17:SER:HB3 | 4:4:33:LYS:CD | 2.40 | 0.51 |
| 8:A:205:PHE:HZ | 8:A:209:HIS:CE1 | 2.09 | 0.51 |
| 9:B:219:PRO:HA | 9:B:222:LEU:CD1 | 2.33 | 0.51 |
| 9:B:248:GLU:OE1 | 24:Q:95:LYS:HD2 | 2.11 | 0.51 |
| 11:D:19:GLN:CD | 11:D:128:PRO:CD | 2.79 | 0.51 |
| 14:G:106:ILE:HG13 | 14:G:107:PRO:O | 2.11 | 0.51 |
| 18:K:243:VAL:O | 18:K:243:VAL:HG12 | 2.09 | 0.51 |
| 19:L:178:ILE:HD11 | 19:L:230:LEU:CA | 2.41 | 0.51 |
| 23:P:156:ALA:O | 23:P:159:ILE:HG22 | 2.10 | 0.51 |
| 23:P:395:ARG:HD2 | 24:Q:357:VAL:CB | 2.41 | 0.51 |
| 25:R:168:ILE:HG13 | 25:R:206:ARG:HH21 | 1.75 | 0.51 |
| 25:R:211:LYS:HZ3 | 25:R:234:SER:HA | 1.75 | 0.51 |
| 29:V:266:LEU:HD23 | 29:V:266:LEU:C | 2.30 | 0.51 |
| 33:Z:301:THR:O | 33:Z:307:HIS:HE1 | 1.94 | 0.51 |
| 33:Z:491:LEU:O | 33:Z:495:ILE:HG13 | 2.11 | 0.51 |
| 33:Z:557:GLU:CD | 33:Z:562:TRP:HZ3 | 2.13 | 0.51 |
| 33:Z:591:ILE:HG22 | 33:Z:593:HIS:CD2 | 2.46 | 0.51 |
| 33:Z:900:LEU:CD2 | 33:Z:903:MET:HE2 | 2.40 | 0.51 |
| 3:3:57:MET:CE | 3:3:89:ARG:NH2 | 2.74 | 0.51 |
| 7:7:48:ASP:OD1 | 7:7:50:SER:N | 2.43 | 0.51 |
| 8:A:164:VAL:HG12 | 9:B:61:LEU:CD2 | 2.39 | 0.51 |
| 13:F:157:TYR:CZ | 14:G:59:VAL:HB | 2.45 | 0.51 |
| 13:F:201:LEU:C | 13:F:202:ARG:HG3 | 2.30 | 0.51 |
| 19:L:246:SER:OG | 19:L:280:MET:HA | 2.11 | 0.51 |
| 21:N:121:GLU:O | 21:N:122:GLN:NE2 | 2.44 | 0.51 |
| 21:N:235:ALA:HA | 21:N:273:LEU:HD21 | 1.92 | 0.51 |
| 21:N:539:MET:HE2 | 21:N:551:GLY:HA2 | 1.90 | 0.51 |
| 25:R:222:ARG:CA | 25:R:224:PHE:CE2 | 2.93 | 0.51 |
| 8:A:117:LEU:CD2 | 8:A:143:PHE:CE1 | 2.94 | 0.51 |
| 13:F:80:ASP:OD2 | 13:F:128:TYR:O | 2.29 | 0.51 |
| 14:G:118:TYR:HE2 | 14:G:131:PHE:HZ | 1.58 | 0.51 |
| 15:H:308:PHE:CE1 | 15:H:351:VAL:CG1 | 2.94 | 0.51 |
| 16:I:204:HIS:CD2 | 33:Z:930:GLY:HA2 | 2.46 | 0.51 |
| 17:J:166:LEU:C | 17:J:174:PHE:CZ | 2.85 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:J:248:ASP:O | 17:J:249:GLU:HB3 | 2.11 | 0.51 |
| 17:J:328:LEU:CD2 | 17:J:343:LEU:HD22 | 2.41 | 0.51 |
| 20:M:384:ASP:N | 20:M:386:PHE:CE1 | 2.77 | 0.51 |
| 21:N:70:TYR:CE1 | 21:N:100:THR:HB | 2.46 | 0.51 |
| 21:N:207:LEU:HB3 | 21:N:232:LEU:HD21 | 1.91 | 0.51 |
| 22:O:151:ASP:O | 22:O:154:GLU:HB2 | 2.11 | 0.51 |
| 24:Q:273:ASN:OD1 | 24:Q:306:TYR:OH | 2.26 | 0.51 |
| 24:Q:311:LEU:HD21 | 24:Q:343:LEU:HD13 | 1.91 | 0.51 |
| 24:Q:391:ASP:OD1 | 25:R:347:THR:HB | 2.11 | 0.51 |
| 33:Z:493:LEU:CD1 | 33:Z:497:PHE:CE1 | 2.84 | 0.51 |
| 33:Z:562:TRP:CD1 | 33:Z:566:LEU:CG | 2.81 | 0.51 |
| 1:1:11:GLY:CA | 1:1:102:TYR:CD1 | 2.94 | 0.50 |
| 3:3:63:ASN:HB3 | 10:C:96:GLN:HE22 | 1.76 | 0.50 |
| 3:3:83:SER:CB | 3:3:121:ILE:HD11 | 2.40 | 0.50 |
| 4:4:17:SER:HB3 | 4:4:33:LYS:HD2 | 1.93 | 0.50 |
| 5:5:179:HIS:CB | 5:5:188:HIS:NE2 | 2.74 | 0.50 |
| 8:A:15:HIS:HB3 | 10:C:6:TYR:CE1 | 2.46 | 0.50 |
| 10:C:38:ILE:HD12 | 10:C:193:ALA:HB2 | 1.93 | 0.50 |
| 15:H:382:LEU:HD23 | 15:H:385:ARG:NH1 | 2.25 | 0.50 |
| 18:K:100:LEU:HB3 | 18:K:109:ILE:O | 2.12 | 0.50 |
| 21:N:32:VAL:HG11 | 21:N:67:LYS:HB2 | 1.94 | 0.50 |
| 21:N:756:THR:HB | 21:N:900:ASN:ND2 | 2.26 | 0.50 |
| 31:X:37:PRO:HA | 31:X:46:TRP:CE3 | 2.46 | 0.50 |
| 33:Z:96:TYR:HB3 | 33:Z:97:PRO:HD3 | 1.93 | 0.50 |
| 33:Z:443:ASP:CB | 33:Z:447:VAL:HB | 2.38 | 0.50 |
| 3:3:57:MET:O | 3:3:61:LYS:HG3 | 2.11 | 0.50 |
| 5:5:76:VAL:CG2 | 5:5:103:GLY:HA3 | 2.41 | 0.50 |
| 8:A:203:VAL:O | 8:A:207:ILE:HG13 | 2.12 | 0.50 |
| 12:E:165:TYR:CD2 | 20:M:434:ALA:HB2 | 2.46 | 0.50 |
| 16:I:208:TYR:CE1 | 16:I:209:GLU:CG | 2.91 | 0.50 |
| 21:N:521:LEU:HD23 | 21:N:524:ILE:HD12 | 1.92 | 0.50 |
| 21:N:579:SER:HA | 21:N:584:ARG:CZ | 2.41 | 0.50 |
| 21:N:599:TYR:CE1 | 21:N:634:LEU:HD22 | 2.46 | 0.50 |
| 22:O:30:GLU:CD | 22:O:58:ARG:HH11 | 2.14 | 0.50 |
| 26:S:203:SER:O | 26:S:204:ASP:CB | 2.60 | 0.50 |
| 27:T:229:VAL:HG12 | 27:T:230:ASN:H | 1.75 | 0.50 |
| 1:1:42:TRP:CD1 | 1:1:178:LEU:HD11 | 2.46 | 0.50 |
| 2:2:217:ILE:HG22 | 3:3:187:VAL:HG22 | 1.93 | 0.50 |
| 3:3:57:MET:HE2 | 3:3:89:ARG:NH2 | 2.26 | 0.50 |
| 8:A:156:LYS:CB | 8:A:166:TYR:CE1 | 2.87 | 0.50 |
| 11:D:7:ALA:N | 12:E:125:GLU:OE1 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:208:TYR:CD1 | 15:H:211:VAL:HG11 | 2.46 | 0.50 |
| 16:I:255:LYS:HG3 | 18:K:284:ALA:O | 2.11 | 0.50 |
| 20:M:196:ALA:HA | 20:M:345:ARG:HH21 | 1.77 | 0.50 |
| 21:N:138:GLU:HG2 | 21:N:162:ARG:HH12 | 1.76 | 0.50 |
| 21:N:749:LEU:HD23 | 21:N:753:PHE:CZ | 2.46 | 0.50 |
| 22:O:146:ALA:O | 22:O:150:LEU:HG | 2.12 | 0.50 |
| 23:P:274:GLY:N | 23:P:277:GLN:HE21 | 2.09 | 0.50 |
| 24:Q:146:TYR:HE1 | 24:Q:184:VAL:CA | 2.05 | 0.50 |
| 25:R:338:TYR:CD1 | 25:R:377:LEU:HD13 | 2.46 | 0.50 |
| 26:S:315:LYS:HZ3 | 26:S:345:TYR:HD1 | 1.50 | 0.50 |
| 27:T:229:VAL:HB | 27:T:234:TYR:CE1 | 2.44 | 0.50 |
| 3:3:60:TYR:CE2 | 10:C:96:GLN:HB2 | 2.45 | 0.50 |
| 14:G:168:ARG:NE | 14:G:172:LYS:HZ2 | 2.06 | 0.50 |
| 15:H:155:PHE:CE2 | 20:M:76:PRO:CB | 2.95 | 0.50 |
| 15:H:172:MET:HG3 | 16:I:129:TYR:HD2 | 1.69 | 0.50 |
| 15:H:358:PRO:HA | 15:H:361:LEU:HD12 | 1.92 | 0.50 |
| 18:K:67:TYR:OH | 21:N:609:LEU:HD21 | 2.12 | 0.50 |
| 21:N:406:TYR:HE1 | 21:N:448:LEU:HB3 | 1.73 | 0.50 |
| 21:N:771:PHE:HE2 | 21:N:773:MET:HG2 | 1.73 | 0.50 |
| 23:P:101:MET:CE | 23:P:119:ILE:HD11 | 2.42 | 0.50 |
| 23:P:425:HIS:CA | 28:U:228:LYS:HZ1 | 2.25 | 0.50 |
| 26:S:288:THR:CG2 | 26:S:292:TYR:HE2 | 2.24 | 0.50 |
| 33:Z:301:THR:C | 33:Z:307:HIS:CE1 | 2.84 | 0.50 |
| 33:Z:303:ASP:C | 33:Z:307:HIS:HD2 | 2.15 | 0.50 |
| 3:3:155:PHE:CE1 | 3:3:189:ARG:CD | 2.88 | 0.50 |
| 7:7:103:TRP:O | 7:7:103:TRP:CG | 2.60 | 0.50 |
| 8:A:229:THR:OG1 | 8:A:232:LYS:HG3 | 2.12 | 0.50 |
| 16:I:228:GLY:O | 16:I:232:LEU:HG | 2.12 | 0.50 |
| 21:N:536:ILE:HD13 | 21:N:555:ILE:HG13 | 1.89 | 0.50 |
| 23:P:203:ILE:CG2 | 23:P:220:TYR:CZ | 2.95 | 0.50 |
| 26:S:316:LEU:O | 26:S:320:ILE:HG13 | 2.12 | 0.50 |
| 27:T:220:PHE:HB3 | 27:T:224:ARG:NH1 | 2.27 | 0.50 |
| 28:U:275:VAL:C | 28:U:278:ILE:HG22 | 2.27 | 0.50 |
| 3:3:100:VAL:HG21 | 3:3:115:PHE:CE1 | 2.47 | 0.50 |
| 5:5:101:ILE:HD12 | 5:5:115:VAL:HG21 | 1.93 | 0.50 |
| 6:6:49:ALA:HB3 | 7:7:127:VAL:HG22 | 1.92 | 0.50 |
| 9:B:139:HIS:HD2 | 9:B:234:ARG:NE | 2.09 | 0.50 |
| 14:G:111:PHE:HD1 | 14:G:114:ARG:CZ | 2.19 | 0.50 |
| 16:I:174:ASP:CG | 17:J:282:PHE:HB2 | 2.31 | 0.50 |
| 21:N:16:ASN:HA | 21:N:21:LYS:NZ | 2.27 | 0.50 |
| 21:N:50:TYR:CD1 | 21:N:62:ALA:HB2 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:756:THR:HB | 21:N:900:ASN:HD22 | 1.77 | 0.50 |
| 24:Q:39:SER:OG | 24:Q:88:PHE:HB2 | 2.11 | 0.50 |
| 26:S:315:LYS:NZ | 26:S:345:TYR:HE1 | 2.06 | 0.50 |
| 31:X:72:GLU:O | 31:X:91:PHE:CD2 | 2.64 | 0.50 |
| 33:Z:298:PHE:CZ | 33:Z:314:LEU:HD22 | 2.46 | 0.50 |
| 33:Z:577:GLN:O | 33:Z:580:GLN:HG2 | 2.12 | 0.50 |
| 6:6:1:GLY:C | 6:6:46:ASN:HD21 | 2.15 | 0.50 |
| 7:7:77:GLU:O | 7:7:77:GLU:HG3 | 2.12 | 0.50 |
| 9:B:75:TYR:HB3 | 9:B:134:LEU:HD23 | 1.91 | 0.50 |
| 9:B:249:ALA:HB1 | 24:Q:94:VAL:HG12 | 1.93 | 0.50 |
| 15:H:295:PHE:CZ | 15:H:336:LEU:CD1 | 2.91 | 0.50 |
| 17:J:247:MET:CE | 17:J:272:MET:HG3 | 2.42 | 0.50 |
| 18:K:241:GLU:HA | 19:L:303:ARG:HH12 | 1.74 | 0.50 |
| 19:L:178:ILE:HD11 | 19:L:230:LEU:HA | 1.93 | 0.50 |
| 19:L:412:PRO:O | 19:L:416:MET:HG3 | 2.11 | 0.50 |
| 22:O:30:GLU:HG2 | 22:O:58:ARG:CZ | 2.42 | 0.50 |
| 26:S:327:ILE:HG21 | 26:S:349:THR:CG2 | 2.42 | 0.50 |
| 33:Z:433:LEU:HD13 | 33:Z:468:GLU:HB3 | 1.93 | 0.50 |
| 4:4:143:LEU:CD2 | 4:4:159:LEU:HD21 | 2.42 | 0.50 |
| 6:6:17:ASP:OD2 | 6:6:189:VAL:HG22 | 2.12 | 0.50 |
| 13:F:43:HIS:CD2 | 13:F:218:LYS:H | 2.29 | 0.50 |
| 14:G:193:LYS:HE2 | 14:G:241:PHE:CB | 2.23 | 0.50 |
| 18:K:98:GLN:NE2 | 18:K:136:SER:CB | 2.69 | 0.50 |
| 19:L:178:ILE:CD1 | 19:L:230:LEU:CD2 | 2.87 | 0.50 |
| 19:L:289:ARG:NH1 | 19:L:333:LEU:C | 2.63 | 0.50 |
| 20:M:75:LEU:HD22 | 20:M:77:TYR:H | 1.77 | 0.50 |
| 20:M:203:ARG:HB3 | 20:M:206:LYS:HD2 | 1.94 | 0.50 |
| 21:N:492:THR:CA | 21:N:528:ARG:HH11 | 2.24 | 0.50 |
| 23:P:152:LYS:HD3 | 23:P:155:GLU:OE1 | 2.12 | 0.50 |
| 25:R:417:TYR:OH | 28:U:292:ILE:CG2 | 2.60 | 0.50 |
| 33:Z:64:TYR:HE2 | 33:Z:111:LEU:HB3 | 1.74 | 0.50 |
| 33:Z:79:THR:O | 33:Z:80:SER:HB3 | 2.11 | 0.50 |
| 1:1:-8:LYS:HZ1 | 2:2:117:GLY:CA | 2.24 | 0.50 |
| 4:4:106:TYR:CE1 | 4:4:185:LYS:HA | 2.47 | 0.50 |
| 8:A:18:ILE:HA | 9:B:128:ARG:HH11 | 1.76 | 0.50 |
| 8:A:130:GLN:HG2 | 9:B:128:ARG:HG2 | 1.93 | 0.50 |
| 16:I:395:MET:HE2 | 16:I:420:LYS:CE | 2.35 | 0.50 |
| 18:K:55:GLU:O | 18:K:59:GLU:HG3 | 2.11 | 0.50 |
| 18:K:159:SER:HG | 18:K:244:HIS:CE1 | 2.18 | 0.50 |
| 21:N:84:ALA:O | 21:N:86:LYS:HG3 | 2.11 | 0.50 |
| 21:N:353:LEU:N | 21:N:354:PRO:CD | 2.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:O:30:GLU:CB | 22:O:58:ARG:NH1 | 2.75 | 0.50 |
| 23:P:160:LEU:HD12 | 23:P:186:LEU:HD12 | 1.93 | 0.50 |
| 23:P:343:LYS:O | 23:P:347:GLU:HG3 | 2.12 | 0.50 |
| 24:Q:9:GLU:HG2 | 24:Q:13:ARG:NH1 | 2.26 | 0.50 |
| 24:Q:38:SER:OG | 24:Q:88:PHE:CD1 | 2.51 | 0.50 |
| 24:Q:38:SER:HG | 24:Q:88:PHE:HE1 | 1.42 | 0.50 |
| 24:Q:61:LEU:CD2 | 24:Q:65:TYR:CZ | 2.94 | 0.50 |
| 26:S:242:LEU:HD13 | 26:S:278:LYS:HD3 | 1.93 | 0.50 |
| 26:S:250:ALA:HB2 | 26:S:279:ILE:HD13 | 1.94 | 0.50 |
| 27:T:247:ASP:CG | 27:T:248:GLU:H | 2.13 | 0.50 |
| 29:V:292:ILE:O | 29:V:296:LEU:HG | 2.12 | 0.50 |
| 33:Z:405:ASN:O | 33:Z:409:LYS:HG3 | 2.12 | 0.50 |
| 33:Z:850:LEU:HD23 | 33:Z:850:LEU:C | 2.31 | 0.50 |
| 3:3:-2:ASN:HD21 | 3:3:48:ALA:N | 2.09 | 0.49 |
| 4:4:103:ILE:HD12 | 4:4:118:ILE:CD1 | 2.40 | 0.49 |
| 7:7:1:THR:H | 7:7:19:LEU:HD23 | 1.77 | 0.49 |
| 10:C:147:GLN:HB3 | 10:C:149:TYR:CE1 | 2.47 | 0.49 |
| 11:D:193:LYS:HG3 | 11:D:197:ARG:HH12 | 1.72 | 0.49 |
| 15:H:147:ILE:HD12 | 15:H:181:TYR:CB | 2.40 | 0.49 |
| 15:H:295:PHE:CE1 | 15:H:336:LEU:HD12 | 2.47 | 0.49 |
| 17:J:363:THR:HA | 18:K:203:ILE:HD11 | 1.93 | 0.49 |
| 18:K:241:GLU:HA | 19:L:303:ARG:HH11 | 1.75 | 0.49 |
| 21:N:174:LEU:HD12 | 21:N:182:ASN:CG | 2.33 | 0.49 |
| 21:N:221:ASP:HB3 | 21:N:894:ARG:HH22 | 1.77 | 0.49 |
| 21:N:304:LEU:HD23 | 21:N:343:THR:O | 2.12 | 0.49 |
| 22:O:195:TYR:CD2 | 22:O:213:LEU:HD22 | 2.46 | 0.49 |
| 22:O:199:LEU:HD12 | 22:O:203:THR:O | 2.11 | 0.49 |
| 22:O:250:TRP:NE1 | 22:O:269:LEU:O | 2.44 | 0.49 |
| 23:P:77:GLU:O | 23:P:81:LEU:HG | 2.12 | 0.49 |
| 25:R:258:LEU:HD11 | 25:R:288:SER:HA | 1.94 | 0.49 |
| 30:W:139:VAL:CG1 | 30:W:157:PHE:HE2 | 2.18 | 0.49 |
| 33:Z:442:VAL:O | 33:Z:443:ASP:HB2 | 2.12 | 0.49 |
| 33:Z:562:TRP:CZ2 | 33:Z:566:LEU:HD21 | 2.46 | 0.49 |
| 33:Z:850:LEU:CD2 | 33:Z:854:LEU:CD1 | 2.89 | 0.49 |
| 1:1:83:LYS:HZ2 | 1:1:117:GLY:C | 2.15 | 0.49 |
| 1:1:112:THR:HG22 | 7:7:27:ARG:NH2 | 2.27 | 0.49 |
| 4:4:37:LEU:HD12 | 4:4:60:GLN:HA | 1.94 | 0.49 |
| 5:5:159:ARG:NH1 | 5:5:204:GLU:HB2 | 2.27 | 0.49 |
| 11:D:13:PRO:HB3 | 12:E:26:TYR:CZ | 2.46 | 0.49 |
| 11:D:236:ILE:CG2 | 11:D:240:LYS:HE3 | 2.42 | 0.49 |
| 14:G:68:VAL:HG12 | 14:G:69:VAL:N | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:172:MET:HB3 | 16:I:129:TYR:HD2 | 1.48 | 0.49 |
| 15:H:385:ARG:O | 15:H:389:PHE:CD2 | 2.65 | 0.49 |
| 17:J:143:PRO:HB2 | 17:J:204:HIS:HB2 | 1.93 | 0.49 |
| 18:K:170:THR:N | 18:K:173:ASP:OD2 | 2.37 | 0.49 |
| 18:K:329:LEU:HA | 18:K:334:LEU:HD23 | 1.93 | 0.49 |
| 21:N:223:LEU:HD22 | 21:N:897:LYS:HB2 | 1.92 | 0.49 |
| 21:N:338:PHE:CE1 | 21:N:749:LEU:HB3 | 2.47 | 0.49 |
| 21:N:515:ARG:NH2 | 21:N:741:TYR:CD2 | 2.80 | 0.49 |
| 24:Q:50:ARG:HH21 | 24:Q:53:GLU:HB2 | 1.74 | 0.49 |
| 25:R:164:THR:HG21 | 25:R:199:GLU:OE1 | 2.11 | 0.49 |
| 27:T:1:MET:HB3 | 27:T:9:LYS:NZ | 2.27 | 0.49 |
| 28:U:52:PHE:CD2 | 28:U:72:TYR:HE2 | 2.30 | 0.49 |
| 33:Z:165:TYR:CE1 | 33:Z:196:SER:HB3 | 2.47 | 0.49 |
| 33:Z:502:ASN:O | 33:Z:505:VAL:HG22 | 2.11 | 0.49 |
| 33:Z:557:GLU:OE1 | 33:Z:562:TRP:HE3 | 1.95 | 0.49 |
| 33:Z:761:PHE:CG | 33:Z:780:MET:HE2 | 2.46 | 0.49 |
| 1:1:55:ILE:HG23 | 1:1:85:LEU:CD1 | 2.42 | 0.49 |
| 6:6:141:LEU:HD12 | 6:6:145:VAL:HG23 | 1.95 | 0.49 |
| 11:D:31:THR:OG1 | 11:D:76:SER:HA | 2.12 | 0.49 |
| 13:F:152:ASN:ND2 | 14:G:81:ILE:HD12 | 2.26 | 0.49 |
| 17:J:142:VAL:O | 17:J:142:VAL:HG12 | 2.12 | 0.49 |
| 21:N:720:ALA:O | 21:N:721:ASP:CG | 2.50 | 0.49 |
| 23:P:241:LEU:HD23 | 23:P:264:ILE:HG13 | 1.93 | 0.49 |
| 28:U:46:ILE:HG21 | 28:U:119:LEU:HD22 | 1.92 | 0.49 |
| 28:U:54:LEU:CD2 | 28:U:72:TYR:CD2 | 2.96 | 0.49 |
| 33:Z:205:LEU:HA | 33:Z:236:PHE:HZ | 1.77 | 0.49 |
| 2:2:109:HIS:HB3 | 2:2:111:PHE:HE2 | 1.77 | 0.49 |
| 7:7:8:TYR:CE2 | 7:7:10:ASN:C | 2.85 | 0.49 |
| 11:D:193:LYS:HE2 | 11:D:197:ARG:NH2 | 2.27 | 0.49 |
| 15:H:307:PHE:CE2 | 15:H:309:ASP:OD1 | 2.66 | 0.49 |
| 17:J:29:GLU:O | 17:J:32:LEU:HB3 | 2.12 | 0.49 |
| 18:K:346:ARG:CG | 18:K:349:ARG:NH2 | 2.61 | 0.49 |
| 20:M:129:LEU:HD21 | 20:M:155:ILE:HG13 | 1.95 | 0.49 |
| 20:M:289:LYS:HD3 | 20:M:305:MET:HE2 | 1.94 | 0.49 |
| 20:M:338:LEU:HD21 | 20:M:346:LYS:NZ | 2.27 | 0.49 |
| 22:O:41:LEU:CD2 | 22:O:62:TYR:HB2 | 2.42 | 0.49 |
| 22:O:384:MET:HE3 | 28:U:190:LEU:CA | 2.42 | 0.49 |
| 23:P:292:LYS:HG2 | 23:P:320:PRO:HB2 | 1.93 | 0.49 |
| 25:R:338:TYR:CZ | 25:R:368:LEU:HD11 | 2.48 | 0.49 |
| 29:V:52:LEU:HD12 | 29:V:69:PHE:HZ | 1.77 | 0.49 |
| 29:V:84:ASP:OD2 | 29:V:87:PHE:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:W:9:VAL:HA | 30:W:52:ILE:HG13 | 1.94 | 0.49 |
| 30:W:35:PHE:CE2 | 30:W:182:TYR:CE2 | 3.00 | 0.49 |
| 33:Z:168:GLN:CD | 33:Z:195:PHE:CE1 | 2.86 | 0.49 |
| 33:Z:532:HIS:O | 33:Z:535:VAL:HG23 | 2.11 | 0.49 |
| 1:1:123:PRO:HG2 | 1:1:124:TYR:CD1 | 2.47 | 0.49 |
| 5:5:1:THR:HA | 5:5:17:ASP:OD2 | 2.13 | 0.49 |
| 6:6:31:GLU:CD | 7:7:129:TYR:HA | 2.33 | 0.49 |
| 8:A:148:GLU:OE2 | 8:A:230:LYS:HG3 | 2.12 | 0.49 |
| 11:D:181:ARG:NH1 | 12:E:57:PRO:O | 2.45 | 0.49 |
| 15:H:274:VAL:HG21 | 15:H:308:PHE:CE2 | 2.48 | 0.49 |
| 15:H:351:VAL:HG11 | 15:H:353:PHE:CE1 | 2.37 | 0.49 |
| 16:I:340:ARG:NH1 | 16:I:343:ARG:HG3 | 2.26 | 0.49 |
| 17:J:162:GLU:HG2 | 17:J:166:LEU:HD12 | 1.94 | 0.49 |
| 21:N:340:HIS:HB2 | 21:N:374:ILE:HG12 | 1.92 | 0.49 |
| 24:Q:176:ASP:O | 24:Q:180:LEU:HG | 2.12 | 0.49 |
| 24:Q:353:PRO:C | 24:Q:354:PHE:CD1 | 2.86 | 0.49 |
| 29:V:254:ARG:O | 29:V:258:GLU:HG3 | 2.13 | 0.49 |
| 33:Z:294:ILE:O | 33:Z:298:PHE:CD2 | 2.65 | 0.49 |
| 33:Z:295:ARG:NH2 | 33:Z:325:GLY:HA3 | 2.27 | 0.49 |
| 33:Z:486:SER:O | 33:Z:490:ILE:CG1 | 2.25 | 0.49 |
| 33:Z:957:LEU:C | 33:Z:957:LEU:HD12 | 2.32 | 0.49 |
| 2:2:113:ILE:HG12 | 2:2:119:THR:HG22 | 1.93 | 0.49 |
| 3:3:100:VAL:HG21 | 3:3:115:PHE:HE1 | 1.78 | 0.49 |
| 9:B:94:HIS:HA | 9:B:98:LYS:CE | 2.43 | 0.49 |
| 16:I:126:PRO:CG | 16:I:154:MET:CE | 2.77 | 0.49 |
| 21:N:162:ARG:CZ | 21:N:165:ILE:CD1 | 2.91 | 0.49 |
| 22:O:250:TRP:CZ2 | 22:O:271:LYS:HG2 | 2.47 | 0.49 |
| 24:Q:246:TYR:HA | 24:Q:249:LEU:HD12 | 1.93 | 0.49 |
| 33:Z:463:HIS:CE1 | 33:Z:497:PHE:CD1 | 3.01 | 0.49 |
| 2:2:59:ILE:O | 2:2:63:ILE:HG12 | 2.13 | 0.49 |
| 3:3:109:LYS:CE | 3:3:125:LYS:NZ | 2.76 | 0.49 |
| 5:5:159:ARG:NH2 | 5:5:203:GLU:OE1 | 2.45 | 0.49 |
| 7:7:-3:VAL:HG23 | 7:7:49:ILE:H | 1.76 | 0.49 |
| 7:7:144:ASN:O | 7:7:148:ARG:HG3 | 2.13 | 0.49 |
| 9:B:159:TRP:CE2 | 10:C:57:LEU:HD13 | 2.48 | 0.49 |
| 15:H:392:HIS:CE1 | 15:H:420:ARG:CG | 2.94 | 0.49 |
| 16:I:117:HIS:O | 16:I:118:ALA:HB2 | 2.12 | 0.49 |
| 18:K:280:LYS:HZ1 | 18:K:296:LEU:CD2 | 2.19 | 0.49 |
| 19:L:133:ASN:ND2 | 28:U:86:LYS:NZ | 2.60 | 0.49 |
| 19:L:165:PRO:HB3 | 19:L:269:TYR:CE2 | 2.48 | 0.49 |
| 21:N:642:ASP:HB2 | 21:N:643:PRO:CD | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:O:188:PHE:HD2 | 22:O:220:SER:HB3 | 1.77 | 0.49 |
| 23:P:237:VAL:CG1 | 23:P:267:PHE:CE2 | 2.95 | 0.49 |
| 24:Q:64:LEU:O | 24:Q:68:MET:HG2 | 2.13 | 0.49 |
| 27:T:32:ILE:HA | 27:T:35:ILE:HD12 | 1.95 | 0.49 |
| 27:T:228:ILE:HG22 | 27:T:229:VAL:O | 2.13 | 0.49 |
| 28:U:67:PHE:CE1 | 30:W:97:THR:HG23 | 2.47 | 0.49 |
| 2:2:73:GLU:O | 2:2:75:ARG:NH1 | 2.45 | 0.49 |
| 4:4:37:LEU:HD12 | 4:4:60:GLN:HG2 | 1.95 | 0.49 |
| 12:E:165:TYR:HE2 | 20:M:433:TYR:O | 1.96 | 0.49 |
| 14:G:98:PHE:CE2 | 14:G:104:THR:HG23 | 2.47 | 0.49 |
| 16:I:193:GLU:OE1 | 16:I:348:ILE:HG12 | 2.12 | 0.49 |
| 17:J:151:GLY:HA3 | 17:J:326:GLU:HG3 | 1.95 | 0.49 |
| 17:J:337:LEU:O | 25:R:204:TRP:NE1 | 2.46 | 0.49 |
| 18:K:281:ARG:NH1 | 18:K:287:GLY:O | 2.46 | 0.49 |
| 18:K:353:PHE:HD1 | 18:K:387:MET:SD | 2.36 | 0.49 |
| 20:M:159:LEU:HB3 | 20:M:160:PRO:HD2 | 1.94 | 0.49 |
| 21:N:83:LEU:HD11 | 21:N:133:LEU:HD21 | 1.95 | 0.49 |
| 21:N:657:MET:CB | 21:N:682:PHE:CE1 | 2.95 | 0.49 |
| 22:O:384:MET:HE1 | 28:U:189:ARG:CB | 2.43 | 0.49 |
| 23:P:90:LYS:HE3 | 23:P:129:LYS:HB3 | 1.95 | 0.49 |
| 24:Q:273:ASN:CB | 24:Q:306:TYR:OH | 2.59 | 0.49 |
| 25:R:356:ALA:O | 32:Y:89:GLN:NE2 | 2.46 | 0.49 |
| 25:R:417:TYR:CZ | 28:U:292:ILE:CG2 | 2.95 | 0.49 |
| 31:X:73:THR:HB | 31:X:129:LEU:HD11 | 1.94 | 0.49 |
| 2:2:160:GLN:NE2 | 2:2:164:TRP:CE2 | 2.80 | 0.49 |
| 5:5:145:LYS:HB3 | 5:5:148:LEU:HG | 1.95 | 0.49 |
| 15:H:246:ILE:HD11 | 15:H:352:MET:HG2 | 1.95 | 0.49 |
| 19:L:117:TYR:CE1 | 19:L:131:VAL:HG13 | 2.44 | 0.49 |
| 19:L:231:LEU:O | 19:L:235:VAL:HG23 | 2.13 | 0.49 |
| 21:N:447:SER:HA | 21:N:450:ILE:HG22 | 1.94 | 0.49 |
| 23:P:203:ILE:CG1 | 23:P:220:TYR:CZ | 2.90 | 0.49 |
| 23:P:308:LEU:HD21 | 23:P:346:ILE:HA | 1.95 | 0.49 |
| 23:P:392:LYS:HG2 | 24:Q:354:PHE:CD2 | 2.47 | 0.49 |
| 24:Q:59:LEU:HD13 | 24:Q:103:LYS:HG2 | 1.95 | 0.49 |
| 26:S:343:LEU:HD12 | 26:S:347:HIS:CE1 | 2.48 | 0.49 |
| 27:T:131:LYS:H | 27:T:135:ASN:ND2 | 2.11 | 0.49 |
| 33:Z:889:VAL:HG23 | 33:Z:891:PRO:HD2 | 1.93 | 0.49 |
| 33:Z:924:LYS:HZ3 | 33:Z:993:GLU:HG3 | 1.74 | 0.49 |
| 1:1:1:THR:HG22 | 1:1:1:THR:O | 2.13 | 0.49 |
| 1:1:120:HIS:CB | 7:7:28:PHE:CE1 | 2.95 | 0.49 |
| 6:6:31:GLU:OE1 | 7:7:129:TYR:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:D:7:ALA:CB | 12:E:125:GLU:OE2 | 2.53 | 0.49 |
| 12:E:45:GLY:HA2 | 12:E:153:TYR:CE1 | 2.47 | 0.49 |
| 17:J:56:ARG:NH2 | 21:N:611:LYS:O | 2.42 | 0.49 |
| 18:K:216:GLY:HA3 | 19:L:342:ARG:HH22 | 1.75 | 0.49 |
| 20:M:59:LEU:O | 20:M:62:ILE:HG22 | 2.13 | 0.49 |
| 23:P:48:GLN:HE22 | 23:P:86:HIS:CG | 2.31 | 0.49 |
| 25:R:113:LEU:HD22 | 25:R:136:ASN:HB3 | 1.94 | 0.49 |
| 25:R:175:ALA:HB2 | 25:R:209:ARG:HD3 | 1.94 | 0.49 |
| 26:S:399:TYR:HB3 | 26:S:402:ILE:HD13 | 1.94 | 0.49 |
| 33:Z:99:LEU:HB2 | 33:Z:119:LEU:HD21 | 1.94 | 0.49 |
| 33:Z:371:SER:HB3 | 33:Z:399:LEU:HD13 | 1.95 | 0.49 |
| 3:3:-2:ASN:ND2 | 3:3:48:ALA:H | 2.11 | 0.48 |
| 8:A:104:PHE:CD1 | 8:A:108:TYR:CD2 | 3.01 | 0.48 |
| 9:B:250:LEU:HD22 | 24:Q:132:PHE:CZ | 2.48 | 0.48 |
| 11:D:6:ARG:HH12 | 13:F:123:TYR:CB | 2.26 | 0.48 |
| 12:E:184:LEU:HD13 | 13:F:56:LEU:HG | 1.94 | 0.48 |
| 15:H:65:GLU:O | 15:H:69:VAL:CG2 | 2.52 | 0.48 |
| 15:H:418:GLU:O | 15:H:422:VAL:HG23 | 2.13 | 0.48 |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:HB | 1.95 | 0.48 |
| 17:J:286:LYS:HE3 | 17:J:289:LYS:NZ | 2.28 | 0.48 |
| 18:K:242:PHE:C | 18:K:244:HIS:N | 2.66 | 0.48 |
| 19:L:228:LYS:HB2 | 19:L:349:ILE:CD1 | 2.43 | 0.48 |
| 20:M:82:VAL:HG11 | 20:M:140:LEU:HB3 | 1.95 | 0.48 |
| 21:N:447:SER:O | 21:N:450:ILE:HG22 | 2.13 | 0.48 |
| 23:P:72:TRP:HH2 | 23:P:103:TYR:HB2 | 1.56 | 0.48 |
| 28:U:293:GLU:CG | 29:V:277:LYS:HE3 | 2.43 | 0.48 |
| 29:V:168:LEU:HD11 | 29:V:188:LEU:HG | 1.95 | 0.48 |
| 33:Z:74:SER:HB3 | 33:Z:79:THR:CG2 | 2.42 | 0.48 |
| 33:Z:290:GLU:HB3 | 33:Z:293:MET:HG3 | 1.95 | 0.48 |
| 33:Z:546:ILE:HG22 | 33:Z:550:PHE:CD2 | 2.48 | 0.48 |
| 1:1:98:ILE:CD1 | 1:1:127:ALA:HB3 | 2.37 | 0.48 |
| 4:4:63:ILE:HD11 | 4:4:82:PHE:CD2 | 2.48 | 0.48 |
| 11:D:120:TYR:CD2 | 11:D:129:PHE:CE1 | 3.01 | 0.48 |
| 12:E:35:SER:OG | 12:E:53:ARG:NE | 2.35 | 0.48 |
| 12:E:157:HIS:CE1 | 12:E:159:GLU:OE2 | 2.65 | 0.48 |
| 15:H:172:MET:C | 16:I:129:TYR:CZ | 2.71 | 0.48 |
| 16:I:362:LEU:CD2 | 16:I:377:LEU:CD2 | 2.91 | 0.48 |
| 17:J:186:ILE:CG2 | 17:J:313:LYS:HG2 | 2.44 | 0.48 |
| 17:J:210:PHE:CE2 | 17:J:212:ARG:HG3 | 2.48 | 0.48 |
| 19:L:92:GLU:CG | 20:M:65:ASN:HD21 | 2.26 | 0.48 |
| 19:L:125:PRO:HG2 | 19:L:127:TYR:OH | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:140:LEU:HD21 | 19:L:158:ILE:HD11 | 1.94 | 0.48 |
| 19:L:193:LEU:HD21 | 19:L:347:VAL:HG21 | 1.94 | 0.48 |
| 19:L:357:ARG:HB3 | 19:L:361:PHE:HE2 | 1.77 | 0.48 |
| 20:M:167:VAL:HG23 | 20:M:269:LEU:CD1 | 2.43 | 0.48 |
| 23:P:306:ASN:OD1 | 23:P:306:ASN:O | 2.31 | 0.48 |
| 23:P:311:TRP:CD1 | 23:P:345:VAL:HG21 | 2.48 | 0.48 |
| 24:Q:141:LEU:HG | 24:Q:145:HIS:HD2 | 1.74 | 0.48 |
| 24:Q:239:PHE:CE2 | 24:Q:264:TYR:HB3 | 2.48 | 0.48 |
| 31:X:120:GLU:O | 31:X:124:LYS:HG3 | 2.13 | 0.48 |
| 33:Z:103:TYR:HE1 | 33:Z:116:ALA:CB | 2.25 | 0.48 |
| 33:Z:781:GLY:HA2 | 33:Z:818:CYS:SG | 2.54 | 0.48 |
| 1:1:143:ARG:HG2 | 1:1:144:GLU:O | 2.14 | 0.48 |
| 2:2:210:THR:HG23 | 3:3:160:GLN:NE2 | 2.27 | 0.48 |
| 4:4:40:HIS:CE1 | 4:4:108:LYS:HD3 | 2.49 | 0.48 |
| 9:B:66:LEU:CD1 | 9:B:235:PHE:CE2 | 2.87 | 0.48 |
| 12:E:14:THR:HG22 | 12:E:22:PHE:HE2 | 1.78 | 0.48 |
| 12:E:121:LEU:HD22 | 13:F:79:PRO:HB3 | 1.95 | 0.48 |
| 15:H:171:GLY:O | 16:I:129:TYR:CE1 | 2.66 | 0.48 |
| 16:I:290:LYS:CE | 16:I:336:PRO:HD3 | 2.43 | 0.48 |
| 17:J:326:GLU:OE2 | 17:J:329:ARG:NH2 | 2.43 | 0.48 |
| 19:L:169:ASN:HD22 | 19:L:262:ILE:HD13 | 1.79 | 0.48 |
| 21:N:223:LEU:O | 21:N:227:LYS:HG3 | 2.13 | 0.48 |
| 21:N:776:TYR:HD2 | 21:N:881:TYR:HB3 | 1.77 | 0.48 |
| 23:P:425:HIS:CG | 28:U:228:LYS:HZ1 | 2.31 | 0.48 |
| 24:Q:164:GLU:O | 24:Q:168:LEU:HB2 | 2.12 | 0.48 |
| 25:R:130:GLN:NE2 | 25:R:134:TRP:NE1 | 2.48 | 0.48 |
| 27:T:108:LEU:HD23 | 27:T:174:PHE:HE1 | 1.76 | 0.48 |
| 33:Z:56:LEU:HD23 | 33:Z:68:LEU:CD2 | 2.41 | 0.48 |
| 6:6:91:LYS:O | 6:6:96:TYR:CE1 | 2.66 | 0.48 |
| 8:A:158:ASP:OD2 | 8:A:162:TYR:HB3 | 2.13 | 0.48 |
| 12:E:70:ILE:HD12 | 12:E:74:ILE:HG22 | 1.95 | 0.48 |
| 13:F:49:LEU:CD2 | 13:F:201:LEU:HD21 | 2.43 | 0.48 |
| 15:H:101:ARG:NH2 | 15:H:150:LYS:HD3 | 2.27 | 0.48 |
| 15:H:246:ILE:HD11 | 15:H:352:MET:CE | 2.42 | 0.48 |
| 16:I:141:LEU:HD21 | 16:I:159:VAL:HB | 1.94 | 0.48 |
| 17:J:146:THR:HG22 | 17:J:149:MET:HB2 | 1.95 | 0.48 |
| 18:K:71:GLU:OE2 | 21:N:576:VAL:CG2 | 2.55 | 0.48 |
| 24:Q:141:LEU:CG | 24:Q:145:HIS:NE2 | 2.76 | 0.48 |
| 26:S:390:THR:HA | 26:S:393:ARG:NH1 | 2.29 | 0.48 |
| 26:S:425:ARG:HH12 | 27:T:155:GLY:N | 2.11 | 0.48 |
| 27:T:220:PHE:HB3 | 27:T:224:ARG:HH12 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:U:293:GLU:HG2 | 29:V:277:LYS:HE3 | 1.94 | 0.48 |
| 33:Z:321:PHE:CZ | 33:Z:349:THR:O | 2.67 | 0.48 |
| 33:Z:481:PRO:O | 33:Z:482:ASP:HB2 | 2.13 | 0.48 |
| 1:1:126:ILE:HD12 | 1:1:131:SER:O | 2.13 | 0.48 |
| 3:3:64:LEU:CD1 | 10:C:92:ARG:HB3 | 2.43 | 0.48 |
| 8:A:117:LEU:HD23 | 8:A:143:PHE:CE1 | 2.49 | 0.48 |
| 10:C:29:ILE:HD11 | 10:C:153:PRO:HD3 | 1.95 | 0.48 |
| 11:D:64:VAL:HG11 | 11:D:213:THR:HG21 | 1.95 | 0.48 |
| 13:F:159:THR:HA | 13:F:169:LYS:CE | 2.40 | 0.48 |
| 15:H:428:MET:CG | 16:I:346:ARG:HH21 | 2.24 | 0.48 |
| 16:I:172:LYS:CD | 17:J:231:ARG:HH12 | 2.27 | 0.48 |
| 16:I:384:LYS:CD | 16:I:420:LYS:HD2 | 2.37 | 0.48 |
| 17:J:32:LEU:HD22 | 26:S:225:HIS:CE1 | 2.49 | 0.48 |
| 19:L:371:THR:HG21 | 19:L:411:ASN:HD22 | 1.78 | 0.48 |
| 20:M:72:ASN:HB3 | 20:M:156:LEU:HD22 | 1.94 | 0.48 |
| 20:M:207:PHE:CD2 | 20:M:212:ILE:HD11 | 2.49 | 0.48 |
| 21:N:183:VAL:HG21 | 21:N:221:ASP:OD2 | 2.13 | 0.48 |
| 23:P:332:GLU:O | 23:P:333:ALA:HB2 | 2.14 | 0.48 |
| 24:Q:165:PHE:CE2 | 24:Q:173:SER:OG | 2.60 | 0.48 |
| 25:R:70:TYR:O | 25:R:70:TYR:CG | 2.63 | 0.48 |
| 26:S:451:ILE:O | 26:S:452:TYR:HB2 | 2.13 | 0.48 |
| 27:T:89:TYR:CE1 | 27:T:102:LYS:HB2 | 2.49 | 0.48 |
| 28:U:24:ARG:HH22 | 29:V:66:VAL:CG1 | 2.27 | 0.48 |
| 29:V:181:ASN:C | 29:V:182:LYS:HG2 | 2.34 | 0.48 |
| 29:V:186:GLN:HG2 | 29:V:190:HIS:CD2 | 2.48 | 0.48 |
| 30:W:20:ASP:HB2 | 30:W:25:ARG:CZ | 2.43 | 0.48 |
| 30:W:133:LYS:HE3 | 30:W:163:ASN:ND2 | 2.22 | 0.48 |
| 31:X:87:PHE:CE2 | 31:X:121:ILE:HG21 | 2.47 | 0.48 |
| 31:X:121:ILE:O | 31:X:125:MET:HG2 | 2.13 | 0.48 |
| 3:3:65:TYR:HD2 | 3:3:73:ILE:HG22 | 1.76 | 0.48 |
| 4:4:72:TYR:OH | 4:4:109:LYS:HB3 | 2.13 | 0.48 |
| 6:6:77:ILE:HD11 | 6:6:102:ILE:HB | 1.95 | 0.48 |
| 8:A:34:ALA:O | 8:A:35:THR:CG2 | 2.61 | 0.48 |
| 10:C:5:ARG:O | 10:C:6:TYR:HD1 | 1.96 | 0.48 |
| 13:F:101:ARG:HH11 | 13:F:103:LEU:HA | 1.65 | 0.48 |
| 13:F:168:ALA:O | 13:F:172:LEU:HG | 2.13 | 0.48 |
| 17:J:200:ARG:HG2 | 17:J:210:PHE:CD2 | 2.48 | 0.48 |
| 21:N:510:HIS:HB2 | 21:N:513:ILE:HD12 | 1.95 | 0.48 |
| 21:N:657:MET:HG2 | 21:N:682:PHE:CE1 | 2.45 | 0.48 |
| 21:N:919:THR:CG2 | 21:N:922:GLN:HG2 | 2.44 | 0.48 |
| 22:O:138:LEU:HD23 | 22:O:138:LEU:C | 2.33 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:P:308:LEU:HD12 | 23:P:349:ASN:OD1 | 2.08 | 0.48 |
| 24:Q:50:ARG:NH2 | 24:Q:53:GLU:HB2 | 2.29 | 0.48 |
| 25:R:209:ARG:NE | 25:R:243:LEU:HD22 | 2.19 | 0.48 |
| 25:R:331:ARG:O | 25:R:371:PHE:CZ | 2.66 | 0.48 |
| 27:T:57:ILE:HG23 | 27:T:58:THR:N | 2.28 | 0.48 |
| 33:Z:407:VAL:HG12 | 33:Z:415:MET:HE1 | 1.96 | 0.48 |
| 33:Z:924:LYS:HA | 33:Z:959:HIS:HD2 | 1.79 | 0.48 |
| 3:3:155:PHE:HB2 | 3:3:180:ILE:CD1 | 2.43 | 0.48 |
| 8:A:58:LYS:HE2 | 19:L:384:ASP:OD1 | 2.14 | 0.48 |
| 20:M:203:ARG:CZ | 20:M:206:LYS:HZ1 | 2.27 | 0.48 |
| 20:M:236:ALA:CA | 20:M:277:ILE:HD12 | 2.43 | 0.48 |
| 21:N:657:MET:CG | 21:N:682:PHE:HE1 | 2.26 | 0.48 |
| 23:P:363:LEU:HG | 23:P:398:LYS:HD3 | 1.94 | 0.48 |
| 25:R:298:ALA:O | 25:R:299:SER:CB | 2.60 | 0.48 |
| 28:U:32:ARG:CD | 28:U:94:HIS:CE1 | 2.97 | 0.48 |
| 33:Z:744:ALA:CB | 33:Z:783:VAL:HG23 | 2.43 | 0.48 |
| 33:Z:884:THR:OG1 | 33:Z:904:LEU:CD2 | 2.61 | 0.48 |
| 2:2:36:ARG:NH1 | 2:2:38:SER:HA | 2.28 | 0.48 |
| 4:4:34:THR:CG2 | 4:4:181:LYS:HZ2 | 2.27 | 0.48 |
| 4:4:39:PRO:HD2 | 4:4:73:GLU:OE2 | 2.14 | 0.48 |
| 8:A:160:ALA:HB1 | 18:K:428:LYS:HG2 | 1.95 | 0.48 |
| 9:B:67:LEU:HD11 | 9:B:73:ALA:CB | 2.39 | 0.48 |
| 9:B:123:GLN:HE22 | 10:C:86:ILE:HG13 | 1.78 | 0.48 |
| 9:B:210:GLU:CG | 9:B:237:LYS:HE3 | 2.20 | 0.48 |
| 9:B:217:GLU:HB3 | 9:B:234:ARG:HG2 | 1.95 | 0.48 |
| 12:E:14:THR:CG2 | 12:E:22:PHE:CE2 | 2.96 | 0.48 |
| 13:F:12:THR:CG2 | 13:F:19:LEU:CD2 | 2.92 | 0.48 |
| 19:L:390:ASP:OD1 | 20:M:338:LEU:HD13 | 2.14 | 0.48 |
| 21:N:263:SER:CB | 21:N:721:ASP:OD2 | 2.62 | 0.48 |
| 21:N:758:VAL:H | 21:N:874:ILE:HD12 | 1.78 | 0.48 |
| 26:S:381:VAL:HG22 | 27:T:150:ARG:HE | 1.78 | 0.48 |
| 28:U:11:ALA:HB3 | 28:U:14:VAL:HG23 | 1.95 | 0.48 |
| 30:W:99:LYS:NZ | 30:W:135:ASN:HB3 | 2.29 | 0.48 |
| 33:Z:233:LEU:O | 33:Z:271:ILE:HD11 | 2.13 | 0.48 |
| 1:1:116:GLY:CA | 7:7:-4:ILE:HD11 | 2.40 | 0.48 |
| 3:3:155:PHE:HB2 | 3:3:180:ILE:HD11 | 1.96 | 0.48 |
| 11:D:174:PHE:HZ | 11:D:197:ARG:HB3 | 1.78 | 0.48 |
| 15:H:168:ILE:HG12 | 15:H:174:VAL:HB | 1.96 | 0.48 |
| 19:L:170:MET:HG2 | 19:L:266:MET:HE3 | 1.96 | 0.48 |
| 20:M:384:ASP:O | 20:M:385:GLU:HB3 | 2.14 | 0.48 |
| 21:N:314:LEU:HD13 | 21:N:336:ASN:OD1 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:61:LEU:HD21 | 24:Q:65:TYR:CZ | 2.44 | 0.48 |
| 24:Q:419:LEU:HD21 | 28:U:286:ILE:HG12 | 1.96 | 0.48 |
| 27:T:89:TYR:CG | 27:T:102:LYS:HD2 | 2.49 | 0.48 |
| 30:W:20:ASP:HB2 | 30:W:25:ARG:NH2 | 2.21 | 0.48 |
| 33:Z:493:LEU:CD2 | 33:Z:497:PHE:CE2 | 2.97 | 0.48 |
| 33:Z:493:LEU:HG | 33:Z:497:PHE:CD2 | 2.48 | 0.48 |
| 33:Z:550:PHE:HZ | 33:Z:566:LEU:C | 2.18 | 0.48 |
| 33:Z:850:LEU:HD23 | 33:Z:850:LEU:O | 2.13 | 0.48 |
| 1:1:138:CYS:HA | 1:1:154:PHE:HZ | 1.78 | 0.48 |
| 5:5:159:ARG:NH1 | 5:5:200:VAL:HG22 | 2.28 | 0.48 |
| 7:7:92:MET:HE2 | 7:7:122:VAL:HG22 | 1.96 | 0.48 |
| 13:F:190:ILE:HG23 | 13:F:213:ILE:HD13 | 1.95 | 0.48 |
| 15:H:254:THR:OG1 | 15:H:377:PHE:CZ | 2.58 | 0.48 |
| 15:H:299:ARG:HH21 | 15:H:345:PRO:HD3 | 1.77 | 0.48 |
| 16:I:137:ASP:HB2 | 16:I:140:LEU:HG | 1.96 | 0.48 |
| 17:J:228:ARG:NH1 | 17:J:232:GLU:CD | 2.66 | 0.48 |
| 18:K:83:GLN:O | 18:K:86:VAL:HG12 | 2.14 | 0.48 |
| 18:K:150:LEU:HD22 | 19:L:112:LEU:HD21 | 1.96 | 0.48 |
| 18:K:258:PHE:CG | 18:K:302:GLN:CB | 2.92 | 0.48 |
| 22:O:48:PHE:CD1 | 22:O:80:LYS:NZ | 2.76 | 0.48 |
| 22:O:255:LEU:HD23 | 22:O:255:LEU:C | 2.34 | 0.48 |
| 24:Q:63:GLN:O | 24:Q:66:VAL:HG22 | 2.13 | 0.48 |
| 25:R:237:THR:OG1 | 25:R:238:PHE:CE1 | 2.65 | 0.48 |
| 26:S:145:PHE:O | 26:S:146:LEU:HB3 | 2.13 | 0.48 |
| 28:U:72:TYR:CZ | 28:U:76:MET:HG3 | 2.49 | 0.48 |
| 28:U:106:ILE:CG2 | 28:U:110:PHE:HE2 | 2.27 | 0.48 |
| 29:V:135:ARG:HD2 | 29:V:157:ARG:CZ | 2.31 | 0.48 |
| 33:Z:92:LEU:HD12 | 33:Z:95:THR:OG1 | 2.14 | 0.48 |
| 33:Z:363:ASP:O | 33:Z:366:LYS:CD | 2.62 | 0.48 |
| 2:2:197:GLU:HB2 | 3:3:142:GLU:OE2 | 2.14 | 0.47 |
| 4:4:37:LEU:HD23 | 4:4:41:THR:HG21 | 1.96 | 0.47 |
| 7:7:124:LEU:HD12 | 7:7:124:LEU:C | 2.34 | 0.47 |
| 8:A:219:SER:H | 8:A:222:ASP:HB2 | 1.79 | 0.47 |
| 11:D:68:ASP:CG | 11:D:97:ARG:NH2 | 2.50 | 0.47 |
| 13:F:91:GLN:HE22 | 13:F:108:ALA:HA | 1.79 | 0.47 |
| 14:G:168:ARG:HE | 14:G:172:LYS:CE | 2.27 | 0.47 |
| 15:H:422:VAL:HG13 | 15:H:446:ALA:HB3 | 1.95 | 0.47 |
| 15:H:434:ARG:HG2 | 33:Z:956:LEU:HB3 | 1.95 | 0.47 |
| 16:I:384:LYS:HD3 | 16:I:420:LYS:CD | 2.37 | 0.47 |
| 17:J:85:LEU:HD23 | 17:J:95:ILE:HG13 | 1.96 | 0.47 |
| 17:J:308:GLY:N | 17:J:311:ASP:OD1 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:140:LEU:HD23 | 19:L:158:ILE:HG12 | 1.96 | 0.47 |
| 19:L:290:ARG:NH1 | 19:L:293:GLU:C | 2.65 | 0.47 |
| 21:N:282:TYR:CE2 | 21:N:286:LEU:HB2 | 2.49 | 0.47 |
| 21:N:666:GLN:HG2 | 21:N:875:LEU:CD2 | 2.43 | 0.47 |
| 21:N:666:GLN:O | 21:N:875:LEU:HD22 | 2.13 | 0.47 |
| 22:O:204:SER:HB3 | 22:O:209:GLU:HG2 | 1.96 | 0.47 |
| 22:O:366:MET:SD | 28:U:229:LEU:HD13 | 2.54 | 0.47 |
| 23:P:270:LEU:HD22 | 23:P:340:ASP:HB2 | 1.96 | 0.47 |
| 27:T:211:PHE:CZ | 27:T:220:PHE:CE2 | 3.02 | 0.47 |
| 28:U:277:TYR:CE1 | 29:V:295:VAL:HG13 | 2.12 | 0.47 |
| 28:U:293:GLU:HG2 | 29:V:277:LYS:HD2 | 1.96 | 0.47 |
| 29:V:49:VAL:HG12 | 29:V:73:GLN:HG2 | 1.95 | 0.47 |
| 32:Y:82:ASP:HB3 | 32:Y:86:ARG:HH12 | 1.76 | 0.47 |
| 33:Z:208:VAL:HG21 | 33:Z:236:PHE:CZ | 2.46 | 0.47 |
| 33:Z:394:TYR:CB | 33:Z:859:LYS:HZ1 | 2.27 | 0.47 |
| 9:B:106:PRO:HD2 | 9:B:109:LEU:HD12 | 1.96 | 0.47 |
| 10:C:18:ARG:HH21 | 11:D:29:ARG:NH2 | 2.10 | 0.47 |
| 15:H:365:LEU:CD2 | 15:H:370:ARG:CZ | 2.92 | 0.47 |
| 15:H:456:LYS:HD3 | 16:I:332:GLU:HB3 | 1.95 | 0.47 |
| 16:I:389:GLY:HA2 | 16:I:392:ILE:HD12 | 1.95 | 0.47 |
| 21:N:325:PHE:HE1 | 29:V:167:ASN:OD1 | 1.96 | 0.47 |
| 21:N:585:ARG:CZ | 21:N:589:ILE:HD11 | 2.44 | 0.47 |
| 22:O:29:PHE:CE2 | 22:O:61:LEU:HD11 | 2.49 | 0.47 |
| 24:Q:114:GLN:HG3 | 24:Q:144:LEU:CD1 | 2.44 | 0.47 |
| 25:R:363:PHE:CE1 | 32:Y:78:LYS:CD | 2.80 | 0.47 |
| 26:S:338:MET:O | 26:S:342:LEU:HG | 2.14 | 0.47 |
| 31:X:104:LYS:HE3 | 31:X:108:ASN:CG | 2.34 | 0.47 |
| 33:Z:474:LEU:O | 33:Z:478:VAL:HG23 | 2.14 | 0.47 |
| 33:Z:535:VAL:HG22 | 33:Z:572:ILE:CG2 | 2.44 | 0.47 |
| 33:Z:846:PHE:HE2 | 33:Z:901:PHE:HE2 | 1.61 | 0.47 |
| 33:Z:850:LEU:HD21 | 33:Z:854:LEU:CD1 | 2.43 | 0.47 |
| 1:1:51:ASP:OD1 | 1:1:93:LEU:CD2 | 2.62 | 0.47 |
| 2:2:55:VAL:HG21 | 2:2:94:ILE:HG21 | 1.96 | 0.47 |
| 5:5:104:TYR:CE1 | 5:5:110:PRO:HD3 | 2.50 | 0.47 |
| 5:5:179:HIS:CB | 5:5:188:HIS:CD2 | 2.97 | 0.47 |
| 6:6:6:ILE:HB | 6:6:13:VAL:HG22 | 1.96 | 0.47 |
| 8:A:18:ILE:HD12 | 9:B:20:GLN:NE2 | 2.29 | 0.47 |
| 8:A:220:LYS:HD2 | 8:A:238:ALA:O | 2.14 | 0.47 |
| 8:A:252:ASP:OD2 | 23:P:85:LYS:CE | 2.57 | 0.47 |
| 9:B:18:LEU:HB2 | 9:B:21:ILE:HD12 | 1.96 | 0.47 |
| 10:C:50:ARG:NH2 | 10:C:211:LEU:O | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:97:LEU:HB2 | 15:H:173:ARG:CD | 2.44 | 0.47 |
| 16:I:358:LYS:NZ | 16:I:385:ASP:CA | 2.77 | 0.47 |
| 17:J:219:VAL:O | 17:J:219:VAL:HG12 | 2.15 | 0.47 |
| 20:M:72:ASN:HB2 | 20:M:156:LEU:HD21 | 1.95 | 0.47 |
| 21:N:147:ALA:O | 21:N:148:SER:HB2 | 2.14 | 0.47 |
| 22:O:213:LEU:O | 22:O:217:LEU:HG | 2.14 | 0.47 |
| 24:Q:309:ARG:NH2 | 24:Q:345:SER:OG | 2.44 | 0.47 |
| 33:Z:294:ILE:HD13 | 33:Z:320:SER:HB2 | 1.97 | 0.47 |
| 33:Z:469:PRO:CG | 33:Z:472:LEU:HD12 | 2.44 | 0.47 |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:CD2 | 2.19 | 0.47 |
| 33:Z:474:LEU:HD22 | 33:Z:493:LEU:CB | 2.43 | 0.47 |
| 33:Z:744:ALA:O | 33:Z:748:LEU:HG | 2.14 | 0.47 |
| 4:4:65:LEU:HD11 | 4:4:69:ARG:HE | 1.80 | 0.47 |
| 5:5:128:CYS:SG | 5:5:140:LEU:HD12 | 2.54 | 0.47 |
| 5:5:199:LYS:HG2 | 5:5:203:GLU:OE1 | 2.15 | 0.47 |
| 15:H:96:PRO:HB2 | 16:I:111:GLU:OE2 | 2.14 | 0.47 |
| 15:H:286:GLU:CD | 15:H:289:ARG:HH21 | 2.18 | 0.47 |
| 15:H:358:PRO:CG | 15:H:374:LYS:HZ1 | 2.27 | 0.47 |
| 21:N:298:TYR:CD1 | 21:N:768:ILE:HD11 | 2.50 | 0.47 |
| 21:N:436:ASP:O | 21:N:439:VAL:HG12 | 2.14 | 0.47 |
| 22:O:131:SER:HB3 | 22:O:135:ARG:HH12 | 1.77 | 0.47 |
| 23:P:264:ILE:HG21 | 23:P:280:LEU:HD11 | 1.95 | 0.47 |
| 25:R:94:PHE:HZ | 25:R:99:TYR:HH | 1.60 | 0.47 |
| 25:R:194:VAL:O | 25:R:197:MET:SD | 2.73 | 0.47 |
| 25:R:217:HIS:O | 25:R:220:ALA:HB3 | 2.15 | 0.47 |
| 25:R:411:LEU:HD23 | 26:S:464:ARG:HH12 | 1.72 | 0.47 |
| 28:U:67:PHE:CZ | 30:W:97:THR:CB | 2.98 | 0.47 |
| 28:U:111:LYS:HA | 28:U:118:PRO:HG3 | 1.95 | 0.47 |
| 30:W:52:ILE:HG22 | 30:W:61:VAL:HA | 1.95 | 0.47 |
| 33:Z:574:TYR:CZ | 33:Z:584:VAL:CB | 2.97 | 0.47 |
| 3:3:136:GLN:HB3 | 3:3:168:ARG:HH21 | 1.80 | 0.47 |
| 10:C:65:LYS:HA | 10:C:67:TYR:CE1 | 2.49 | 0.47 |
| 11:D:188:VAL:HG21 | 11:D:216:LYS:HE2 | 1.96 | 0.47 |
| 12:E:45:GLY:HA3 | 12:E:193:LEU:HD13 | 1.96 | 0.47 |
| 13:F:102:LYS:O | 13:F:103:LEU:HB3 | 2.14 | 0.47 |
| 13:F:114:ASP:O | 13:F:118:LYS:HG3 | 2.14 | 0.47 |
| 13:F:179:PHE:CE1 | 13:F:192:ALA:HB2 | 2.49 | 0.47 |
| 17:J:342:ASN:OD1 | 17:J:344:ARG:HB2 | 2.15 | 0.47 |
| 21:N:490:LEU:HD23 | 21:N:490:LEU:C | 2.35 | 0.47 |
| 21:N:584:ARG:HD2 | 21:N:614:ASN:ND2 | 2.29 | 0.47 |
| 21:N:762:ARG:CG | 21:N:890:PHE:HE2 | 2.24 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:O:62:TYR:HD2 | 22:O:82:LEU:CD1 | 2.03 | 0.47 |
| 26:S:151:GLU:OE1 | 26:S:154:GLN:CB | 2.62 | 0.47 |
| 27:T:115:SER:HB2 | 27:T:180:ILE:HG21 | 1.96 | 0.47 |
| 29:V:71:MET:HE1 | 29:V:83:VAL:HG13 | 1.95 | 0.47 |
| 33:Z:50:GLU:OE2 | 33:Z:55:ARG:NE | 2.48 | 0.47 |
| 1:1:19:ARG:HH21 | 1:1:171:GLY:HA2 | 1.74 | 0.47 |
| 1:1:175:MET:HB2 | 1:1:186:LEU:HB2 | 1.97 | 0.47 |
| 5:5:8:PHE:CD1 | 5:5:13:ILE:HG12 | 2.46 | 0.47 |
| 7:7:131:SER:HB3 | 7:7:134:LEU:CD2 | 2.45 | 0.47 |
| 8:A:30:TYR:CD1 | 14:G:16:PRO:HB3 | 2.49 | 0.47 |
| 9:B:139:HIS:CE1 | 9:B:145:PHE:CE1 | 3.03 | 0.47 |
| 11:D:189:GLU:HG3 | 11:D:232:TYR:OH | 2.14 | 0.47 |
| 13:F:146:GLU:OE2 | 13:F:148:GLN:NE2 | 2.45 | 0.47 |
| 17:J:332:SER:HB2 | 17:J:337:LEU:HD12 | 1.96 | 0.47 |
| 17:J:376:HIS:CG | 25:R:235:LEU:HD22 | 2.49 | 0.47 |
| 20:M:303:ARG:HH12 | 20:M:307:GLU:CB | 2.25 | 0.47 |
| 21:N:682:PHE:CE2 | 21:N:702:ALA:HB1 | 2.50 | 0.47 |
| 22:O:15:ARG:HA | 30:W:20:ASP:OD1 | 2.13 | 0.47 |
| 27:T:266:TYR:CD1 | 27:T:267:ALA:N | 2.82 | 0.47 |
| 1:1:175:MET:HE3 | 1:1:188:PHE:HE1 | 1.80 | 0.47 |
| 3:3:155:PHE:CD1 | 3:3:189:ARG:HD2 | 2.50 | 0.47 |
| 4:4:69:ARG:HG2 | 11:D:90:ARG:HD3 | 1.95 | 0.47 |
| 6:6:38:GLY:O | 6:6:39:ASP:HB2 | 2.15 | 0.47 |
| 9:B:67:LEU:CD1 | 9:B:73:ALA:HB2 | 2.43 | 0.47 |
| 11:D:6:ARG:HH12 | 13:F:123:TYR:HB2 | 1.80 | 0.47 |
| 12:E:220:SER:HA | 12:E:231:TYR:CD1 | 2.49 | 0.47 |
| 14:G:111:PHE:CD1 | 14:G:114:ARG:CZ | 2.97 | 0.47 |
| 16:I:278:ILE:HG21 | 16:I:325:ILE:CD1 | 2.44 | 0.47 |
| 17:J:232:GLU:O | 17:J:235:VAL:HB | 2.15 | 0.47 |
| 18:K:48:TYR:CE2 | 21:N:156:ILE:HD11 | 2.49 | 0.47 |
| 18:K:161:MET:HE3 | 18:K:257:VAL:HG21 | 1.95 | 0.47 |
| 19:L:82:ARG:CG | 19:L:86:LYS:HE3 | 2.45 | 0.47 |
| 19:L:92:GLU:HG2 | 20:M:65:ASN:HD21 | 1.80 | 0.47 |
| 19:L:170:MET:CE | 19:L:265:GLU:HB3 | 2.45 | 0.47 |
| 20:M:74:GLN:O | 20:M:77:TYR:CD1 | 2.66 | 0.47 |
| 20:M:129:LEU:CD2 | 20:M:155:ILE:HG13 | 2.45 | 0.47 |
| 21:N:329:HIS:CE1 | 21:N:363:ALA:HB1 | 2.49 | 0.47 |
| 21:N:362:TRP:CH2 | 29:V:23:THR:CB | 2.97 | 0.47 |
| 22:O:317:THR:O | 22:O:318:HIS:HB2 | 2.15 | 0.47 |
| 23:P:61:LYS:O | 23:P:65:LEU:HG | 2.15 | 0.47 |
| 23:P:143:LEU:HG | 23:P:147:LYS:HE3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:P:184:MET:HB2 | 23:P:223:LEU:CD1 | 2.38 | 0.47 |
| 23:P:264:ILE:HG22 | 23:P:280:LEU:HD11 | 1.97 | 0.47 |
| 24:Q:66:VAL:HG11 | 24:Q:107:VAL:HG23 | 1.97 | 0.47 |
| 24:Q:188:LEU:O | 24:Q:189:ARG:HB2 | 2.15 | 0.47 |
| 24:Q:325:LEU:HD21 | 24:Q:335:PHE:CE2 | 2.49 | 0.47 |
| 25:R:241:ILE:HG22 | 25:R:242:GLU:CG | 2.28 | 0.47 |
| 25:R:316:LEU:CD2 | 25:R:322:LEU:HB3 | 2.43 | 0.47 |
| 25:R:397:ASN:ND2 | 26:S:450:ASN:O | 2.48 | 0.47 |
| 27:T:20:TYR:CE1 | 27:T:71:GLN:HG3 | 2.49 | 0.47 |
| 27:T:236:ASN:CG | 27:T:238:GLN:HB2 | 2.34 | 0.47 |
| 28:U:65:VAL:CG1 | 30:W:96:LEU:CD1 | 2.93 | 0.47 |
| 28:U:92:TRP:CZ2 | 28:U:120:LEU:HD11 | 2.47 | 0.47 |
| 30:W:35:PHE:CD2 | 30:W:182:TYR:CD2 | 3.02 | 0.47 |
| 30:W:141:ILE:CG2 | 30:W:154:LEU:HD13 | 2.40 | 0.47 |
| 33:Z:205:LEU:HD23 | 33:Z:236:PHE:CE1 | 2.49 | 0.47 |
| 33:Z:301:THR:HG22 | 33:Z:307:HIS:ND1 | 2.23 | 0.47 |
| 33:Z:436:LEU:CD2 | 33:Z:455:ILE:CG1 | 2.92 | 0.47 |
| 1:1:48:SER:O | 1:1:52:THR:HG23 | 2.15 | 0.47 |
| 7:7:33:ARG:HH21 | 7:7:46:SER:N | 2.09 | 0.47 |
| 10:C:173:GLN:NE2 | 11:D:52:LEU:HB2 | 2.29 | 0.47 |
| 12:E:14:THR:HG22 | 12:E:22:PHE:CE2 | 2.50 | 0.47 |
| 13:F:159:THR:HA | 13:F:169:LYS:CD | 2.45 | 0.47 |
| 16:I:97:GLU:HB2 | 16:I:100:ARG:HH21 | 1.80 | 0.47 |
| 19:L:163:THR:OG1 | 19:L:265:GLU:HG3 | 2.14 | 0.47 |
| 20:M:76:PRO:C | 20:M:77:TYR:CD1 | 2.89 | 0.47 |
| 21:N:53:ASP:CB | 21:N:58:ARG:HH21 | 2.27 | 0.47 |
| 21:N:329:HIS:HB2 | 29:V:182:LYS:NZ | 1.90 | 0.47 |
| 24:Q:83:GLU:HA | 24:Q:86:MET:HG2 | 1.96 | 0.47 |
| 25:R:259:PHE:HE1 | 25:R:332:GLU:CB | 2.28 | 0.47 |
| 33:Z:985:LYS:CD | 33:Z:991:GLU:H | 2.28 | 0.47 |
| 3:3:177:VAL:CG1 | 3:3:190:TYR:CE1 | 2.98 | 0.47 |
| 6:6:56:VAL:HG12 | 6:6:60:LYS:HE3 | 1.97 | 0.47 |
| 6:6:91:LYS:O | 6:6:96:TYR:CD1 | 2.68 | 0.47 |
| 10:C:15:PRO:HG3 | 15:H:456:LYS:NZ | 2.29 | 0.47 |
| 13:F:12:THR:HG22 | 13:F:19:LEU:CD2 | 2.45 | 0.47 |
| 14:G:111:PHE:HB2 | 14:G:114:ARG:NH2 | 2.30 | 0.47 |
| 15:H:246:ILE:HD11 | 15:H:352:MET:HE3 | 1.97 | 0.47 |
| 15:H:423:CYS:HA | 15:H:443:PHE:HE1 | 1.80 | 0.47 |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:CB | 2.44 | 0.47 |
| 19:L:357:ARG:NH1 | 19:L:386:PHE:HB2 | 2.17 | 0.47 |
| 20:M:179:THR:HG1 | 20:M:182:ASP:CG | 2.17 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:137:PHE:O | 21:N:141:ILE:HG12 | 2.14 | 0.47 |
| 21:N:536:ILE:CD1 | 21:N:555:ILE:HG13 | 2.43 | 0.47 |
| 23:P:298:SER:O | 23:P:302:LEU:HG | 2.13 | 0.47 |
| 24:Q:348:CYS:SG | 24:Q:386:PHE:CD1 | 3.08 | 0.47 |
| 26:S:271:ARG:HG2 | 26:S:309:PHE:CE1 | 2.50 | 0.47 |
| 30:W:40:LYS:HZ1 | 30:W:111:VAL:HG21 | 1.80 | 0.47 |
| 33:Z:75:ILE:CG2 | 33:Z:121:ILE:HD13 | 2.44 | 0.47 |
| 1:1:51:ASP:CG | 1:1:93:LEU:HD22 | 2.35 | 0.47 |
| 1:1:66:TYR:HE2 | 1:1:73:PRO:CA | 2.27 | 0.47 |
| 4:4:95:ARG:CZ | 5:5:88:TYR:OH | 2.63 | 0.47 |
| 4:4:106:TYR:CE2 | 4:4:185:LYS:HB3 | 2.50 | 0.47 |
| 7:7:17:ASP:HA | 7:7:187:PHE:HA | 1.97 | 0.47 |
| 8:A:237:SER:O | 8:A:241:ILE:HG13 | 2.15 | 0.47 |
| 11:D:102:ASP:OD1 | 11:D:103:PRO:HD2 | 2.13 | 0.47 |
| 14:G:164:THR:HA | 14:G:168:ARG:HD2 | 1.98 | 0.47 |
| 15:H:334:LEU:CD1 | 20:M:285:ALA:HB2 | 2.44 | 0.47 |
| 15:H:365:LEU:HA | 15:H:370:ARG:NH1 | 2.30 | 0.47 |
| 16:I:78:ASN:O | 16:I:82:LEU:HG | 2.15 | 0.47 |
| 21:N:302:PHE:CE1 | 21:N:306:ASN:ND2 | 2.83 | 0.47 |
| 23:P:154:ASP:OD1 | 23:P:190:LYS:CE | 2.62 | 0.47 |
| 24:Q:382:LEU:CD1 | 25:R:263:ARG:NH1 | 2.77 | 0.47 |
| 26:S:234:ILE:HG13 | 26:S:257:LEU:HD13 | 1.97 | 0.47 |
| 31:X:76:VAL:HB | 31:X:88:ALA:HB3 | 1.96 | 0.47 |
| 33:Z:65:GLU:HA | 33:Z:111:LEU:HD21 | 1.96 | 0.47 |
| 33:Z:160:GLU:OE2 | 33:Z:164:VAL:HG21 | 2.15 | 0.47 |
| 33:Z:385:PHE:CZ | 33:Z:389:PHE:HE2 | 1.98 | 0.47 |
| 33:Z:813:PHE:CD2 | 33:Z:888:LEU:CD2 | 2.97 | 0.47 |
| 33:Z:833:GLN:NE2 | 33:Z:837:TYR:CZ | 2.81 | 0.47 |
| 7:7:6:MET:HE1 | 7:7:150:VAL:HG11 | 1.96 | 0.46 |
| 11:D:37:LYS:HD3 | 11:D:147:LEU:CB | 2.45 | 0.46 |
| 11:D:193:LYS:CG | 11:D:197:ARG:CZ | 2.93 | 0.46 |
| 16:I:119:ILE:HG23 | 16:I:127:ASP:OD1 | 2.14 | 0.46 |
| 16:I:245:LEU:CG | 16:I:247:ILE:HD11 | 2.41 | 0.46 |
| 17:J:143:PRO:O | 17:J:204:HIS:ND1 | 2.48 | 0.46 |
| 21:N:32:VAL:CG2 | 21:N:64:ILE:HG23 | 2.45 | 0.46 |
| 21:N:368:THR:O | 21:N:371:LEU:HB2 | 2.15 | 0.46 |
| 22:O:137:TYR:HB3 | 22:O:141:ASN:HD21 | 1.80 | 0.46 |
| 22:O:291:ILE:HG23 | 22:O:292:CYS:N | 2.30 | 0.46 |
| 23:P:203:ILE:HG23 | 23:P:220:TYR:CE2 | 2.49 | 0.46 |
| 24:Q:373:VAL:HG12 | 24:Q:377:LEU:CD1 | 2.45 | 0.46 |
| 28:U:19:LEU:HD11 | 29:V:212:MET:HB2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:U:20:ASP:CG | 28:U:24:ARG:HE | 2.12 | 0.46 |
| 28:U:77:ASN:ND2 | 28:U:81:LYS:HE3 | 2.30 | 0.46 |
| 33:Z:71:LEU:CD2 | 33:Z:118:VAL:HG13 | 2.45 | 0.46 |
| 33:Z:124:MET:C | 33:Z:124:MET:SD | 2.94 | 0.46 |
| 33:Z:376:SER:OG | 33:Z:379:GLN:HB2 | 2.14 | 0.46 |
| 33:Z:497:PHE:CG | 33:Z:505:VAL:HG11 | 2.51 | 0.46 |
| 2:2:59:ILE:CD1 | 2:2:82:MET:HB3 | 2.42 | 0.46 |
| 3:3:37:TYR:CE1 | 3:3:59:ARG:HB2 | 2.49 | 0.46 |
| 3:3:133:ALA:O | 3:3:137:LEU:HG | 2.16 | 0.46 |
| 4:4:43:MET:HE3 | 4:4:103:ILE:CD1 | 2.45 | 0.46 |
| 6:6:68:PHE:HZ | 13:F:67:ASP:CA | 2.28 | 0.46 |
| 6:6:68:PHE:HE1 | 13:F:65:LYS:HG2 | 1.79 | 0.46 |
| 15:H:335:GLU:OE1 | 20:M:249:PRO:HB2 | 2.15 | 0.46 |
| 16:I:190:GLN:OE1 | 16:I:190:GLN:N | 2.46 | 0.46 |
| 18:K:67:TYR:CD1 | 21:N:572:LEU:HB3 | 2.49 | 0.46 |
| 21:N:193:ALA:O | 21:N:197:VAL:HB | 2.16 | 0.46 |
| 21:N:230:VAL:HG22 | 21:N:265:ALA:HB2 | 1.97 | 0.46 |
| 21:N:710:GLY:O | 21:N:711:ARG:HB2 | 2.15 | 0.46 |
| 22:O:356:ARG:NH2 | 28:U:234:ASN:OD1 | 2.48 | 0.46 |
| 22:O:377:VAL:CG2 | 28:U:200:LEU:CD1 | 2.88 | 0.46 |
| 23:P:140:THR:HG21 | 23:P:163:LEU:HD22 | 1.97 | 0.46 |
| 24:Q:11:ALA:CB | 24:Q:27:TYR:CE1 | 2.98 | 0.46 |
| 24:Q:289:GLU:CD | 24:Q:291:TYR:CE1 | 2.86 | 0.46 |
| 24:Q:409:TYR:HB2 | 25:R:399:GLN:HG2 | 1.96 | 0.46 |
| 25:R:67:CYS:SG | 25:R:92:ILE:O | 2.73 | 0.46 |
| 26:S:425:ARG:CZ | 27:T:153:MET:O | 2.63 | 0.46 |
| 27:T:130:ASP:HB3 | 27:T:135:ASN:HD21 | 1.80 | 0.46 |
| 33:Z:64:TYR:CE1 | 33:Z:68:LEU:HD21 | 2.50 | 0.46 |
| 33:Z:217:GLU:O | 33:Z:221:VAL:HG23 | 2.15 | 0.46 |
| 33:Z:229:SER:OG | 33:Z:233:LEU:HG | 2.15 | 0.46 |
| 33:Z:393:GLY:O | 33:Z:394:TYR:HB2 | 2.16 | 0.46 |
| 33:Z:493:LEU:HD11 | 33:Z:497:PHE:HZ | 1.55 | 0.46 |
| 2:2:191:LEU:C | 2:2:193:PRO:HD3 | 2.35 | 0.46 |
| 10:C:21:GLN:NE2 | 10:C:129:ARG:HA | 2.30 | 0.46 |
| 11:D:214:VAL:HB | 11:D:222:VAL:CG1 | 2.45 | 0.46 |
| 14:G:33:GLY:O | 14:G:166:LYS:HG3 | 2.16 | 0.46 |
| 14:G:111:PHE:CE2 | 14:G:115:LEU:CD1 | 2.98 | 0.46 |
| 15:H:367:ARG:NH1 | 20:M:223:PRO:HB3 | 2.29 | 0.46 |
| 16:I:290:LYS:NZ | 16:I:336:PRO:HD3 | 2.30 | 0.46 |
| 17:J:135:SER:O | 17:J:136:LEU:HG | 2.14 | 0.46 |
| 18:K:212:TYR:OH | 18:K:320:ARG:HA | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:L:331:ASP:OD2 | 20:M:292:ASP:O | 2.33 | 0.46 |
| 21:N:85:ALA:O | 21:N:86:LYS:HB2 | 2.16 | 0.46 |
| 21:N:117:TYR:OH | 21:N:202:PHE:HA | 2.15 | 0.46 |
| 22:O:41:LEU:HG | 22:O:58:ARG:HD2 | 1.97 | 0.46 |
| 22:O:58:ARG:HB2 | 22:O:61:LEU:HD12 | 1.97 | 0.46 |
| 23:P:315:GLN:OE1 | 23:P:341:LEU:HD13 | 2.15 | 0.46 |
| 27:T:270:ILE:HD11 | 29:V:288:LEU:CD2 | 2.45 | 0.46 |
| 28:U:273:LEU:HD11 | 29:V:298:ALA:CB | 2.45 | 0.46 |
| 31:X:104:LYS:HZ1 | 31:X:107:GLY:C | 2.17 | 0.46 |
| 33:Z:809:MET:CE | 33:Z:847:ILE:HD11 | 2.45 | 0.46 |
| 3:3:60:TYR:HD2 | 10:C:96:GLN:HB3 | 1.72 | 0.46 |
| 15:H:173:ARG:HH21 | 16:I:119:ILE:HG21 | 1.80 | 0.46 |
| 16:I:76:VAL:HG12 | 33:Z:621:LEU:CD1 | 2.45 | 0.46 |
| 16:I:246:ARG:HE | 17:J:274:GLU:HB3 | 1.80 | 0.46 |
| 17:J:132:PRO:HG3 | 17:J:139:VAL:H | 1.79 | 0.46 |
| 18:K:132:LYS:HB3 | 18:K:133:PRO:HD2 | 1.97 | 0.46 |
| 20:M:354:GLU:HG2 | 20:M:357:ARG:HH22 | 1.80 | 0.46 |
| 20:M:379:LEU:O | 20:M:383:THR:HG23 | 2.15 | 0.46 |
| 21:N:53:ASP:CA | 21:N:58:ARG:NH2 | 2.60 | 0.46 |
| 25:R:354:ALA:HA | 25:R:364:LEU:CD2 | 2.45 | 0.46 |
| 27:T:51:TYR:O | 27:T:54:ASP:HB2 | 2.15 | 0.46 |
| 31:X:45:PHE:CE2 | 31:X:67:ILE:HD13 | 2.51 | 0.46 |
| 33:Z:187:SER:CA | 33:Z:198:GLU:HG2 | 2.44 | 0.46 |
| 33:Z:207:ILE:HA | 33:Z:210:TYR:HD2 | 1.80 | 0.46 |
| 1:1:84:GLU:O | 1:1:88:GLU:HG3 | 2.16 | 0.46 |
| 2:2:59:ILE:CD1 | 2:2:86:HIS:CE1 | 2.98 | 0.46 |
| 3:3:7:THR:CG2 | 3:3:112:ILE:CD1 | 2.93 | 0.46 |
| 3:3:37:TYR:HE1 | 3:3:59:ARG:CG | 2.22 | 0.46 |
| 9:B:18:LEU:HD12 | 9:B:21:ILE:HD12 | 1.98 | 0.46 |
| 10:C:107:PRO:HB3 | 10:C:143:ARG:HH22 | 1.76 | 0.46 |
| 13:F:67:ASP:OD2 | 13:F:69:HIS:NE2 | 2.48 | 0.46 |
| 15:H:329:VAL:HG11 | 16:I:300:ARG:CZ | 2.45 | 0.46 |
| 17:J:193:THR:HB | 17:J:316:PHE:HE2 | 1.80 | 0.46 |
| 18:K:212:TYR:CD1 | 18:K:321:ALA:HB2 | 2.50 | 0.46 |
| 19:L:145:ARG:NE | 19:L:162:GLU:CG | 2.76 | 0.46 |
| 21:N:10:LEU:HD22 | 21:N:42:GLU:HG3 | 1.96 | 0.46 |
| 22:O:185:PHE:CD1 | 22:O:223:LEU:HD13 | 2.50 | 0.46 |
| 24:Q:141:LEU:HG | 24:Q:145:HIS:NE2 | 2.30 | 0.46 |
| 24:Q:315:ASN:OD1 | 24:Q:339:TYR:HE1 | 1.99 | 0.46 |
| 28:U:111:LYS:HA | 28:U:118:PRO:CG | 2.45 | 0.46 |
| 28:U:293:GLU:HG2 | 29:V:277:LYS:HZ2 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:B:48:GLU:CG | 9:B:200:VAL:HG11 | 2.44 | 0.46 |
| 11:D:216:LYS:HB3 | 11:D:217:PRO:HD2 | 1.97 | 0.46 |
| 13:F:3:ARG:NH2 | 15:H:359:ASN:HD21 | 1.98 | 0.46 |
| 13:F:110:HIS:CE1 | 14:G:85:ARG:HB3 | 2.50 | 0.46 |
| 13:F:159:THR:CB | 13:F:169:LYS:HZ3 | 2.29 | 0.46 |
| 16:I:418:GLN:HB3 | 16:I:422:ARG:HH12 | 1.81 | 0.46 |
| 17:J:59:LYS:HG2 | 17:J:63:ARG:HH12 | 1.80 | 0.46 |
| 17:J:210:PHE:HE2 | 17:J:212:ARG:HD2 | 1.79 | 0.46 |
| 20:M:160:PRO:HB2 | 20:M:166:ARG:NH2 | 2.28 | 0.46 |
| 22:O:106:PHE:CG | 22:O:106:PHE:O | 2.68 | 0.46 |
| 24:Q:382:LEU:CB | 25:R:263:ARG:HH12 | 2.29 | 0.46 |
| 25:R:209:ARG:CZ | 25:R:243:LEU:HD13 | 2.45 | 0.46 |
| 26:S:283:GLN:O | 26:S:284:LEU:HB2 | 2.15 | 0.46 |
| 27:T:115:SER:HB2 | 27:T:180:ILE:CG2 | 2.45 | 0.46 |
| 28:U:67:PHE:HD2 | 30:W:100:HIS:HE1 | 1.58 | 0.46 |
| 30:W:89:THR:HG22 | 30:W:93:ILE:HD12 | 1.98 | 0.46 |
| 33:Z:212:LEU:HD23 | 33:Z:217:GLU:HG2 | 1.97 | 0.46 |
| 33:Z:440:LEU:HD12 | 33:Z:455:ILE:HD11 | 1.97 | 0.46 |
| 33:Z:866:VAL:HB | 33:Z:873:LEU:CD1 | 2.46 | 0.46 |
| 33:Z:957:LEU:HB2 | 33:Z:961:GLU:CD | 2.35 | 0.46 |
| 1:1:112:THR:HG21 | 7:7:27:ARG:HH21 | 1.81 | 0.46 |
| 5:5:4:LEU:HD12 | 5:5:4:LEU:O | 2.15 | 0.46 |
| 8:A:218:PHE:CD2 | 8:A:223:LEU:HD21 | 2.50 | 0.46 |
| 11:D:48:ARG:NH1 | 11:D:57:THR:HB | 2.29 | 0.46 |
| 13:F:65:LYS:CG | 13:F:222:PHE:CD2 | 2.95 | 0.46 |
| 13:F:101:ARG:NH1 | 13:F:104:ALA:H | 2.14 | 0.46 |
| 16:I:253:ILE:O | 16:I:253:ILE:HG22 | 2.15 | 0.46 |
| 17:J:145:SER:OG | 17:J:201:ALA:N | 2.49 | 0.46 |
| 20:M:159:LEU:HB3 | 20:M:160:PRO:CD | 2.45 | 0.46 |
| 21:N:232:LEU:HD12 | 21:N:237:LEU:HD11 | 1.97 | 0.46 |
| 21:N:427:ILE:CD1 | 21:N:450:ILE:HG12 | 2.46 | 0.46 |
| 21:N:892:PRO:HA | 21:N:905:LEU:HG | 1.97 | 0.46 |
| 23:P:138:ARG:NH1 | 23:P:141:LYS:HD3 | 2.31 | 0.46 |
| 23:P:395:ARG:HD2 | 24:Q:357:VAL:HB | 1.96 | 0.46 |
| 24:Q:165:PHE:CE1 | 24:Q:170:ASP:HB2 | 2.51 | 0.46 |
| 25:R:73:ASN:HB2 | 25:R:76:GLN:NE2 | 2.31 | 0.46 |
| 25:R:140:TYR:CD2 | 25:R:141:TYR:CD1 | 3.03 | 0.46 |
| 26:S:327:ILE:HG21 | 26:S:349:THR:HG21 | 1.98 | 0.46 |
| 27:T:89:TYR:CE2 | 27:T:102:LYS:HG3 | 2.51 | 0.46 |
| 28:U:283:ARG:NH1 | 29:V:291:ASN:CG | 2.65 | 0.46 |
| 33:Z:61:SER:HA | 33:Z:111:LEU:HD11 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:213:LYS:HA | 33:Z:240:ASN:HD21 | 1.80 | 0.46 |
| 6:6:66:TYR:CE2 | 6:6:73:LYS:C | 2.84 | 0.46 |
| 7:7:13:ILE:CG2 | 7:7:169:ILE:HG13 | 2.46 | 0.46 |
| 8:A:91:ARG:HH12 | 8:A:95:LEU:HB2 | 1.79 | 0.46 |
| 9:B:217:GLU:OE1 | 9:B:222:LEU:HD21 | 2.16 | 0.46 |
| 9:B:231:LYS:HD3 | 9:B:234:ARG:NH2 | 2.28 | 0.46 |
| 14:G:122:HIS:ND1 | 14:G:128:VAL:HG12 | 2.28 | 0.46 |
| 16:I:317:ASP:CB | 16:I:343:ARG:NH2 | 2.69 | 0.46 |
| 20:M:203:ARG:HD3 | 20:M:206:LYS:HZ2 | 1.80 | 0.46 |
| 20:M:308:LEU:O | 20:M:312:LEU:HG | 2.15 | 0.46 |
| 21:N:21:LYS:HD3 | 21:N:49:LEU:CD2 | 2.46 | 0.46 |
| 22:O:117:ASN:OD1 | 22:O:118:GLY:N | 2.48 | 0.46 |
| 23:P:141:LYS:HG3 | 23:P:182:GLU:OE2 | 2.16 | 0.46 |
| 23:P:344:ARG:NH2 | 23:P:347:GLU:OE2 | 2.49 | 0.46 |
| 24:Q:146:TYR:CD1 | 24:Q:151:TYR:CD1 | 3.03 | 0.46 |
| 25:R:354:ALA:CB | 25:R:364:LEU:HD23 | 2.44 | 0.46 |
| 33:Z:130:GLY:O | 33:Z:131:LYS:CG | 2.64 | 0.46 |
| 1:1:38:HIS:HB3 | 1:1:41:ILE:HB | 1.98 | 0.46 |
| 3:3:29:ASN:OD1 | 3:3:174:TRP:HE3 | 1.99 | 0.46 |
| 4:4:59:ILE:O | 4:4:63:ILE:HG12 | 2.16 | 0.46 |
| 14:G:51:LYS:HE2 | 14:G:63:ASN:CB | 2.44 | 0.46 |
| 15:H:292:ARG:NH1 | 15:H:296:GLU:OE2 | 2.48 | 0.46 |
| 16:I:349:LEU:C | 16:I:349:LEU:HD12 | 2.37 | 0.46 |
| 18:K:210:LEU:HB2 | 18:K:334:LEU:HD11 | 1.98 | 0.46 |
| 18:K:280:LYS:CE | 18:K:296:LEU:HD22 | 2.46 | 0.46 |
| 21:N:443:LEU:HD21 | 21:N:469:VAL:HG22 | 1.97 | 0.46 |
| 22:O:370:LEU:HD22 | 28:U:207:VAL:HG21 | 1.97 | 0.46 |
| 24:Q:232:TYR:CB | 24:Q:272:LEU:HD21 | 2.39 | 0.46 |
| 27:T:183:SER:HA | 27:T:186:ARG:CD | 2.45 | 0.46 |
| 33:Z:165:TYR:CE1 | 33:Z:190:THR:OG1 | 2.57 | 0.46 |
| 33:Z:339:PHE:HB3 | 33:Z:341:TYR:CE1 | 2.51 | 0.46 |
| 33:Z:394:TYR:HB3 | 33:Z:859:LYS:CE | 2.46 | 0.46 |
| 1:1:82:PHE:CB | 1:1:113:ILE:CD1 | 2.94 | 0.46 |
| 3:3:75:PRO:HD2 | 3:3:104:ASN:ND2 | 2.31 | 0.46 |
| 7:7:13:ILE:HG21 | 7:7:169:ILE:HG13 | 1.98 | 0.46 |
| 7:7:178:TYR:OH | 7:7:210:LYS:NZ | 2.28 | 0.46 |
| 8:A:66:PRO:HG2 | 8:A:67:THR:HG23 | 1.98 | 0.46 |
| 13:F:85:SER:O | 13:F:89:ARG:HG3 | 2.15 | 0.46 |
| 15:H:328:GLU:HG2 | 15:H:331:ARG:HH21 | 1.80 | 0.46 |
| 18:K:123:LEU:HD12 | 18:K:147:VAL:O | 2.16 | 0.46 |
| 20:M:72:ASN:O | 20:M:77:TYR:CE2 | 2.69 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:256:GLN:OE1 | 21:N:904:VAL:N | 2.49 | 0.46 |
| 21:N:466:LEU:O | 21:N:469:VAL:HB | 2.16 | 0.46 |
| 23:P:131:PHE:CD1 | 23:P:136:ARG:HD2 | 2.50 | 0.46 |
| 23:P:137:ALA:HB1 | 23:P:179:PHE:CZ | 2.50 | 0.46 |
| 23:P:369:LEU:HD12 | 23:P:376:THR:HG23 | 1.97 | 0.46 |
| 24:Q:141:LEU:O | 24:Q:145:HIS:CD2 | 2.69 | 0.46 |
| 26:S:286:TYR:OH | 26:S:323:LEU:HD22 | 2.16 | 0.46 |
| 28:U:24:ARG:HH22 | 29:V:66:VAL:HG12 | 1.81 | 0.46 |
| 28:U:293:GLU:HG2 | 29:V:277:LYS:CD | 2.46 | 0.46 |
| 33:Z:501:LYS:HG3 | 33:Z:534:PHE:CD2 | 2.50 | 0.46 |
| 5:5:159:ARG:HH11 | 5:5:200:VAL:HG13 | 1.81 | 0.45 |
| 9:B:35:LEU:C | 9:B:35:LEU:HD12 | 2.37 | 0.45 |
| 10:C:106:ILE:HG12 | 10:C:107:PRO:O | 2.15 | 0.45 |
| 11:D:10:ILE:HD11 | 12:E:10:ARG:HB3 | 1.99 | 0.45 |
| 11:D:11:PHE:HA | 11:D:17:ILE:HD12 | 1.96 | 0.45 |
| 11:D:193:LYS:HZ2 | 11:D:236:ILE:HG13 | 1.80 | 0.45 |
| 12:E:68:VAL:HG12 | 12:E:93:ARG:NH2 | 2.31 | 0.45 |
| 14:G:59:VAL:CG2 | 14:G:60:PRO:HD2 | 2.45 | 0.45 |
| 15:H:49:LEU:O | 33:Z:765:MET:CE | 2.63 | 0.45 |
| 17:J:337:LEU:N | 25:R:204:TRP:HE1 | 1.98 | 0.45 |
| 19:L:118:ILE:HG12 | 19:L:128:ILE:CD1 | 2.46 | 0.45 |
| 22:O:33:TYR:CE2 | 22:O:34:GLU:OE2 | 2.69 | 0.45 |
| 22:O:122:HIS:C | 22:O:166:ARG:HH12 | 2.20 | 0.45 |
| 22:O:277:ILE:HG22 | 22:O:279:ILE:H | 1.81 | 0.45 |
| 26:S:288:THR:CG2 | 26:S:292:TYR:CE2 | 2.99 | 0.45 |
| 27:T:229:VAL:CG1 | 27:T:230:ASN:N | 2.80 | 0.45 |
| 29:V:247:ILE:HD12 | 29:V:250:GLN:HB2 | 1.98 | 0.45 |
| 31:X:38:ASN:OD1 | 31:X:43:LEU:CD1 | 2.64 | 0.45 |
| 33:Z:103:TYR:CZ | 33:Z:137:TYR:CD1 | 3.04 | 0.45 |
| 33:Z:486:SER:O | 33:Z:489:ALA:HB3 | 2.16 | 0.45 |
| 33:Z:884:THR:CB | 33:Z:904:LEU:HD21 | 2.46 | 0.45 |
| 9:B:39:ALA:O | 9:B:40:THR:HG23 | 2.16 | 0.45 |
| 12:E:157:HIS:HB3 | 12:E:167:TYR:CE1 | 2.51 | 0.45 |
| 14:G:200:TYR:CD1 | 14:G:200:TYR:C | 2.89 | 0.45 |
| 15:H:59:ILE:CD1 | 16:I:92:GLU:CD | 2.69 | 0.45 |
| 15:H:62:ARG:HH21 | 16:I:92:GLU:HG2 | 1.81 | 0.45 |
| 15:H:97:LEU:CB | 15:H:173:ARG:CG | 2.94 | 0.45 |
| 15:H:326:ASP:CA | 15:H:329:VAL:HG22 | 2.45 | 0.45 |
| 18:K:224:LYS:NZ | 18:K:236:ARG:NH2 | 2.51 | 0.45 |
| 18:K:342:SER:O | 18:K:343:LEU:CB | 2.62 | 0.45 |
| 19:L:389:ALA:CA | 20:M:339:ARG:HE | 2.29 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:423:LEU:O | 21:N:426:ILE:HB | 2.16 | 0.45 |
| 21:N:664:LEU:CD2 | 21:N:672:ASN:ND2 | 2.80 | 0.45 |
| 23:P:170:SER:HA | 23:P:173:MET:HE3 | 1.98 | 0.45 |
| 23:P:184:MET:SD | 23:P:223:LEU:HD12 | 2.56 | 0.45 |
| 23:P:366:ASN:HD21 | 23:P:373:GLU:CA | 2.15 | 0.45 |
| 23:P:375:GLN:O | 23:P:379:TYR:CD2 | 2.69 | 0.45 |
| 24:Q:263:LYS:CE | 24:Q:295:GLY:HA3 | 2.43 | 0.45 |
| 25:R:214:TYR:HE2 | 25:R:226:GLU:O | 1.99 | 0.45 |
| 26:S:443:ILE:HG22 | 26:S:445:THR:CG2 | 2.47 | 0.45 |
| 27:T:89:TYR:HB3 | 27:T:90:PHE:CD1 | 2.51 | 0.45 |
| 30:W:21:PHE:CE1 | 30:W:25:ARG:NH2 | 2.81 | 0.45 |
| 31:X:48:PHE:CG | 31:X:68:LEU:HD11 | 2.51 | 0.45 |
| 33:Z:65:GLU:N | 33:Z:111:LEU:HD21 | 2.31 | 0.45 |
| 33:Z:138:ARG:CZ | 33:Z:157:LEU:HA | 2.46 | 0.45 |
| 33:Z:403:ASN:ND2 | 33:Z:406:TRP:HB2 | 2.31 | 0.45 |
| 33:Z:457:ILE:HG23 | 33:Z:905:ASN:ND2 | 2.32 | 0.45 |
| 33:Z:748:LEU:HD11 | 33:Z:782:ILE:O | 2.15 | 0.45 |
| 1:1:82:PHE:HB2 | 1:1:113:ILE:CD1 | 2.46 | 0.45 |
| 8:A:135:ARG:HD3 | 14:G:124:LEU:HD23 | 1.98 | 0.45 |
| 11:D:146:LYS:HE2 | 11:D:148:TYR:CE2 | 2.51 | 0.45 |
| 14:G:108:ILE:HD12 | 14:G:146:HIS:HB2 | 1.97 | 0.45 |
| 15:H:311:ILE:CD1 | 15:H:361:LEU:HD13 | 2.46 | 0.45 |
| 15:H:381:ASP:C | 15:H:381:ASP:OD1 | 2.55 | 0.45 |
| 16:I:380:LEU:O | 16:I:384:LYS:HG3 | 2.16 | 0.45 |
| 16:I:416:PHE:O | 16:I:420:LYS:HG2 | 2.16 | 0.45 |
| 17:J:170:HIS:NE2 | 25:R:124:ASP:HB3 | 2.32 | 0.45 |
| 19:L:67:HIS:N | 19:L:70:TYR:HD2 | 2.14 | 0.45 |
| 19:L:123:SER:HB3 | 20:M:125:GLN:HE21 | 1.82 | 0.45 |
| 21:N:208:ARG:HG2 | 21:N:232:LEU:HD13 | 1.97 | 0.45 |
| 23:P:94:GLN:OE1 | 23:P:136:ARG:CG | 2.62 | 0.45 |
| 24:Q:275:ILE:CG1 | 24:Q:306:TYR:HD2 | 2.28 | 0.45 |
| 25:R:161:ALA:O | 25:R:162:ILE:HG23 | 2.17 | 0.45 |
| 26:S:145:PHE:HD2 | 26:S:152:LEU:HD23 | 1.81 | 0.45 |
| 28:U:298:ASN:O | 28:U:302:GLN:HG3 | 2.16 | 0.45 |
| 31:X:104:LYS:NZ | 31:X:107:GLY:O | 2.40 | 0.45 |
| 33:Z:65:GLU:HA | 33:Z:111:LEU:CD2 | 2.46 | 0.45 |
| 33:Z:290:GLU:CG | 33:Z:293:MET:CE | 2.83 | 0.45 |
| 33:Z:322:GLU:CG | 33:Z:464:ASP:OD2 | 2.53 | 0.45 |
| 33:Z:510:LEU:N | 33:Z:511:PRO:HD2 | 2.31 | 0.45 |
| 33:Z:761:PHE:HD2 | 33:Z:780:MET:HE1 | 1.79 | 0.45 |
| 1:1:173:ILE:HD12 | 1:1:193:TYR:CG | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:88:PHE:O | 2:2:91:GLN:NE2 | 2.48 | 0.45 |
| 4:4:106:TYR:CZ | 4:4:185:LYS:HA | 2.52 | 0.45 |
| 5:5:118:ASP:OD1 | 5:5:118:ASP:O | 2.33 | 0.45 |
| 6:6:34:VAL:HG12 | 6:6:196:LEU:CD1 | 2.44 | 0.45 |
| 9:B:184:GLU:HG2 | 9:B:186:GLU:N | 2.30 | 0.45 |
| 11:D:37:LYS:HG2 | 11:D:42:VAL:HG23 | 1.97 | 0.45 |
| 11:D:106:VAL:HB | 11:D:146:LYS:CE | 2.47 | 0.45 |
| 11:D:120:TYR:CG | 11:D:126:VAL:HG21 | 2.50 | 0.45 |
| 15:H:340:LEU:HD12 | 15:H:370:ARG:HG3 | 1.95 | 0.45 |
| 16:I:103:PRO:CB | 17:J:120:TYR:CZ | 2.94 | 0.45 |
| 17:J:167:PRO:HA | 17:J:174:PHE:CE2 | 2.47 | 0.45 |
| 18:K:186:GLU:HA | 18:K:190:LEU:CD1 | 2.43 | 0.45 |
| 19:L:190:ILE:O | 19:L:194:ARG:HG3 | 2.16 | 0.45 |
| 20:M:303:ARG:NH2 | 20:M:307:GLU:OE1 | 2.49 | 0.45 |
| 23:P:203:ILE:HG13 | 23:P:220:TYR:OH | 2.08 | 0.45 |
| 23:P:287:ASP:HB3 | 23:P:297:GLU:CD | 2.37 | 0.45 |
| 25:R:304:TYR:HD2 | 25:R:305:PHE:CD1 | 2.34 | 0.45 |
| 26:S:138:MET:O | 26:S:142:VAL:HG23 | 2.16 | 0.45 |
| 28:U:76:MET:SD | 29:V:94:MET:HG3 | 2.56 | 0.45 |
| 30:W:21:PHE:HB3 | 30:W:22:PRO:HD2 | 1.97 | 0.45 |
| 33:Z:483:THR:HB | 33:Z:521:GLU:HG3 | 1.99 | 0.45 |
| 33:Z:886:VAL:HG13 | 33:Z:893:PHE:CE2 | 2.48 | 0.45 |
| 11:D:215:VAL:HG22 | 11:D:221:ILE:HG12 | 1.98 | 0.45 |
| 19:L:400:PHE:HZ | 20:M:215:PRO:HD3 | 1.82 | 0.45 |
| 20:M:203:ARG:HH11 | 20:M:206:LYS:HZ2 | 1.63 | 0.45 |
| 21:N:63:LEU:HD22 | 21:N:88:ARG:HB3 | 1.99 | 0.45 |
| 21:N:771:PHE:CE2 | 21:N:773:MET:CG | 2.99 | 0.45 |
| 22:O:76:LEU:HD22 | 22:O:124:ASP:N | 2.31 | 0.45 |
| 23:P:299:LEU:HD12 | 23:P:302:LEU:HD12 | 1.97 | 0.45 |
| 23:P:422:LEU:HD12 | 28:U:262:GLN:HE22 | 1.81 | 0.45 |
| 24:Q:309:ARG:NE | 24:Q:345:SER:CB | 2.51 | 0.45 |
| 27:T:109:TYR:O | 27:T:113:LEU:HG | 2.17 | 0.45 |
| 28:U:191:THR:CG2 | 28:U:195:LYS:HE3 | 2.47 | 0.45 |
| 29:V:48:GLU:OE2 | 29:V:111:HIS:ND1 | 2.49 | 0.45 |
| 33:Z:865:ASP:OD1 | 33:Z:909:ARG:NH2 | 2.42 | 0.45 |
| 1:1:14:LEU:HD21 | 1:1:100:ALA:HB3 | 0.57 | 0.45 |
| 1:1:19:ARG:CZ | 1:1:170:GLY:C | 2.85 | 0.45 |
| 3:3:104:ASN:HB3 | 3:3:107:SER:OG | 2.16 | 0.45 |
| 6:6:115:SER:OG | 6:6:128:ARG:HG2 | 2.17 | 0.45 |
| 10:C:221:ASN:ND2 | 10:C:226:TYR:HE1 | 2.14 | 0.45 |
| 15:H:174:VAL:HG11 | 15:H:183:ILE:HG21 | 1.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:298:ALA:HB2 | 15:H:306:ILE:HD11 | 1.98 | 0.45 |
| 17:J:115:LEU:HD13 | 17:J:122:LEU:CD2 | 2.46 | 0.45 |
| 20:M:216:LYS:HZ1 | 20:M:321:VAL:HB | 1.80 | 0.45 |
| 20:M:216:LYS:HZ2 | 20:M:321:VAL:HB | 1.81 | 0.45 |
| 23:P:440:HIS:CE1 | 28:U:209:GLU:CB | 2.96 | 0.45 |
| 24:Q:429:LYS:HD2 | 29:V:269:ARG:CZ | 2.46 | 0.45 |
| 27:T:29:PRO:HA | 27:T:32:ILE:HD12 | 1.97 | 0.45 |
| 27:T:112:ASN:CA | 27:T:177:PHE:CZ | 3.00 | 0.45 |
| 28:U:36:VAL:HB | 28:U:54:LEU:HD11 | 1.99 | 0.45 |
| 28:U:138:VAL:CG1 | 28:U:157:LEU:HD11 | 2.47 | 0.45 |
| 31:X:7:VAL:HG12 | 31:X:8:ILE:HG13 | 1.99 | 0.45 |
| 5:5:178:TYR:HD2 | 5:5:185:TRP:CE3 | 2.35 | 0.45 |
| 9:B:96:SER:O | 9:B:97:TYR:CD1 | 2.70 | 0.45 |
| 12:E:53:ARG:NH1 | 12:E:209:GLU:OE2 | 2.50 | 0.45 |
| 14:G:7:TYR:CD1 | 14:G:13:VAL:CG2 | 2.97 | 0.45 |
| 15:H:171:GLY:O | 16:I:129:TYR:CZ | 2.70 | 0.45 |
| 17:J:162:GLU:HG2 | 17:J:166:LEU:CD1 | 2.46 | 0.45 |
| 18:K:92:VAL:HA | 18:K:94:LEU:HG | 1.99 | 0.45 |
| 18:K:191:PRO:HG2 | 18:K:313:LYS:HZ2 | 1.80 | 0.45 |
| 19:L:298:ASP:OD1 | 19:L:301:ILE:CD1 | 2.63 | 0.45 |
| 21:N:207:LEU:CD1 | 21:N:232:LEU:CD2 | 2.94 | 0.45 |
| 21:N:324:LYS:CG | 21:N:325:PHE:HD2 | 2.28 | 0.45 |
| 21:N:330:THR:HG21 | 21:N:739:PHE:CZ | 2.48 | 0.45 |
| 21:N:515:ARG:NE | 21:N:741:TYR:CD2 | 2.85 | 0.45 |
| 23:P:237:VAL:HG12 | 23:P:267:PHE:CE2 | 2.51 | 0.45 |
| 25:R:127:GLU:HB3 | 25:R:162:ILE:HD13 | 1.98 | 0.45 |
| 25:R:128:LEU:HD23 | 25:R:162:ILE:HD11 | 1.99 | 0.45 |
| 25:R:312:TYR:CE2 | 25:R:317:ILE:HD11 | 2.52 | 0.45 |
| 25:R:350:LEU:HB2 | 25:R:388:VAL:HG23 | 1.98 | 0.45 |
| 26:S:456:ASP:HB2 | 26:S:457:PRO:HD3 | 1.98 | 0.45 |
| 27:T:152:LEU:HD12 | 27:T:157:TYR:HE1 | 1.82 | 0.45 |
| 33:Z:172:ASP:HB3 | 33:Z:177:THR:OG1 | 2.16 | 0.45 |
| 33:Z:286:VAL:HG21 | 33:Z:317:GLN:HG2 | 1.98 | 0.45 |
| 33:Z:321:PHE:CE2 | 33:Z:351:PRO:CG | 2.79 | 0.45 |
| 8:A:91:ARG:NH1 | 8:A:95:LEU:HB2 | 2.32 | 0.45 |
| 8:A:154:ILE:HG23 | 8:A:166:TYR:HB2 | 1.99 | 0.45 |
| 14:G:68:VAL:CG1 | 14:G:69:VAL:N | 2.80 | 0.45 |
| 15:H:168:ILE:HG22 | 15:H:172:MET:HA | 1.99 | 0.45 |
| 15:H:284:VAL:CG1 | 20:M:253:GLN:CA | 2.94 | 0.45 |
| 19:L:193:LEU:HA | 19:L:196:VAL:HG22 | 1.98 | 0.45 |
| 22:O:222:LEU:HB3 | 22:O:280:LEU:CD1 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:O:243:VAL:HG23 | 22:O:248:TYR:CD2 | 2.52 | 0.45 |
| 22:O:296:LEU:HD13 | 22:O:312:ASP:HB3 | 1.98 | 0.45 |
| 25:R:58:GLU:O | 25:R:144:ILE:HD12 | 2.17 | 0.45 |
| 25:R:161:ALA:O | 25:R:162:ILE:CG2 | 2.65 | 0.45 |
| 27:T:104:LYS:O | 27:T:108:LEU:HG | 2.16 | 0.45 |
| 29:V:154:ASP:CB | 29:V:156:PHE:CZ | 2.97 | 0.45 |
| 33:Z:49:LEU:C | 33:Z:49:LEU:HD12 | 2.37 | 0.45 |
| 33:Z:436:LEU:CD2 | 33:Z:455:ILE:HG12 | 2.46 | 0.45 |
| 1:1:-8:LYS:CE | 2:2:117:GLY:HA3 | 2.47 | 0.45 |
| 1:1:11:GLY:HA3 | 1:1:102:TYR:CE1 | 2.52 | 0.45 |
| 2:2:8:PHE:CD2 | 2:2:11:GLY:N | 2.84 | 0.45 |
| 2:2:63:ILE:O | 2:2:66:HIS:HB3 | 2.17 | 0.45 |
| 3:3:63:ASN:O | 3:3:67:LEU:HG | 2.16 | 0.45 |
| 3:3:158:ILE:HG23 | 3:3:159:SER:N | 2.30 | 0.45 |
| 4:4:13:ILE:CG2 | 4:4:160:LEU:HD11 | 2.47 | 0.45 |
| 4:4:26:VAL:CG1 | 4:4:28:LYS:O | 2.65 | 0.45 |
| 4:4:106:TYR:OH | 4:4:185:LYS:HB3 | 2.17 | 0.45 |
| 6:6:81:ALA:HB2 | 6:6:102:ILE:HD11 | 1.99 | 0.45 |
| 6:6:190:GLY:O | 6:6:191:ASP:HB2 | 2.17 | 0.45 |
| 10:C:4:ARG:NH1 | 12:E:11:GLY:HA2 | 2.32 | 0.45 |
| 10:C:194:LEU:HD11 | 10:C:238:ILE:HG22 | 1.99 | 0.45 |
| 15:H:244:LYS:NZ | 15:H:244:LYS:HB3 | 2.31 | 0.45 |
| 17:J:224:GLY:O | 17:J:225:GLU:C | 2.55 | 0.45 |
| 21:N:668:THR:HG21 | 21:N:783:SER:O | 2.17 | 0.45 |
| 24:Q:165:PHE:CZ | 24:Q:173:SER:CB | 2.99 | 0.45 |
| 33:Z:75:ILE:HD13 | 33:Z:121:ILE:HG21 | 1.99 | 0.45 |
| 33:Z:272:TYR:HE2 | 33:Z:284:LEU:CD1 | 2.27 | 0.45 |
| 33:Z:506:LEU:HB2 | 33:Z:534:PHE:CZ | 2.47 | 0.45 |
| 1:1:57:ASP:CA | 8:A:106:TYR:HE1 | 2.29 | 0.45 |
| 6:6:68:PHE:CE2 | 13:F:66:CYS:O | 2.70 | 0.45 |
| 11:D:11:PHE:HE2 | 12:E:26:TYR:C | 2.19 | 0.45 |
| 15:H:382:LEU:HD23 | 15:H:385:ARG:HH11 | 1.82 | 0.45 |
| 18:K:67:TYR:CD1 | 21:N:572:LEU:HD22 | 2.52 | 0.45 |
| 18:K:174:VAL:CG2 | 18:K:177:LEU:HD11 | 2.47 | 0.45 |
| 18:K:196:ASP:O | 18:K:200:GLN:HG3 | 2.17 | 0.45 |
| 18:K:344:ARG:HE | 18:K:380:GLY:N | 2.15 | 0.45 |
| 21:N:31:VAL:CG2 | 21:N:35:LEU:CD1 | 2.94 | 0.45 |
| 21:N:539:MET:HE2 | 21:N:551:GLY:N | 2.32 | 0.45 |
| 22:O:96:LEU:HD22 | 22:O:137:TYR:CE1 | 2.51 | 0.45 |
| 22:O:250:TRP:HA | 22:O:269:LEU:CG | 2.45 | 0.45 |
| 24:Q:263:LYS:HE2 | 24:Q:295:GLY:CA | 2.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:R:72:VAL:O | 25:R:72:VAL:HG12 | 2.16 | 0.45 |
| 25:R:397:ASN:HD22 | 26:S:451:ILE:C | 2.20 | 0.45 |
| 26:S:461:PHE:CZ | 28:U:278:ILE:N | 2.85 | 0.45 |
| 33:Z:546:ILE:O | 33:Z:550:PHE:CD2 | 2.70 | 0.45 |
| 3:3:1:GLY:HA3 | 3:3:33:LYS:HZ3 | 1.81 | 0.44 |
| 9:B:221:LEU:HD11 | 9:B:236:ARG:HD2 | 1.99 | 0.44 |
| 12:E:51:GLU:HG2 | 12:E:53:ARG:HG3 | 1.99 | 0.44 |
| 13:F:65:LYS:HG3 | 13:F:222:PHE:HD2 | 1.77 | 0.44 |
| 13:F:74:LEU:HD22 | 13:F:81:ALA:HB1 | 1.98 | 0.44 |
| 15:H:282:LYS:N | 16:I:257:LEU:HG | 2.32 | 0.44 |
| 17:J:109:ALA:O | 17:J:110:SER:HB2 | 2.17 | 0.44 |
| 22:O:253:GLN:OE1 | 22:O:269:LEU:HG | 2.17 | 0.44 |
| 22:O:310:PHE:HE1 | 22:O:348:VAL:HG22 | 1.81 | 0.44 |
| 25:R:259:PHE:O | 25:R:259:PHE:CD1 | 2.70 | 0.44 |
| 25:R:417:TYR:CZ | 28:U:292:ILE:HG21 | 2.52 | 0.44 |
| 33:Z:457:ILE:HD11 | 33:Z:902:TYR:CG | 2.52 | 0.44 |
| 33:Z:463:HIS:HE1 | 33:Z:497:PHE:HE1 | 1.63 | 0.44 |
| 33:Z:562:TRP:CE2 | 33:Z:566:LEU:CG | 2.91 | 0.44 |
| 33:Z:911:LYS:CB | 33:Z:962:ARG:HG3 | 2.47 | 0.44 |
| 7:7:17:ASP:C | 7:7:17:ASP:OD1 | 2.56 | 0.44 |
| 8:A:42:SER:HB2 | 8:A:171:THR:CG2 | 2.47 | 0.44 |
| 16:I:257:LEU:HD13 | 16:I:304:ARG:HD3 | 1.99 | 0.44 |
| 19:L:88:TYR:O | 19:L:91:THR:HB | 2.18 | 0.44 |
| 19:L:361:PHE:CE1 | 19:L:391:ILE:HD12 | 2.47 | 0.44 |
| 19:L:416:MET:HB3 | 19:L:420:ARG:HH12 | 1.82 | 0.44 |
| 20:M:129:LEU:C | 20:M:129:LEU:HD12 | 2.38 | 0.44 |
| 20:M:358:ALA:O | 20:M:362:GLN:HG2 | 2.16 | 0.44 |
| 20:M:397:GLU:O | 20:M:400:MET:HB2 | 2.18 | 0.44 |
| 21:N:255:ALA:O | 21:N:259:PHE:HD2 | 2.00 | 0.44 |
| 21:N:376:LYS:HA | 21:N:411:ILE:HG12 | 1.98 | 0.44 |
| 22:O:373:TRP:CZ3 | 28:U:200:LEU:CD2 | 3.00 | 0.44 |
| 23:P:176:LYS:NZ | 23:P:206:LYS:NZ | 2.64 | 0.44 |
| 25:R:171:MET:HG3 | 25:R:209:ARG:NH1 | 2.32 | 0.44 |
| 25:R:249:ILE:HG23 | 25:R:250:ALA:N | 2.33 | 0.44 |
| 26:S:147:TRP:CE3 | 26:S:148:ASP:HB2 | 2.51 | 0.44 |
| 26:S:188:TYR:OH | 26:S:240:ASP:CB | 2.66 | 0.44 |
| 30:W:16:SER:HA | 30:W:25:ARG:HB3 | 1.99 | 0.44 |
| 30:W:76:LEU:C | 30:W:79:THR:HG23 | 2.37 | 0.44 |
| 33:Z:59:ASP:O | 33:Z:60:ASP:HB2 | 2.17 | 0.44 |
| 33:Z:440:LEU:HD23 | 33:Z:440:LEU:C | 2.37 | 0.44 |
| 33:Z:812:ILE:CG2 | 33:Z:847:ILE:HG22 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:59:ARG:NH2 | 10:C:100:LYS:HA | 2.32 | 0.44 |
| 3:3:69:GLU:HG3 | 3:3:71:ARG:H | 1.82 | 0.44 |
| 6:6:37:CYS:HG | 6:6:59:PHE:HD2 | 1.65 | 0.44 |
| 7:7:16:ALA:HB3 | 7:7:34:LEU:HG | 2.00 | 0.44 |
| 7:7:31:VAL:HG11 | 7:7:49:ILE:HD12 | 1.99 | 0.44 |
| 9:B:160:LYS:HB3 | 10:C:58:GLU:HG2 | 1.99 | 0.44 |
| 9:B:180:ASN:HD22 | 24:Q:168:LEU:HD23 | 1.83 | 0.44 |
| 10:C:147:GLN:HB3 | 10:C:149:TYR:HE1 | 1.83 | 0.44 |
| 11:D:37:LYS:HD3 | 11:D:147:LEU:HB3 | 2.00 | 0.44 |
| 13:F:52:ASN:ND2 | 13:F:54:ASP:O | 2.51 | 0.44 |
| 14:G:168:ARG:NE | 14:G:172:LYS:HZ1 | 2.07 | 0.44 |
| 14:G:205:ASP:O | 14:G:206:ASN:OD1 | 2.35 | 0.44 |
| 15:H:62:ARG:HH12 | 16:I:95:GLN:HB2 | 1.82 | 0.44 |
| 15:H:149:LEU:HD22 | 15:H:177:ASP:HB3 | 2.00 | 0.44 |
| 16:I:124:THR:O | 16:I:125:MET:HB2 | 2.18 | 0.44 |
| 17:J:377:VAL:CG1 | 17:J:382:PHE:CZ | 3.01 | 0.44 |
| 18:K:123:LEU:HD11 | 18:K:147:VAL:HA | 1.99 | 0.44 |
| 18:K:237:VAL:CG1 | 18:K:242:PHE:HZ | 2.31 | 0.44 |
| 21:N:539:MET:CE | 21:N:551:GLY:CA | 2.88 | 0.44 |
| 21:N:770:LYS:HE3 | 21:N:917:ILE:CD1 | 2.43 | 0.44 |
| 22:O:59:LEU:CD2 | 22:O:85:SER:HB2 | 2.47 | 0.44 |
| 29:V:159:ILE:HD11 | 29:V:188:LEU:HD11 | 1.98 | 0.44 |
| 30:W:29:GLN:NE2 | 30:W:115:CYS:SG | 2.90 | 0.44 |
| 30:W:118:ILE:CD1 | 30:W:153:LEU:HD12 | 2.47 | 0.44 |
| 33:Z:64:TYR:CD2 | 33:Z:111:LEU:HD11 | 2.25 | 0.44 |
| 33:Z:623:ARG:HG2 | 33:Z:739:ALA:HB2 | 1.99 | 0.44 |
| 15:H:152:ILE:O | 15:H:153:ALA:HB3 | 2.17 | 0.44 |
| 17:J:193:THR:HG23 | 17:J:355:GLY:H | 1.81 | 0.44 |
| 19:L:114:GLU:HB3 | 19:L:137:ARG:CD | 2.45 | 0.44 |
| 19:L:193:LEU:CD2 | 19:L:347:VAL:HG21 | 2.47 | 0.44 |
| 20:M:290:ARG:HH11 | 20:M:294:GLU:HB3 | 1.82 | 0.44 |
| 21:N:584:ARG:NH1 | 21:N:614:ASN:ND2 | 2.35 | 0.44 |
| 21:N:641:LEU:HD12 | 21:N:660:LEU:HD23 | 1.98 | 0.44 |
| 21:N:739:PHE:CD1 | 21:N:743:PHE:O | 2.70 | 0.44 |
| 23:P:241:LEU:HD23 | 23:P:264:ILE:HG12 | 2.00 | 0.44 |
| 25:R:164:THR:CG2 | 25:R:199:GLU:OE1 | 2.65 | 0.44 |
| 26:S:315:LYS:CE | 26:S:345:TYR:HE1 | 2.27 | 0.44 |
| 27:T:53:ASN:H | 27:T:57:ILE:HB | 1.83 | 0.44 |
| 29:V:247:ILE:O | 29:V:247:ILE:HG13 | 2.16 | 0.44 |
| 31:X:46:TRP:HE1 | 31:X:132:SER:CA | 2.30 | 0.44 |
| 33:Z:339:PHE:HB3 | 33:Z:341:TYR:CZ | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:363:ASP:O | 33:Z:366:LYS:HE2 | 2.16 | 0.44 |
| 33:Z:752:ILE:O | 33:Z:756:MET:HG2 | 2.17 | 0.44 |
| 2:2:54:ALA:CB | 3:3:87:TYR:CE1 | 3.00 | 0.44 |
| 5:5:111:THR:HG21 | 5:5:113:TYR:CE2 | 2.51 | 0.44 |
| 17:J:79:VAL:HG22 | 17:J:83:LYS:O | 2.17 | 0.44 |
| 17:J:101:ASP:C | 17:J:102:ILE:HG23 | 2.38 | 0.44 |
| 17:J:135:SER:O | 18:K:293:GLN:NE2 | 2.42 | 0.44 |
| 17:J:167:PRO:HB3 | 17:J:174:PHE:CD2 | 2.44 | 0.44 |
| 17:J:210:PHE:CE2 | 17:J:212:ARG:CG | 3.00 | 0.44 |
| 19:L:189:GLN:HE21 | 19:L:350:PRO:HD2 | 1.69 | 0.44 |
| 20:M:131:MET:SD | 20:M:137:PRO:HB3 | 2.57 | 0.44 |
| 22:O:60:ARG:HH21 | 22:O:94:GLU:CD | 2.20 | 0.44 |
| 24:Q:38:SER:CB | 24:Q:88:PHE:CE1 | 2.99 | 0.44 |
| 24:Q:343:LEU:CD1 | 24:Q:368:LEU:HD11 | 2.36 | 0.44 |
| 24:Q:373:VAL:HG12 | 24:Q:377:LEU:HD12 | 1.99 | 0.44 |
| 25:R:197:MET:HB3 | 25:R:198:ILE:H | 1.55 | 0.44 |
| 25:R:301:TYR:CD1 | 25:R:305:PHE:CE1 | 3.03 | 0.44 |
| 27:T:188:GLU:O | 27:T:192:ASN:ND2 | 2.50 | 0.44 |
| 29:V:127:LYS:O | 29:V:131:GLN:HG2 | 2.16 | 0.44 |
| 30:W:25:ARG:O | 30:W:29:GLN:HG3 | 2.17 | 0.44 |
| 3:3:52:THR:CG2 | 4:4:84:ARG:CZ | 2.94 | 0.44 |
| 6:6:14:LEU:HD22 | 6:6:42:VAL:HG23 | 2.00 | 0.44 |
| 12:E:52:LYS:HE2 | 12:E:217:ALA:O | 2.17 | 0.44 |
| 16:I:97:GLU:HA | 16:I:100:ARG:HE | 1.83 | 0.44 |
| 18:K:209:VAL:CG1 | 18:K:338:ILE:HD12 | 2.48 | 0.44 |
| 21:N:32:VAL:HG21 | 21:N:64:ILE:HG23 | 2.00 | 0.44 |
| 21:N:222:TYR:CZ | 21:N:253:LEU:HD21 | 2.53 | 0.44 |
| 21:N:329:HIS:O | 21:N:332:VAL:HG12 | 2.18 | 0.44 |
| 21:N:697:PHE:CE1 | 21:N:739:PHE:CZ | 3.05 | 0.44 |
| 21:N:758:VAL:HG23 | 21:N:874:ILE:HD13 | 1.99 | 0.44 |
| 22:O:72:LYS:HG2 | 22:O:73:ILE:HG12 | 1.99 | 0.44 |
| 23:P:272:PRO:O | 23:P:273:TYR:CE1 | 2.67 | 0.44 |
| 25:R:105:LYS:HE2 | 25:R:109:LYS:CE | 2.47 | 0.44 |
| 25:R:252:TYR:CE2 | 25:R:321:TYR:HD2 | 2.35 | 0.44 |
| 26:S:156:VAL:HG22 | 26:S:187:ILE:HG23 | 1.99 | 0.44 |
| 26:S:295:ALA:HA | 26:S:298:ARG:HE | 1.81 | 0.44 |
| 26:S:302:HIS:CD2 | 26:S:303:ASN:CG | 2.91 | 0.44 |
| 33:Z:56:LEU:HD22 | 33:Z:68:LEU:HD23 | 1.90 | 0.44 |
| 33:Z:135:LEU:HD21 | 33:Z:195:PHE:HA | 2.00 | 0.44 |
| 33:Z:249:MET:HE3 | 33:Z:268:ALA:HB2 | 1.98 | 0.44 |
| 33:Z:598:ALA:O | 33:Z:601:VAL:HG22 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Z:911:LYS:HB3 | 33:Z:962:ARG:HG3 | 2.00 | 0.44 |
| 2:2:36:ARG:NH2 | 2:2:39:PRO:N | 2.66 | 0.44 |
| 10:C:4:ARG:HD3 | 12:E:125:GLU:HG3 | 2.00 | 0.44 |
| 15:H:168:ILE:HG22 | 15:H:172:MET:SD | 2.58 | 0.44 |
| 15:H:267:THR:O | 15:H:268:ASP:HB3 | 2.18 | 0.44 |
| 18:K:423:LYS:HE3 | 18:K:424:PHE:CE2 | 2.48 | 0.44 |
| 19:L:289:ARG:CD | 19:L:334:ASP:OD1 | 2.66 | 0.44 |
| 21:N:123:PHE:CD1 | 21:N:129:ILE:HD13 | 2.53 | 0.44 |
| 21:N:515:ARG:NH2 | 21:N:738:GLN:CD | 2.65 | 0.44 |
| 22:O:384:MET:HE1 | 28:U:189:ARG:HB3 | 2.00 | 0.44 |
| 24:Q:171:LYS:HB2 | 24:Q:172:PRO:HD3 | 1.99 | 0.44 |
| 24:Q:262:LEU:HD23 | 24:Q:296:ILE:CD1 | 2.47 | 0.44 |
| 24:Q:278:VAL:O | 24:Q:282:LEU:HG | 2.17 | 0.44 |
| 25:R:55:LYS:HG2 | 25:R:98:LEU:HD13 | 2.00 | 0.44 |
| 25:R:158:LEU:HD21 | 25:R:197:MET:CE | 2.48 | 0.44 |
| 25:R:209:ARG:HH21 | 25:R:243:LEU:CD2 | 2.31 | 0.44 |
| 25:R:224:PHE:CE2 | 25:R:328:PHE:CE1 | 3.05 | 0.44 |
| 25:R:335:ARG:CA | 25:R:371:PHE:CE2 | 3.01 | 0.44 |
| 27:T:26:LEU:HB3 | 27:T:30:ILE:HD11 | 1.99 | 0.44 |
| 30:W:65:PHE:HZ | 30:W:98:LEU:HD23 | 1.83 | 0.44 |
| 33:Z:53:VAL:CG2 | 33:Z:91:PHE:CD2 | 3.01 | 0.44 |
| 33:Z:207:ILE:HA | 33:Z:210:TYR:CD2 | 2.53 | 0.44 |
| 33:Z:397:ASP:HB2 | 33:Z:425:ILE:HG21 | 1.99 | 0.44 |
| 33:Z:518:LEU:CD1 | 33:Z:562:TRP:HE3 | 2.28 | 0.44 |
| 2:2:83:LEU:CD1 | 2:2:100:VAL:HG21 | 2.48 | 0.44 |
| 2:2:171:SER:OG | 2:2:172:ASN:N | 2.49 | 0.44 |
| 5:5:4:LEU:HD11 | 5:5:15:ALA:HB3 | 2.00 | 0.44 |
| 6:6:195:ILE:HG22 | 6:6:197:ILE:HG13 | 2.00 | 0.44 |
| 13:F:43:HIS:CE1 | 13:F:218:LYS:HB3 | 2.53 | 0.44 |
| 15:H:223:GLU:HB3 | 20:M:400:MET:HE3 | 1.99 | 0.44 |
| 16:I:106:ILE:HD13 | 16:I:160:LEU:CD2 | 2.48 | 0.44 |
| 16:I:126:PRO:HB2 | 16:I:128:TYR:CE2 | 2.39 | 0.44 |
| 16:I:137:ASP:H | 16:I:140:LEU:HD12 | 1.82 | 0.44 |
| 16:I:257:LEU:HB2 | 16:I:304:ARG:NH2 | 2.33 | 0.44 |
| 17:J:248:ASP:O | 17:J:249:GLU:CB | 2.66 | 0.44 |
| 18:K:85:GLU:O | 18:K:89:ILE:HG12 | 2.17 | 0.44 |
| 19:L:389:ALA:HA | 20:M:339:ARG:HE | 1.83 | 0.44 |
| 21:N:584:ARG:HH11 | 21:N:614:ASN:HD22 | 0.71 | 0.44 |
| 23:P:245:TYR:CE2 | 23:P:257:TRP:NE1 | 2.86 | 0.44 |
| 25:R:34:THR:HG22 | 25:R:70:TYR:HB2 | 2.00 | 0.44 |
| 25:R:258:LEU:HD22 | 25:R:296:LEU:HD12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:S:204:ASP:O | 26:S:208:ILE:HD12 | 2.17 | 0.44 |
| 27:T:15:PHE:CZ | 27:T:67:LEU:CB | 2.94 | 0.44 |
| 27:T:245:TYR:O | 27:T:246:GLU:HB3 | 2.15 | 0.44 |
| 33:Z:312:TYR:CE1 | 33:Z:348:LEU:CD2 | 2.99 | 0.44 |
| 2:2:104:ASP:HB3 | 2:2:105:PRO:CD | 2.45 | 0.44 |
| 2:2:213:LEU:HB2 | 3:3:192:LYS:HB2 | 2.00 | 0.44 |
| 3:3:37:TYR:OH | 3:3:55:ASN:O | 2.35 | 0.44 |
| 4:4:51:ASP:OD1 | 5:5:88:TYR:CE1 | 2.71 | 0.44 |
| 6:6:17:ASP:C | 6:6:17:ASP:OD1 | 2.56 | 0.44 |
| 9:B:196:LEU:O | 9:B:200:VAL:HG22 | 2.18 | 0.44 |
| 10:C:49:GLU:HG3 | 10:C:210:ARG:O | 2.18 | 0.44 |
| 11:D:146:LYS:HB3 | 11:D:148:TYR:CE2 | 2.52 | 0.44 |
| 15:H:223:GLU:HB3 | 20:M:400:MET:HE1 | 1.97 | 0.44 |
| 15:H:284:VAL:HG12 | 20:M:253:GLN:CA | 2.47 | 0.44 |
| 22:O:41:LEU:C | 22:O:41:LEU:HD12 | 2.39 | 0.44 |
| 25:R:62:TYR:CZ | 25:R:180:PHE:CB | 2.99 | 0.44 |
| 25:R:312:TYR:HA | 25:R:316:LEU:HD12 | 1.98 | 0.44 |
| 27:T:108:LEU:HD23 | 27:T:174:PHE:CD1 | 2.53 | 0.44 |
| 27:T:139:ASP:CB | 27:T:142:LEU:HD12 | 2.46 | 0.44 |
| 29:V:23:THR:N | 29:V:167:ASN:HB2 | 2.33 | 0.44 |
| 30:W:14:GLU:O | 30:W:18:ASN:ND2 | 2.51 | 0.44 |
| 30:W:46:GLU:O | 30:W:47:ASN:ND2 | 2.50 | 0.44 |
| 33:Z:100:CYS:SG | 33:Z:137:TYR:OH | 2.63 | 0.44 |
| 33:Z:234:PRO:HA | 33:Z:271:ILE:HG12 | 2.00 | 0.44 |
| 33:Z:269:TYR:CZ | 33:Z:293:MET:HB3 | 2.53 | 0.44 |
| 33:Z:863:THR:CG2 | 33:Z:911:LYS:HZ2 | 2.14 | 0.44 |
| 3:3:129:VAL:HG21 | 3:3:138:PHE:CD1 | 2.50 | 0.43 |
| 17:J:377:VAL:HG11 | 17:J:382:PHE:CZ | 2.52 | 0.43 |
| 18:K:95:VAL:HG12 | 19:L:127:TYR:CE1 | 2.53 | 0.43 |
| 21:N:328:PHE:HB2 | 29:V:181:ASN:CG | 2.38 | 0.43 |
| 21:N:492:THR:C | 21:N:528:ARG:HH11 | 2.20 | 0.43 |
| 21:N:602:VAL:HG11 | 21:N:625:LEU:HD23 | 2.00 | 0.43 |
| 21:N:925:ASP:OD1 | 21:N:925:ASP:O | 2.36 | 0.43 |
| 24:Q:429:LYS:CB | 29:V:269:ARG:NH2 | 2.57 | 0.43 |
| 25:R:31:PHE:CD1 | 25:R:320:LYS:HG2 | 2.53 | 0.43 |
| 26:S:205:ASN:OD1 | 27:T:44:LEU:HD22 | 2.18 | 0.43 |
| 33:Z:64:TYR:CE2 | 33:Z:68:LEU:CD1 | 2.88 | 0.43 |
| 5:5:7:ARG:CZ | 5:5:110:PRO:HG2 | 2.48 | 0.43 |
| 6:6:2:THR:N | 6:6:46:ASN:HD21 | 2.16 | 0.43 |
| 6:6:10:ASP:OD1 | 6:6:11:PHE:CD1 | 2.60 | 0.43 |
| 9:B:239:THR:O | 9:B:243:ILE:HG13 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:D:67:ILE:HD11 | 11:D:73:LEU:HB2 | 2.00 | 0.43 |
| 13:F:7:ASP:HB3 | 13:F:21:GLN:NE2 | 2.34 | 0.43 |
| 15:H:62:ARG:HD2 | 16:I:96:LEU:CD2 | 2.49 | 0.43 |
| 15:H:156:VAL:HA | 15:H:181:TYR:CZ | 2.53 | 0.43 |
| 17:J:135:SER:OG | 18:K:280:LYS:HD3 | 2.17 | 0.43 |
| 18:K:88:ARG:HH11 | 29:V:149:GLY:HA3 | 1.82 | 0.43 |
| 20:M:384:ASP:N | 20:M:386:PHE:CD1 | 2.86 | 0.43 |
| 21:N:109:TYR:CE1 | 21:N:129:ILE:HD12 | 2.50 | 0.43 |
| 22:O:15:ARG:NH2 | 22:O:73:ILE:CD1 | 2.71 | 0.43 |
| 22:O:190:TYR:CE2 | 22:O:194:LEU:HD11 | 2.53 | 0.43 |
| 23:P:350:LEU:HD13 | 23:P:383:LEU:HD12 | 2.00 | 0.43 |
| 25:R:408:ASP:OD1 | 26:S:464:ARG:NH1 | 2.46 | 0.43 |
| 27:T:89:TYR:CZ | 27:T:102:LYS:HB2 | 2.53 | 0.43 |
| 30:W:21:PHE:CE1 | 30:W:25:ARG:HG3 | 2.53 | 0.43 |
| 33:Z:301:THR:CG2 | 33:Z:307:HIS:ND1 | 2.81 | 0.43 |
| 33:Z:415:MET:HG2 | 33:Z:446:GLU:HB2 | 1.99 | 0.43 |
| 33:Z:766:HIS:CD2 | 33:Z:767:TYR:CD1 | 3.06 | 0.43 |
| 33:Z:972:SER:OG | 33:Z:976:HIS:N | 2.50 | 0.43 |
| 1:1:82:PHE:HB2 | 1:1:113:ILE:HD13 | 2.00 | 0.43 |
| 7:7:91:VAL:HG12 | 7:7:102:LEU:HD11 | 1.99 | 0.43 |
| 11:D:203:VAL:O | 11:D:204:GLN:CB | 2.66 | 0.43 |
| 13:F:215:ILE:HG22 | 13:F:223:THR:O | 2.19 | 0.43 |
| 15:H:155:PHE:CE2 | 20:M:76:PRO:HB2 | 2.53 | 0.43 |
| 15:H:282:LYS:HB2 | 16:I:257:LEU:HB3 | 1.99 | 0.43 |
| 16:I:204:HIS:CB | 16:I:207:LEU:HB2 | 2.26 | 0.43 |
| 16:I:207:LEU:CG | 33:Z:930:GLY:HA2 | 2.48 | 0.43 |
| 17:J:79:VAL:O | 17:J:104:VAL:HG21 | 2.17 | 0.43 |
| 19:L:85:GLU:HG3 | 20:M:58:MET:CE | 2.48 | 0.43 |
| 20:M:130:PRO:HD2 | 20:M:154:LEU:CD2 | 2.47 | 0.43 |
| 21:N:344:THR:O | 21:N:344:THR:HG22 | 2.18 | 0.43 |
| 22:O:384:MET:CE | 28:U:190:LEU:HA | 2.48 | 0.43 |
| 23:P:138:ARG:HH11 | 23:P:141:LYS:HD3 | 1.83 | 0.43 |
| 23:P:265:VAL:HG12 | 23:P:296:GLN:HE21 | 1.83 | 0.43 |
| 23:P:415:TRP:HD1 | 28:U:265:LEU:HB2 | 1.83 | 0.43 |
| 25:R:422:ARG:NH1 | 26:S:474:GLU:CG | 2.81 | 0.43 |
| 29:V:41:GLY:HA2 | 29:V:49:VAL:CG2 | 2.48 | 0.43 |
| 30:W:178:PRO:O | 30:W:179:ARG:HB2 | 2.17 | 0.43 |
| 33:Z:473:LEU:C | 33:Z:477:TYR:CD2 | 2.92 | 0.43 |
| 1:1:114:PRO:CG | 1:1:118:SER:HB2 | 2.45 | 0.43 |
| 3:3:-2:ASN:HA | 3:3:21:GLY:H | 1.83 | 0.43 |
| 3:3:17:ASP:C | 3:3:17:ASP:OD1 | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:6:91:LYS:HB2 | 6:6:96:TYR:CE1 | 2.47 | 0.43 |
| 7:7:187:PHE:CE2 | 7:7:204:LEU:CD1 | 3.02 | 0.43 |
| 9:B:48:GLU:HB3 | 9:B:50:LYS:HE3 | 1.99 | 0.43 |
| 14:G:111:PHE:HB2 | 14:G:114:ARG:HH21 | 1.83 | 0.43 |
| 15:H:99:VAL:O | 15:H:173:ARG:CD | 2.65 | 0.43 |
| 17:J:71:TYR:HE1 | 18:K:118:TYR:HE2 | 1.66 | 0.43 |
| 17:J:177:LEU:HD23 | 17:J:179:ILE:HG22 | 1.93 | 0.43 |
| 18:K:131:LEU:HA | 18:K:135:MET:SD | 2.58 | 0.43 |
| 19:L:67:HIS:HD2 | 19:L:68:ARG:HG3 | 1.82 | 0.43 |
| 21:N:641:LEU:HD13 | 21:N:660:LEU:HD23 | 1.99 | 0.43 |
| 25:R:338:TYR:CE1 | 25:R:377:LEU:HD13 | 2.53 | 0.43 |
| 25:R:421:VAL:O | 25:R:422:ARG:CB | 2.66 | 0.43 |
| 31:X:37:PRO:HB3 | 31:X:46:TRP:CE3 | 2.53 | 0.43 |
| 31:X:75:TRP:CH2 | 31:X:125:MET:HE3 | 2.26 | 0.43 |
| 33:Z:100:CYS:O | 33:Z:103:TYR:HB3 | 2.18 | 0.43 |
| 33:Z:301:THR:HG22 | 33:Z:307:HIS:NE2 | 2.26 | 0.43 |
| 33:Z:762:GLY:HA2 | 33:Z:765:MET:CE | 2.49 | 0.43 |
| 33:Z:900:LEU:HB3 | 33:Z:903:MET:HE2 | 2.00 | 0.43 |
| 1:1:83:LYS:HZ2 | 1:1:118:SER:CA | 2.15 | 0.43 |
| 6:6:141:LEU:CD1 | 6:6:145:VAL:CG2 | 2.95 | 0.43 |
| 9:B:205:ASN:O | 9:B:209:ILE:HG13 | 2.18 | 0.43 |
| 10:C:144:TYR:CB | 10:C:147:GLN:NE2 | 2.79 | 0.43 |
| 10:C:162:ALA:CB | 10:C:176:LEU:HD21 | 2.47 | 0.43 |
| 15:H:317:ALA:HB2 | 15:H:360:THR:HB | 2.00 | 0.43 |
| 16:I:128:TYR:HD2 | 16:I:154:MET:HG3 | 1.81 | 0.43 |
| 19:L:170:MET:HE1 | 19:L:265:GLU:HB3 | 1.99 | 0.43 |
| 19:L:353:ASN:HB2 | 19:L:356:GLY:H | 1.84 | 0.43 |
| 20:M:258:GLU:O | 20:M:262:LEU:HG | 2.18 | 0.43 |
| 20:M:263:VAL:HG21 | 20:M:304:THR:HG23 | 1.99 | 0.43 |
| 21:N:525:ASN:ND2 | 21:N:554:THR:HG23 | 2.33 | 0.43 |
| 23:P:129:LYS:O | 23:P:130:ILE:HB | 2.19 | 0.43 |
| 33:Z:249:MET:HE1 | 33:Z:268:ALA:HB2 | 2.00 | 0.43 |
| 33:Z:383:SER:HA | 33:Z:849:ARG:NH1 | 2.33 | 0.43 |
| 33:Z:518:LEU:HD11 | 33:Z:562:TRP:CD2 | 2.54 | 0.43 |
| 2:2:160:GLN:HG3 | 2:2:164:TRP:CD1 | 2.53 | 0.43 |
| 2:2:163:ILE:HG23 | 2:2:170:GLY:HA2 | 2.01 | 0.43 |
| 4:4:153:THR:HG21 | 4:4:182:ILE:HD13 | 2.00 | 0.43 |
| 6:6:112:ALA:HB1 | 6:6:114:TYR:CE1 | 2.53 | 0.43 |
| 10:C:66:LEU:HD12 | 10:C:212:GLU:HG2 | 1.99 | 0.43 |
| 13:F:72:LEU:C | 13:F:72:LEU:HD12 | 2.39 | 0.43 |
| 14:G:59:VAL:HG23 | 14:G:60:PRO:HD2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:144:LYS:HB2 | 20:M:74:GLN:CD | 2.39 | 0.43 |
| 15:H:147:ILE:HG23 | 15:H:181:TYR:HD2 | 1.83 | 0.43 |
| 15:H:168:ILE:HG21 | 15:H:172:MET:O | 2.18 | 0.43 |
| 15:H:328:GLU:HA | 15:H:331:ARG:CZ | 2.49 | 0.43 |
| 20:M:164:ASP:CG | 20:M:165:SER:H | 2.22 | 0.43 |
| 21:N:67:LYS:HG3 | 21:N:97:PHE:CE1 | 2.53 | 0.43 |
| 22:O:4:ASN:HB2 | 22:O:39:PHE:CD1 | 2.54 | 0.43 |
| 23:P:302:LEU:HD11 | 23:P:314:VAL:HG11 | 2.01 | 0.43 |
| 26:S:227:ASN:HB2 | 26:S:263:ASP:OD2 | 2.18 | 0.43 |
| 27:T:89:TYR:CE1 | 27:T:102:LYS:CD | 2.97 | 0.43 |
| 28:U:13:LEU:HD11 | 29:V:36:LYS:CG | 2.45 | 0.43 |
| 31:X:37:PRO:O | 31:X:38:ASN:CB | 2.67 | 0.43 |
| 33:Z:368:VAL:HG12 | 33:Z:369:PHE:N | 2.32 | 0.43 |
| 1:1:11:GLY:HA2 | 1:1:102:TYR:CE1 | 2.53 | 0.43 |
| 1:1:54:ALA:HB1 | 2:2:88:PHE:CE1 | 2.53 | 0.43 |
| 7:7:180:ASP:OD1 | 7:7:182:ARG:HB2 | 2.18 | 0.43 |
| 12:E:208:MET:SD | 12:E:210:GLU:O | 2.77 | 0.43 |
| 13:F:54:ASP:HB3 | 13:F:57:SER:H | 1.83 | 0.43 |
| 18:K:411:TYR:O | 18:K:415:VAL:HG22 | 2.18 | 0.43 |
| 19:L:166:LEU:HD22 | 19:L:168:TYR:CZ | 2.54 | 0.43 |
| 19:L:336:ALA:O | 19:L:342:ARG:NH1 | 2.47 | 0.43 |
| 20:M:195:GLU:HG3 | 20:M:199:LEU:HD12 | 2.01 | 0.43 |
| 21:N:58:ARG:HG3 | 21:N:59:GLU:N | 2.34 | 0.43 |
| 24:Q:355:GLU:CG | 24:Q:397:LEU:HG | 2.47 | 0.43 |
| 26:S:180:ASN:OD1 | 26:S:182:LYS:HG3 | 2.18 | 0.43 |
| 28:U:173:HIS:CE1 | 29:V:150:LYS:HB2 | 2.54 | 0.43 |
| 29:V:135:ARG:CD | 29:V:157:ARG:NH1 | 2.80 | 0.43 |
| 29:V:153:ILE:O | 29:V:154:ASP:OD1 | 2.37 | 0.43 |
| 31:X:61:LEU:HD22 | 31:X:97:TYR:CD2 | 2.53 | 0.43 |
| 33:Z:64:TYR:HB3 | 33:Z:111:LEU:HD11 | 2.01 | 0.43 |
| 33:Z:103:TYR:CE1 | 33:Z:116:ALA:HB2 | 2.47 | 0.43 |
| 33:Z:312:TYR:CZ | 33:Z:348:LEU:CD2 | 3.02 | 0.43 |
| 33:Z:394:TYR:CB | 33:Z:859:LYS:NZ | 2.81 | 0.43 |
| 33:Z:958:ASN:N | 33:Z:961:GLU:OE2 | 2.45 | 0.43 |
| 7:7:8:TYR:CZ | 7:7:11:GLY:CA | 3.01 | 0.43 |
| 7:7:133:THR:HG21 | 7:7:148:ARG:HG2 | 2.01 | 0.43 |
| 9:B:160:LYS:HE3 | 10:C:56:LEU:HD23 | 2.00 | 0.43 |
| 15:H:351:VAL:HG12 | 15:H:353:PHE:CD1 | 2.51 | 0.43 |
| 19:L:218:VAL:HB | 19:L:324:ILE:HG12 | 2.00 | 0.43 |
| 20:M:368:MET:HG3 | 20:M:369:THR:O | 2.18 | 0.43 |
| 21:N:602:VAL:HG12 | 21:N:625:LEU:CD2 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:N:627:ILE:HG23 | 21:N:717:LEU:HD21 | 2.01 | 0.43 |
| 25:R:241:ILE:HG22 | 25:R:242:GLU:N | 2.34 | 0.43 |
| 26:S:321:GLN:O | 26:S:324:MET:HG2 | 2.19 | 0.43 |
| 27:T:157:TYR:CD1 | 27:T:185:ILE:HG23 | 2.54 | 0.43 |
| 28:U:46:ILE:HG23 | 28:U:90:ILE:HD12 | 2.00 | 0.43 |
| 28:U:290:ASP:OD2 | 29:V:281:SER:HA | 2.19 | 0.43 |
| 30:W:8:LEU:HD11 | 30:W:113:PHE:HE2 | 1.84 | 0.43 |
| 33:Z:410:THR:CG2 | 33:Z:414:GLY:HA3 | 2.49 | 0.43 |
| 33:Z:763:HIS:C | 33:Z:766:HIS:ND1 | 2.71 | 0.43 |
| 33:Z:805:LEU:HD22 | 33:Z:841:GLU:OE1 | 2.14 | 0.43 |
| 33:Z:968:ASP:OD2 | 33:Z:983:LEU:HD21 | 2.19 | 0.43 |
| 3:3:100:VAL:CG2 | 3:3:115:PHE:CE1 | 3.01 | 0.43 |
| 11:D:159:TRP:CZ3 | 12:E:59:LEU:CD1 | 2.97 | 0.43 |
| 12:E:182:GLU:OE1 | 12:E:203:ILE:HG12 | 2.19 | 0.43 |
| 13:F:6:TYR:HB2 | 13:F:20:PHE:HD2 | 1.84 | 0.43 |
| 16:I:164:ALA:O | 16:I:165:ASP:CB | 2.62 | 0.43 |
| 16:I:395:MET:SD | 16:I:420:LYS:HE2 | 2.58 | 0.43 |
| 19:L:278:ILE:HG22 | 19:L:280:MET:HG3 | 2.00 | 0.43 |
| 20:M:81:ASN:HB2 | 20:M:163:PHE:CE1 | 2.53 | 0.43 |
| 21:N:302:PHE:CZ | 21:N:757:THR:CB | 3.01 | 0.43 |
| 22:O:255:LEU:HD23 | 22:O:255:LEU:O | 2.18 | 0.43 |
| 23:P:237:VAL:HG11 | 23:P:267:PHE:CE2 | 2.53 | 0.43 |
| 23:P:263:HIS:ND1 | 23:P:325:ASP:OD1 | 2.51 | 0.43 |
| 26:S:443:ILE:HG22 | 26:S:445:THR:HG23 | 2.00 | 0.43 |
| 28:U:62:ASN:CG | 28:U:65:VAL:HG23 | 2.39 | 0.43 |
| 28:U:286:ILE:HG21 | 29:V:261:LEU:HD23 | 2.00 | 0.43 |
| 29:V:145:GLN:CG | 29:V:148:LYS:HE3 | 2.31 | 0.43 |
| 33:Z:519:PRO:HD3 | 33:Z:556:ILE:HG23 | 1.99 | 0.43 |
| 33:Z:893:PHE:HB3 | 33:Z:894:MET:H | 1.53 | 0.43 |
| 1:1:141:ASN:CB | 1:1:154:PHE:HE1 | 2.27 | 0.43 |
| 1:1:177:VAL:HG12 | 1:1:179:THR:CG2 | 2.44 | 0.43 |
| 5:5:32:LYS:O | 5:5:33:ARG:HG2 | 2.18 | 0.43 |
| 7:7:92:MET:SD | 7:7:106:ILE:HD12 | 2.59 | 0.43 |
| 7:7:193:ASP:OD1 | 7:7:195:ASN:N | 2.43 | 0.43 |
| 11:D:60:THR:HG22 | 11:D:61:PRO:O | 2.18 | 0.43 |
| 12:E:67:ILE:HG22 | 12:E:228:PHE:HZ | 1.83 | 0.43 |
| 12:E:166:ARG:HB2 | 13:F:60:GLN:NE2 | 2.34 | 0.43 |
| 13:F:128:TYR:HB3 | 13:F:130:VAL:HG12 | 2.00 | 0.43 |
| 13:F:145:LEU:HD23 | 13:F:146:GLU:N | 2.33 | 0.43 |
| 15:H:291:VAL:O | 15:H:295:PHE:HD1 | 2.02 | 0.43 |
| 16:I:285:ASP:OD1 | 16:I:286:ALA:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:M:330:VAL:O | 20:M:330:VAL:HG13 | 2.19 | 0.43 |
| 21:N:145:LEU:CB | 21:N:173:LYS:NZ | 2.79 | 0.43 |
| 22:O:40:GLN:HB2 | 22:O:58:ARG:HE | 1.81 | 0.43 |
| 23:P:72:TRP:CD2 | 23:P:104:LEU:HD23 | 2.53 | 0.43 |
| 24:Q:167:LYS:HG3 | 24:Q:168:LEU:HG | 2.01 | 0.43 |
| 24:Q:412:ALA:O | 24:Q:416:VAL:HG23 | 2.18 | 0.43 |
| 26:S:425:ARG:NH1 | 27:T:155:GLY:HA2 | 2.29 | 0.43 |
| 26:S:455:GLU:H | 28:U:274:MET:CE | 2.32 | 0.43 |
| 28:U:121:LEU:HD11 | 28:U:134:THR:CG2 | 2.48 | 0.43 |
| 28:U:175:LEU:HD21 | 29:V:213:LEU:HB2 | 1.99 | 0.43 |
| 31:X:122:TYR:O | 31:X:126:ILE:HG12 | 2.19 | 0.43 |
| 33:Z:394:TYR:CG | 33:Z:859:LYS:NZ | 2.83 | 0.43 |
| 33:Z:401:VAL:HG22 | 33:Z:439:TYR:HE2 | 1.84 | 0.43 |
| 2:2:6:VAL:CG1 | 2:2:13:VAL:HB | 2.49 | 0.42 |
| 3:3:7:THR:HG21 | 3:3:125:LYS:HB3 | 2.01 | 0.42 |
| 4:4:142:LEU:HD12 | 4:4:146:HIS:ND1 | 2.33 | 0.42 |
| 4:4:167:LEU:O | 4:4:171:MET:HB3 | 2.19 | 0.42 |
| 7:7:33:ARG:NH2 | 7:7:45:ILE:C | 2.73 | 0.42 |
| 12:E:165:TYR:CE2 | 20:M:434:ALA:HB2 | 2.53 | 0.42 |
| 13:F:86:ASN:HA | 13:F:89:ARG:NH2 | 2.34 | 0.42 |
| 15:H:402:ILE:HG13 | 15:H:440:GLU:HG2 | 1.99 | 0.42 |
| 17:J:199:ALA:CB | 17:J:210:PHE:CE1 | 3.01 | 0.42 |
| 17:J:374:ARG:HH21 | 17:J:381:ASP:CG | 2.21 | 0.42 |
| 20:M:396:VAL:O | 20:M:400:MET:HG2 | 2.18 | 0.42 |
| 23:P:212:LYS:HD3 | 23:P:247:THR:CG2 | 2.46 | 0.42 |
| 23:P:266:TYR:CE1 | 23:P:322:LEU:HA | 2.54 | 0.42 |
| 23:P:315:GLN:O | 23:P:319:GLU:HG3 | 2.19 | 0.42 |
| 24:Q:148:LYS:O | 24:Q:149:LYS:CB | 2.66 | 0.42 |
| 26:S:428:ARG:CA | 27:T:195:LEU:HD22 | 2.42 | 0.42 |
| 29:V:93:ASP:O | 29:V:96:LYS:HB3 | 2.19 | 0.42 |
| 33:Z:103:TYR:CE2 | 33:Z:137:TYR:CE1 | 3.07 | 0.42 |
| 33:Z:410:THR:HG22 | 33:Z:414:GLY:HA3 | 1.99 | 0.42 |
| 33:Z:744:ALA:CA | 33:Z:783:VAL:HG22 | 2.48 | 0.42 |
| 33:Z:805:LEU:CD2 | 33:Z:841:GLU:CD | 2.72 | 0.42 |
| 33:Z:886:VAL:HA | 33:Z:893:PHE:CZ | 2.50 | 0.42 |
| 1:1:-2:LEU:HD12 | 1:1:-2:LEU:C | 2.39 | 0.42 |
| 2:2:87:LEU:HD23 | 2:2:94:ILE:HB | 2.00 | 0.42 |
| 3:3:63:ASN:CB | 10:C:96:GLN:NE2 | 2.82 | 0.42 |
| 5:5:35:ILE:HG21 | 5:5:56:GLU:HB2 | 2.01 | 0.42 |
| 6:6:36:ASP:OD1 | 6:6:38:GLY:N | 2.51 | 0.42 |
| 8:A:21:PRO:HB3 | 9:B:23:TYR:CE1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:F:14:SER:OG | 13:F:18:ARG:O | 2.35 | 0.42 |
| 15:H:102:CYS:HB2 | 15:H:105:ILE:CD1 | 2.27 | 0.42 |
| 15:H:156:VAL:CG2 | 15:H:181:TYR:CZ | 2.83 | 0.42 |
| 15:H:285:GLY:H | 15:H:331:ARG:NH1 | 2.15 | 0.42 |
| 15:H:311:ILE:HD12 | 15:H:361:LEU:HD13 | 2.00 | 0.42 |
| 19:L:149:ASP:CB | 19:L:152:THR:HB | 2.48 | 0.42 |
| 19:L:290:ARG:CZ | 19:L:293:GLU:HA | 2.49 | 0.42 |
| 21:N:303:LEU:HD13 | 21:N:342:GLY:HA3 | 2.01 | 0.42 |
| 21:N:596:LEU:CD2 | 21:N:717:LEU:HD13 | 2.42 | 0.42 |
| 21:N:669:GLU:O | 21:N:670:LYS:HB2 | 2.19 | 0.42 |
| 22:O:223:LEU:HD23 | 22:O:280:LEU:HB2 | 2.01 | 0.42 |
| 23:P:281:ILE:HD11 | 23:P:297:GLU:HG3 | 2.00 | 0.42 |
| 26:S:201:ILE:HD13 | 26:S:205:ASN:HD22 | 1.84 | 0.42 |
| 33:Z:542:ILE:HG21 | 33:Z:573:LEU:HD11 | 2.01 | 0.42 |
| 33:Z:584:VAL:O | 33:Z:588:ILE:HG13 | 2.19 | 0.42 |
| 1:1:46:SER:OG | 1:1:96:GLY:O | 2.33 | 0.42 |
| 1:1:66:TYR:HE2 | 1:1:73:PRO:HA | 1.85 | 0.42 |
| 2:2:197:GLU:O | 3:3:142:GLU:OE2 | 2.37 | 0.42 |
| 5:5:34:VAL:HG11 | 5:5:42:LEU:HD22 | 2.00 | 0.42 |
| 6:6:171:VAL:O | 6:6:175:VAL:HG23 | 2.20 | 0.42 |
| 8:A:18:ILE:HD12 | 9:B:20:GLN:HE22 | 1.84 | 0.42 |
| 9:B:2:THR:HB | 14:G:127:SER:OG | 2.19 | 0.42 |
| 9:B:43:VAL:HG11 | 9:B:137:ALA:CB | 2.41 | 0.42 |
| 10:C:18:ARG:NH2 | 11:D:29:ARG:HH22 | 2.11 | 0.42 |
| 10:C:50:ARG:HH12 | 10:C:232:PRO:HG3 | 1.85 | 0.42 |
| 12:E:56:SER:OG | 12:E:59:LEU:HB2 | 2.19 | 0.42 |
| 15:H:210:ASP:HA | 15:H:388:ILE:HG12 | 2.00 | 0.42 |
| 16:I:172:LYS:HD3 | 17:J:231:ARG:HH12 | 1.84 | 0.42 |
| 17:J:349:LYS:NZ | 17:J:383:GLU:HB2 | 2.35 | 0.42 |
| 18:K:346:ARG:CG | 18:K:349:ARG:HH22 | 2.25 | 0.42 |
| 21:N:162:ARG:HD3 | 21:N:165:ILE:HG13 | 1.97 | 0.42 |
| 21:N:221:ASP:HA | 21:N:894:ARG:NH1 | 2.34 | 0.42 |
| 22:O:291:ILE:HD12 | 22:O:294:MET:HE1 | 2.00 | 0.42 |
| 22:O:365:LYS:HB3 | 22:O:369:ARG:HH12 | 1.83 | 0.42 |
| 24:Q:190:ASN:HD21 | 24:Q:193:LYS:HE3 | 1.85 | 0.42 |
| 24:Q:245:SER:O | 24:Q:249:LEU:HG | 2.18 | 0.42 |
| 24:Q:373:VAL:O | 24:Q:377:LEU:HG | 2.19 | 0.42 |
| 1:1:36:ARG:HD3 | 1:1:42:TRP:CZ2 | 2.54 | 0.42 |
| 3:3:7:THR:HG23 | 3:3:112:ILE:HD13 | 2.01 | 0.42 |
| 8:A:18:ILE:HB | 9:B:20:GLN:NE2 | 2.33 | 0.42 |
| 9:B:43:VAL:HG21 | 9:B:146:SER:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:C:13:PHE:CD1 | 10:C:19:LEU:HD21 | 2.54 | 0.42 |
| 12:E:166:ARG:HB2 | 13:F:60:GLN:CD | 2.40 | 0.42 |
| 13:F:7:ASP:O | 13:F:21:GLN:NE2 | 2.52 | 0.42 |
| 15:H:284:VAL:CG2 | 20:M:254:MET:CA | 2.79 | 0.42 |
| 15:H:423:CYS:HA | 15:H:443:PHE:CE1 | 2.54 | 0.42 |
| 16:I:128:TYR:CE2 | 16:I:154:MET:HG3 | 2.53 | 0.42 |
| 17:J:301:ASP:O | 17:J:304:LEU:HB2 | 2.19 | 0.42 |
| 18:K:197:LEU:HD23 | 18:K:200:GLN:OE1 | 2.20 | 0.42 |
| 19:L:125:PRO:HB2 | 19:L:127:TYR:HE2 | 1.72 | 0.42 |
| 19:L:141:LYS:O | 19:L:144:VAL:HG23 | 2.18 | 0.42 |
| 20:M:75:LEU:HD22 | 20:M:77:TYR:O | 2.19 | 0.42 |
| 20:M:401:ILE:HG12 | 20:M:404:ARG:NH2 | 2.35 | 0.42 |
| 21:N:4:THR:HG21 | 26:S:215:MET:SD | 2.60 | 0.42 |
| 21:N:525:ASN:HA | 21:N:528:ARG:HD3 | 2.01 | 0.42 |
| 21:N:745:LEU:O | 21:N:748:PHE:CD1 | 2.73 | 0.42 |
| 23:P:95:TYR:CE2 | 23:P:96:MET:CE | 3.00 | 0.42 |
| 26:S:223:LEU:O | 26:S:224:LYS:HD3 | 2.19 | 0.42 |
| 26:S:461:PHE:HA | 28:U:281:LEU:HD11 | 2.01 | 0.42 |
| 33:Z:112:LYS:HA | 33:Z:115:LEU:HD12 | 2.01 | 0.42 |
| 33:Z:224:LEU:HD21 | 33:Z:236:PHE:HD2 | 1.76 | 0.42 |
| 1:1:63:LEU:HD22 | 1:1:73:PRO:HG3 | 2.01 | 0.42 |
| 2:2:55:VAL:HG21 | 2:2:94:ILE:CG2 | 2.49 | 0.42 |
| 2:2:97:TYR:CZ | 2:2:115:ALA:CB | 3.02 | 0.42 |
| 3:3:42:LEU:HD22 | 3:3:78:PHE:HZ | 1.83 | 0.42 |
| 8:A:52:VAL:CG1 | 8:A:203:VAL:HG22 | 2.49 | 0.42 |
| 8:A:87:ILE:O | 8:A:87:ILE:CG2 | 2.67 | 0.42 |
| 13:F:101:ARG:HG2 | 13:F:103:LEU:N | 2.19 | 0.42 |
| 14:G:175:LEU:O | 14:G:179:VAL:HG23 | 2.19 | 0.42 |
| 20:M:221:TYR:O | 20:M:349:PHE:HD1 | 2.03 | 0.42 |
| 21:N:106:ILE:O | 21:N:110:VAL:HG23 | 2.19 | 0.42 |
| 21:N:207:LEU:CD1 | 21:N:232:LEU:HD23 | 2.49 | 0.42 |
| 21:N:770:LYS:CD | 21:N:917:ILE:HG21 | 2.50 | 0.42 |
| 23:P:101:MET:HE2 | 23:P:119:ILE:HD11 | 2.01 | 0.42 |
| 23:P:303:PHE:CZ | 23:P:345:VAL:HG22 | 2.46 | 0.42 |
| 23:P:326:ASP:OD1 | 23:P:327:LEU:HG | 2.20 | 0.42 |
| 23:P:422:LEU:CD1 | 28:U:262:GLN:NE2 | 2.82 | 0.42 |
| 24:Q:52:ASN:HD21 | 24:Q:92:LYS:NZ | 2.18 | 0.42 |
| 26:S:436:ILE:HG23 | 27:T:197:TYR:CD2 | 2.55 | 0.42 |
| 28:U:12:PRO:HD2 | 28:U:167:GLU:OE2 | 2.19 | 0.42 |
| 33:Z:354:PRO:O | 33:Z:357:ILE:CG1 | 2.66 | 0.42 |
| 3:3:6:MET:HE1 | 3:3:157:THR:HG22 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:83:VAL:HG11 | 8:A:90:ALA:HA | 2.01 | 0.42 |
| 8:A:123:ASN:HB3 | 9:B:84:VAL:HG22 | 2.01 | 0.42 |
| 9:B:75:TYR:HB3 | 9:B:134:LEU:CD2 | 2.49 | 0.42 |
| 12:E:46:VAL:HG11 | 12:E:145:ALA:CB | 2.47 | 0.42 |
| 12:E:50:VAL:HG22 | 12:E:67:ILE:CD1 | 2.45 | 0.42 |
| 15:H:56:LEU:HD21 | 33:Z:768:GLY:HA2 | 2.01 | 0.42 |
| 17:J:247:MET:HE2 | 17:J:272:MET:HG3 | 2.01 | 0.42 |
| 18:K:280:LYS:NZ | 18:K:293:GLN:OE1 | 2.50 | 0.42 |
| 21:N:211:PHE:O | 21:N:215:MET:HG2 | 2.18 | 0.42 |
| 22:O:46:THR:CG2 | 22:O:50:ASP:OD2 | 2.68 | 0.42 |
| 22:O:58:ARG:CB | 22:O:61:LEU:HD12 | 2.49 | 0.42 |
| 23:P:154:ASP:OD1 | 23:P:190:LYS:HD3 | 2.20 | 0.42 |
| 23:P:324:GLU:O | 23:P:325:ASP:CG | 2.58 | 0.42 |
| 24:Q:151:TYR:CD2 | 24:Q:188:LEU:HD21 | 2.55 | 0.42 |
| 26:S:162:VAL:HG12 | 26:S:167:LEU:HD22 | 2.00 | 0.42 |
| 26:S:343:LEU:CG | 26:S:347:HIS:HE1 | 2.30 | 0.42 |
| 29:V:88:GLN:NE2 | 29:V:89:ALA:HB2 | 2.34 | 0.42 |
| 33:Z:89:LEU:CD1 | 33:Z:125:THR:CG2 | 2.97 | 0.42 |
| 33:Z:407:VAL:HG12 | 33:Z:415:MET:CE | 2.50 | 0.42 |
| 1:1:55:ILE:HD12 | 1:1:95:ALA:HB2 | 2.00 | 0.42 |
| 5:5:4:LEU:HD12 | 5:5:4:LEU:C | 2.40 | 0.42 |
| 5:5:135:PHE:CE2 | 5:5:163:ALA:CB | 2.83 | 0.42 |
| 6:6:48:PHE:CE2 | 6:6:50:ALA:CB | 2.95 | 0.42 |
| 9:B:122:THR:OG1 | 9:B:129:PRO:HG3 | 2.19 | 0.42 |
| 10:C:72:LYS:HG2 | 10:C:225:VAL:HG11 | 2.01 | 0.42 |
| 12:E:180:GLN:HA | 12:E:183:LEU:HD12 | 2.02 | 0.42 |
| 13:F:74:LEU:C | 13:F:74:LEU:HD12 | 2.40 | 0.42 |
| 15:H:101:ARG:NH2 | 15:H:150:LYS:HG3 | 2.35 | 0.42 |
| 16:I:207:LEU:CD2 | 33:Z:930:GLY:HA2 | 2.49 | 0.42 |
| 16:I:395:MET:HG3 | 16:I:420:LYS:CD | 2.44 | 0.42 |
| 17:J:183:LYS:O | 17:J:276:LEU:HD13 | 2.20 | 0.42 |
| 18:K:220:THR:HG22 | 18:K:224:LYS:HE3 | 2.01 | 0.42 |
| 18:K:385:ALA:HA | 19:L:340:PRO:HD2 | 2.01 | 0.42 |
| 19:L:221:TYR:OH | 19:L:348:GLU:HB3 | 2.20 | 0.42 |
| 21:N:45:ASP:O | 21:N:48:ALA:HB3 | 2.19 | 0.42 |
| 21:N:394:ARG:HA | 21:N:401:LYS:HZ3 | 1.84 | 0.42 |
| 22:O:138:LEU:HG | 22:O:146:ALA:HB1 | 2.00 | 0.42 |
| 24:Q:9:GLU:CG | 24:Q:13:ARG:HH12 | 2.32 | 0.42 |
| 25:R:31:PHE:CE1 | 25:R:35:GLN:HG3 | 2.54 | 0.42 |
| 25:R:392:ARG:HG3 | 25:R:394:ASP:O | 2.20 | 0.42 |
| 25:R:411:LEU:HD22 | 26:S:464:ARG:NH1 | 2.21 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:T:183:SER:O | 27:T:186:ARG:HG2 | 2.19 | 0.42 |
| 28:U:195:LYS:HB3 | 29:V:233:LYS:HD3 | 2.02 | 0.42 |
| 28:U:278:ILE:HA | 28:U:281:LEU:HD12 | 2.01 | 0.42 |
| 31:X:79:LYS:HE3 | 31:X:98:PHE:CD2 | 2.51 | 0.42 |
| 33:Z:497:PHE:CD2 | 33:Z:505:VAL:CB | 3.02 | 0.42 |
| 33:Z:532:HIS:CD2 | 33:Z:572:ILE:HD13 | 2.54 | 0.42 |
| 1:1:6:VAL:HG13 | 1:1:142:PHE:CD1 | 2.54 | 0.42 |
| 3:3:36:HIS:HB3 | 3:3:41:PHE:CD2 | 2.55 | 0.42 |
| 5:5:57:THR:HG21 | 6:6:82:ARG:NH1 | 2.35 | 0.42 |
| 6:6:175:VAL:HG13 | 6:6:179:PHE:HE2 | 1.84 | 0.42 |
| 7:7:70:ASN:N | 7:7:71:PRO:HD3 | 2.33 | 0.42 |
| 8:A:54:ILE:CD1 | 8:A:207:ILE:HG13 | 2.49 | 0.42 |
| 13:F:65:LYS:CA | 13:F:222:PHE:CE2 | 3.02 | 0.42 |
| 14:G:111:PHE:CG | 14:G:114:ARG:NH2 | 2.85 | 0.42 |
| 16:I:320:GLY:HA2 | 16:I:323:LYS:NZ | 2.34 | 0.42 |
| 17:J:377:VAL:CG1 | 17:J:378:THR:N | 2.82 | 0.42 |
| 18:K:156:SER:HB3 | 18:K:253:MET:SD | 2.60 | 0.42 |
| 19:L:169:ASN:ND2 | 19:L:262:ILE:HD13 | 2.34 | 0.42 |
| 21:N:405:LEU:CD1 | 21:N:446:ALA:HB2 | 2.49 | 0.42 |
| 25:R:73:ASN:N | 25:R:76:GLN:HE21 | 2.17 | 0.42 |
| 27:T:157:TYR:HB3 | 27:T:189:ILE:HD11 | 2.02 | 0.42 |
| 28:U:62:ASN:OD1 | 28:U:64:ASP:N | 2.46 | 0.42 |
| 28:U:173:HIS:ND1 | 29:V:150:LYS:HA | 2.35 | 0.42 |
| 29:V:140:VAL:HG11 | 29:V:156:PHE:HE2 | 1.83 | 0.42 |
| 31:X:100:TRP:CZ3 | 31:X:102:GLN:CA | 2.92 | 0.42 |
| 33:Z:357:ILE:HD11 | 33:Z:980:VAL:HG21 | 2.01 | 0.42 |
| 33:Z:408:TYR:CE1 | 33:Z:411:LYS:NZ | 2.88 | 0.42 |
| 1:1:57:ASP:HB3 | 8:A:106:TYR:OH | 2.19 | 0.42 |
| 4:4:28:LYS:HE2 | 4:4:31:ASP:HB2 | 2.01 | 0.42 |
| 4:4:181:LYS:HE2 | 4:4:190:GLN:HG2 | 2.01 | 0.42 |
| 8:A:63:LEU:HD21 | 14:G:176:GLU:HA | 2.02 | 0.42 |
| 9:B:239:THR:CG2 | 9:B:240:SER:N | 2.83 | 0.42 |
| 11:D:19:GLN:OE1 | 11:D:128:PRO:HD3 | 2.20 | 0.42 |
| 12:E:15:PHE:HZ | 13:F:126:ARG:NH2 | 2.13 | 0.42 |
| 18:K:241:GLU:CA | 19:L:303:ARG:NH1 | 2.72 | 0.42 |
| 19:L:93:ASN:O | 19:L:96:LYS:HB2 | 2.20 | 0.42 |
| 19:L:178:ILE:HD11 | 19:L:230:LEU:O | 2.20 | 0.42 |
| 21:N:229:VAL:HG11 | 21:N:238:ALA:HB2 | 2.02 | 0.42 |
| 21:N:302:PHE:HD1 | 21:N:871:MET:HG3 | 1.83 | 0.42 |
| 21:N:324:LYS:HD2 | 21:N:325:PHE:CE2 | 2.55 | 0.42 |
| 23:P:369:LEU:CD1 | 23:P:376:THR:HG23 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:R:171:MET:HG3 | 25:R:209:ARG:HH11 | 1.84 | 0.42 |
| 25:R:334:ARG:HH11 | 25:R:363:PHE:HZ | 1.60 | 0.42 |
| 26:S:258:GLU:O | 26:S:259:TYR:CG | 2.73 | 0.42 |
| 27:T:112:ASN:HA | 27:T:177:PHE:CZ | 2.55 | 0.42 |
| 27:T:158:GLN:OE1 | 27:T:210:PHE:HE1 | 2.03 | 0.42 |
| 27:T:254:ASP:HB2 | 27:T:257:THR:OG1 | 2.19 | 0.42 |
| 28:U:8:VAL:CG1 | 28:U:10:ILE:HD11 | 2.50 | 0.42 |
| 31:X:45:PHE:CZ | 31:X:67:ILE:HD13 | 2.55 | 0.42 |
| 33:Z:483:THR:HG22 | 33:Z:521:GLU:HG3 | 2.02 | 0.42 |
| 2:2:1:THR:HG21 | 2:2:33:LYS:HE3 | 2.02 | 0.42 |
| 2:2:7:LYS:O | 2:2:146:LEU:CD2 | 2.63 | 0.42 |
| 4:4:13:ILE:CG2 | 4:4:160:LEU:CD1 | 2.97 | 0.42 |
| 4:4:65:LEU:O | 4:4:69:ARG:HG3 | 2.19 | 0.42 |
| 6:6:193:LEU:HD21 | 6:6:195:ILE:HD11 | 2.02 | 0.42 |
| 7:7:145:PRO:CA | 7:7:148:ARG:HH21 | 2.32 | 0.42 |
| 8:A:78:THR:HG22 | 8:A:231:ASP:C | 2.40 | 0.42 |
| 13:F:65:LYS:CE | 13:F:222:PHE:HD2 | 2.25 | 0.42 |
| 13:F:211:LEU:HD12 | 13:F:234:ILE:HD11 | 2.01 | 0.42 |
| 15:H:247:LEU:HB2 | 15:H:371:ILE:HG21 | 2.02 | 0.42 |
| 16:I:172:LYS:HE2 | 17:J:278:GLN:HB2 | 2.01 | 0.42 |
| 16:I:384:LYS:NZ | 16:I:420:LYS:HZ1 | 2.10 | 0.42 |
| 17:J:84:VAL:HG23 | 17:J:98:VAL:CG1 | 2.49 | 0.42 |
| 18:K:140:HIS:ND1 | 18:K:143:SER:N | 2.68 | 0.42 |
| 18:K:187:ALA:O | 18:K:313:LYS:NZ | 2.53 | 0.42 |
| 19:L:149:ASP:OD2 | 19:L:152:THR:CB | 2.68 | 0.42 |
| 19:L:224:PRO:O | 20:M:342:ARG:NH1 | 2.37 | 0.42 |
| 21:N:21:LYS:HD3 | 21:N:49:LEU:HD22 | 2.02 | 0.42 |
| 21:N:338:PHE:HZ | 21:N:736:PHE:HE1 | 1.67 | 0.42 |
| 21:N:489:MET:HE1 | 21:N:494:LYS:HG3 | 2.00 | 0.42 |
| 21:N:645:THR:HG22 | 21:N:656:ALA:HB1 | 2.02 | 0.42 |
| 22:O:250:TRP:CG | 22:O:269:LEU:HD23 | 2.53 | 0.42 |
| 24:Q:165:PHE:HE1 | 24:Q:170:ASP:HB2 | 1.85 | 0.42 |
| 25:R:118:GLN:O | 25:R:122:GLU:HG3 | 2.20 | 0.42 |
| 25:R:225:LYS:O | 25:R:228:ALA:HB3 | 2.19 | 0.42 |
| 31:X:49:GLU:HG2 | 31:X:65:SER:OG | 2.20 | 0.42 |
| 31:X:79:LYS:HD3 | 31:X:98:PHE:HE2 | 1.84 | 0.42 |
| 33:Z:392:LEU:HD13 | 33:Z:424:SER:C | 2.38 | 0.42 |
| 33:Z:823:ASN:O | 33:Z:827:LEU:HD12 | 2.20 | 0.42 |
| 1:1:3:ILE:HD12 | 1:1:44:CYS:HB2 | 2.02 | 0.41 |
| 3:3:60:TYR:CD2 | 10:C:96:GLN:CB | 2.83 | 0.41 |
| 6:6:91:LYS:HD2 | 6:6:96:TYR:OH | 2.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:54:ILE:HD12 | 8:A:206:ALA:HB3 | 2.01 | 0.41 |
| 9:B:249:ALA:CB | 24:Q:94:VAL:HG12 | 2.50 | 0.41 |
| 10:C:2:GLY:HA2 | 13:F:123:TYR:CZ | 2.55 | 0.41 |
| 12:E:184:LEU:HA | 13:F:56:LEU:HD11 | 2.02 | 0.41 |
| 12:E:223:THR:HB | 12:E:226:ASP:OD1 | 2.20 | 0.41 |
| 15:H:278:GLU:CD | 16:I:262:ARG:HH11 | 2.22 | 0.41 |
| 19:L:282:GLU:OE2 | 20:M:306:LEU:CD1 | 2.67 | 0.41 |
| 19:L:383:SER:HB3 | 19:L:386:PHE:HD2 | 1.85 | 0.41 |
| 20:M:283:LEU:O | 20:M:283:LEU:HG | 2.19 | 0.41 |
| 20:M:424:ALA:O | 20:M:425:ARG:CB | 2.64 | 0.41 |
| 21:N:414:GLY:HA3 | 21:N:728:LYS:HE2 | 2.02 | 0.41 |
| 21:N:739:PHE:HD1 | 21:N:743:PHE:O | 2.02 | 0.41 |
| 22:O:41:LEU:HG | 22:O:58:ARG:CG | 2.50 | 0.41 |
| 22:O:133:ILE:HG23 | 22:O:134:ALA:N | 2.34 | 0.41 |
| 22:O:166:ARG:HG3 | 22:O:167:ILE:N | 2.35 | 0.41 |
| 24:Q:141:LEU:CG | 24:Q:145:HIS:CD2 | 2.99 | 0.41 |
| 24:Q:146:TYR:HD1 | 24:Q:184:VAL:HG22 | 1.84 | 0.41 |
| 24:Q:419:LEU:CD2 | 28:U:289:ASP:OD2 | 2.68 | 0.41 |
| 28:U:65:VAL:CG1 | 30:W:96:LEU:HD11 | 2.49 | 0.41 |
| 29:V:51:GLY:HA2 | 29:V:71:MET:HG3 | 2.02 | 0.41 |
| 29:V:186:GLN:HG2 | 29:V:190:HIS:HD2 | 1.85 | 0.41 |
| 33:Z:591:ILE:HG22 | 33:Z:593:HIS:HD2 | 1.85 | 0.41 |
| 33:Z:827:LEU:HD13 | 33:Z:855:LEU:HD22 | 2.02 | 0.41 |
| 3:3:63:ASN:HB3 | 10:C:96:GLN:NE2 | 2.35 | 0.41 |
| 3:3:100:VAL:CG2 | 3:3:115:PHE:HE1 | 2.33 | 0.41 |
| 3:3:140:MET:HE3 | 3:3:144:LEU:HD11 | 2.00 | 0.41 |
| 5:5:54:PHE:HB2 | 6:6:85:GLN:HE22 | 1.85 | 0.41 |
| 13:F:11:VAL:HG22 | 13:F:120:THR:O | 2.20 | 0.41 |
| 13:F:72:LEU:HD23 | 13:F:88:LEU:HD23 | 2.01 | 0.41 |
| 15:H:147:ILE:HG13 | 15:H:183:ILE:CD1 | 2.50 | 0.41 |
| 15:H:168:ILE:HD12 | 15:H:187:LEU:CD1 | 2.42 | 0.41 |
| 15:H:379:LEU:HD23 | 15:H:415:THR:HG22 | 1.95 | 0.41 |
| 16:I:245:LEU:HG | 16:I:247:ILE:CD1 | 2.43 | 0.41 |
| 16:I:320:GLY:HA2 | 16:I:323:LYS:HZ3 | 1.85 | 0.41 |
| 19:L:163:THR:HG21 | 19:L:264:ARG:NH2 | 2.34 | 0.41 |
| 19:L:361:PHE:CE2 | 19:L:391:ILE:HD12 | 2.51 | 0.41 |
| 20:M:148:VAL:HG22 | 20:M:155:ILE:CG1 | 2.34 | 0.41 |
| 21:N:293:LEU:HD22 | 21:N:379:LEU:CD1 | 2.27 | 0.41 |
| 22:O:321:LYS:O | 22:O:325:GLU:HG3 | 2.20 | 0.41 |
| 23:P:131:PHE:CB | 23:P:136:ARG:NH1 | 2.80 | 0.41 |
| 24:Q:38:SER:OG | 24:Q:39:SER:N | 2.45 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:120:LYS:O | 24:Q:123:GLU:HB2 | 2.20 | 0.41 |
| 25:R:73:ASN:N | 25:R:76:GLN:NE2 | 2.68 | 0.41 |
| 25:R:131:ALA:O | 25:R:135:ILE:HG13 | 2.20 | 0.41 |
| 25:R:237:THR:O | 25:R:246:TYR:CE1 | 2.72 | 0.41 |
| 25:R:298:ALA:O | 25:R:299:SER:HB3 | 2.20 | 0.41 |
| 25:R:367:ASP:OD1 | 25:R:370:LYS:HD2 | 2.19 | 0.41 |
| 26:S:388:ILE:HG21 | 26:S:422:MET:HE3 | 2.03 | 0.41 |
| 27:T:92:ASN:O | 27:T:130:ASP:OD1 | 2.38 | 0.41 |
| 28:U:189:ARG:CZ | 29:V:296:LEU:HD22 | 2.50 | 0.41 |
| 29:V:202:ASP:OD1 | 29:V:203:TYR:N | 2.53 | 0.41 |
| 30:W:2:VAL:HG23 | 30:W:4:GLU:HG3 | 2.02 | 0.41 |
| 30:W:37:PHE:CE2 | 30:W:69:PHE:HB3 | 2.55 | 0.41 |
| 30:W:129:ALA:O | 30:W:161:VAL:HG23 | 2.20 | 0.41 |
| 31:X:91:PHE:O | 31:X:96:ARG:NE | 2.42 | 0.41 |
| 33:Z:303:ASP:N | 33:Z:307:HIS:NE2 | 2.67 | 0.41 |
| 33:Z:392:LEU:HD11 | 33:Z:427:GLN:OE1 | 2.20 | 0.41 |
| 33:Z:497:PHE:HB2 | 33:Z:533:VAL:CG2 | 2.46 | 0.41 |
| 3:3:116:ASP:CG | 3:3:117:LEU:H | 2.23 | 0.41 |
| 5:5:159:ARG:NH1 | 5:5:200:VAL:HG13 | 2.35 | 0.41 |
| 7:7:137:GLY:O | 7:7:140:ALA:HB3 | 2.19 | 0.41 |
| 10:C:4:ARG:NH1 | 12:E:125:GLU:HG3 | 2.36 | 0.41 |
| 10:C:86:ILE:O | 10:C:90:THR:HG23 | 2.20 | 0.41 |
| 13:F:37:GLY:HA2 | 13:F:46:LEU:HD23 | 2.02 | 0.41 |
| 13:F:101:ARG:HH11 | 13:F:104:ALA:H | 1.68 | 0.41 |
| 13:F:194:VAL:O | 13:F:197:ILE:HG22 | 2.20 | 0.41 |
| 14:G:61:GLN:HG2 | 14:G:214:GLU:OE1 | 2.20 | 0.41 |
| 14:G:168:ARG:HH21 | 14:G:172:LYS:HZ1 | 1.68 | 0.41 |
| 15:H:206:VAL:CG2 | 15:H:261:ARG:NE | 2.64 | 0.41 |
| 17:J:166:LEU:O | 17:J:174:PHE:CE1 | 2.74 | 0.41 |
| 20:M:152:SER:O | 20:M:154:LEU:HG | 2.20 | 0.41 |
| 20:M:200:PRO:HB2 | 20:M:319:ASP:OD2 | 2.20 | 0.41 |
| 22:O:15:ARG:NH1 | 22:O:72:LYS:HG2 | 2.35 | 0.41 |
| 22:O:23:HIS:CG | 22:O:24:PRO:HD2 | 2.55 | 0.41 |
| 24:Q:343:LEU:O | 24:Q:347:LEU:HG | 2.20 | 0.41 |
| 24:Q:369:ASP:C | 24:Q:369:ASP:OD1 | 2.59 | 0.41 |
| 25:R:37:LYS:HG3 | 25:R:38:VAL:HG23 | 2.01 | 0.41 |
| 31:X:48:PHE:HE1 | 31:X:128:VAL:HG11 | 1.85 | 0.41 |
| 3:3:-2:ASN:ND2 | 3:3:48:ALA:HB2 | 2.36 | 0.41 |
| 3:3:65:TYR:CD2 | 3:3:73:ILE:HG22 | 2.54 | 0.41 |
| 6:6:43:MET:HG3 | 6:6:102:ILE:CG2 | 2.41 | 0.41 |
| 8:A:137:LEU:HD21 | 14:G:124:LEU:HD11 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:C:208:TYR:HB3 | 10:C:239:LEU:HD12 | 2.00 | 0.41 |
| 10:C:244:ILE:O | 10:C:244:ILE:HG22 | 2.21 | 0.41 |
| 11:D:127:ARG:HD2 | 11:D:127:ARG:O | 2.19 | 0.41 |
| 13:F:14:SER:HB2 | 13:F:15:PRO:HD2 | 2.02 | 0.41 |
| 13:F:101:ARG:NH2 | 13:F:103:LEU:CD1 | 2.82 | 0.41 |
| 15:H:331:ARG:HD2 | 20:M:252:VAL:HG11 | 2.01 | 0.41 |
| 17:J:177:LEU:CD2 | 17:J:179:ILE:HB | 2.51 | 0.41 |
| 17:J:349:LYS:HZ3 | 17:J:383:GLU:HB2 | 1.85 | 0.41 |
| 18:K:234:PHE:CE2 | 18:K:236:ARG:HB2 | 2.56 | 0.41 |
| 19:L:284:ASP:HB2 | 20:M:295:LYS:HE3 | 2.03 | 0.41 |
| 20:M:196:ALA:CA | 20:M:345:ARG:HH21 | 2.32 | 0.41 |
| 21:N:406:TYR:CE1 | 21:N:448:LEU:HD13 | 2.56 | 0.41 |
| 22:O:383:LYS:NZ | 27:T:252:GLU:HG3 | 2.34 | 0.41 |
| 26:S:323:LEU:HD21 | 26:S:383:LEU:HD23 | 2.02 | 0.41 |
| 27:T:57:ILE:CG2 | 27:T:58:THR:N | 2.83 | 0.41 |
| 28:U:67:PHE:CE1 | 30:W:97:THR:CG2 | 3.04 | 0.41 |
| 29:V:69:PHE:C | 29:V:108:TYR:HH | 2.24 | 0.41 |
| 33:Z:103:TYR:CE2 | 33:Z:137:TYR:HE1 | 2.38 | 0.41 |
| 33:Z:153:TYR:CZ | 33:Z:157:LEU:HD22 | 2.55 | 0.41 |
| 33:Z:483:THR:CB | 33:Z:521:GLU:HG3 | 2.51 | 0.41 |
| 33:Z:562:TRP:CE2 | 33:Z:566:LEU:CD2 | 2.91 | 0.41 |
| 2:2:43:CYS:SG | 2:2:100:VAL:HG22 | 2.61 | 0.41 |
| 4:4:55:PHE:O | 4:4:59:ILE:HG12 | 2.21 | 0.41 |
| 6:6:14:LEU:CD2 | 6:6:42:VAL:HG23 | 2.50 | 0.41 |
| 7:7:5:SER:OG | 7:7:119:LEU:HD11 | 2.20 | 0.41 |
| 10:C:177:GLN:HE22 | 11:D:52:LEU:HB3 | 1.84 | 0.41 |
| 11:D:16:HIS:HB2 | 11:D:21:GLU:OE2 | 2.20 | 0.41 |
| 12:E:35:SER:HG | 12:E:53:ARG:HE | 1.63 | 0.41 |
| 15:H:61:ALA:O | 15:H:65:GLU:HG3 | 2.21 | 0.41 |
| 15:H:62:ARG:CD | 16:I:96:LEU:HD21 | 2.50 | 0.41 |
| 15:H:382:LEU:HD22 | 15:H:408:SER:C | 2.41 | 0.41 |
| 16:I:172:LYS:NZ | 17:J:234:PHE:CE2 | 2.89 | 0.41 |
| 16:I:354:ASP:OD1 | 16:I:354:ASP:C | 2.59 | 0.41 |
| 17:J:91:GLU:HB3 | 17:J:94:TYR:OH | 2.20 | 0.41 |
| 20:M:197:ILE:C | 20:M:200:PRO:HD2 | 2.40 | 0.41 |
| 23:P:72:TRP:CE3 | 23:P:104:LEU:CD2 | 3.03 | 0.41 |
| 23:P:130:ILE:O | 23:P:130:ILE:CG2 | 2.65 | 0.41 |
| 24:Q:88:PHE:CE2 | 24:Q:89:ALA:CB | 3.04 | 0.41 |
| 24:Q:348:CYS:SG | 24:Q:380:MET:HG3 | 2.60 | 0.41 |
| 25:R:243:LEU:O | 25:R:244:THR:HB | 2.20 | 0.41 |
| 25:R:378:ASN:HB3 | 25:R:391:ASN:CG | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:T:28:PRO:O | 27:T:31:LYS:HB2 | 2.20 | 0.41 |
| 28:U:288:PHE:CE2 | 28:U:292:ILE:HD11 | 2.56 | 0.41 |
| 30:W:21:PHE:HZ | 30:W:25:ARG:HH12 | 1.58 | 0.41 |
| 31:X:31:GLY:HA2 | 31:X:53:THR:HG23 | 2.02 | 0.41 |
| 33:Z:452:LEU:HD22 | 33:Z:477:TYR:CD2 | 2.56 | 0.41 |
| 33:Z:865:ASP:CG | 33:Z:909:ARG:CZ | 2.81 | 0.41 |
| 33:Z:971:ILE:HG22 | 33:Z:972:SER:O | 2.20 | 0.41 |
| 4:4:117:GLN:NE2 | 4:4:130:GLY:HA3 | 2.34 | 0.41 |
| 5:5:66:HIS:CE1 | 5:5:70:GLU:CD | 2.94 | 0.41 |
| 6:6:19:ARG:HE | 6:6:190:GLY:HA3 | 1.85 | 0.41 |
| 6:6:56:VAL:O | 6:6:60:LYS:HG3 | 2.20 | 0.41 |
| 11:D:48:ARG:HH12 | 11:D:57:THR:CB | 2.30 | 0.41 |
| 11:D:174:PHE:CZ | 11:D:197:ARG:HB3 | 2.56 | 0.41 |
| 16:I:104:LEU:HD21 | 16:I:149:LEU:N | 2.36 | 0.41 |
| 16:I:126:PRO:CG | 16:I:154:MET:HE2 | 2.47 | 0.41 |
| 16:I:128:TYR:CD2 | 16:I:154:MET:CG | 3.01 | 0.41 |
| 16:I:371:LEU:HA | 16:I:411:VAL:H | 1.86 | 0.41 |
| 20:M:278:ILE:HB | 20:M:323:VAL:HG22 | 2.02 | 0.41 |
| 21:N:205:SER:O | 21:N:209:LYS:HG3 | 2.20 | 0.41 |
| 21:N:321:LEU:C | 21:N:321:LEU:HD12 | 2.41 | 0.41 |
| 21:N:340:HIS:HB3 | 21:N:374:ILE:HG12 | 2.03 | 0.41 |
| 21:N:692:GLU:O | 21:N:696:LYS:HG3 | 2.20 | 0.41 |
| 21:N:892:PRO:CA | 21:N:905:LEU:HG | 2.51 | 0.41 |
| 22:O:225:ASP:HA | 22:O:287:LEU:HD21 | 2.02 | 0.41 |
| 22:O:266:PHE:CE1 | 22:O:284:GLU:OE1 | 2.73 | 0.41 |
| 22:O:310:PHE:CD2 | 22:O:346:GLU:HA | 2.56 | 0.41 |
| 23:P:119:ILE:HD13 | 23:P:143:LEU:HB2 | 2.02 | 0.41 |
| 24:Q:88:PHE:CD2 | 24:Q:89:ALA:CB | 3.04 | 0.41 |
| 25:R:140:TYR:CD2 | 25:R:141:TYR:CE1 | 3.08 | 0.41 |
| 25:R:308:LEU:HD13 | 25:R:333:MET:HE2 | 2.03 | 0.41 |
| 25:R:381:ILE:O | 25:R:381:ILE:HG13 | 2.21 | 0.41 |
| 28:U:277:TYR:OH | 29:V:295:VAL:HG12 | 2.19 | 0.41 |
| 33:Z:436:LEU:CD2 | 33:Z:455:ILE:HG13 | 2.49 | 0.41 |
| 5:5:162:LEU:HD23 | 5:5:200:VAL:HG11 | 2.03 | 0.41 |
| 7:7:33:ARG:HH21 | 7:7:45:ILE:C | 2.24 | 0.41 |
| 7:7:33:ARG:NH2 | 7:7:46:SER:C | 2.74 | 0.41 |
| 9:B:58:SER:HA | 9:B:61:LEU:HD12 | 2.03 | 0.41 |
| 10:C:50:ARG:HH21 | 10:C:209:ASP:HA | 1.86 | 0.41 |
| 11:D:27:VAL:HG21 | 11:D:132:SER:OG | 2.20 | 0.41 |
| 11:D:151:GLU:HB2 | 11:D:152:PRO:HD2 | 2.02 | 0.41 |
| 11:D:214:VAL:HB | 11:D:222:VAL:HG13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:H:308:PHE:CD1 | 15:H:351:VAL:CG1 | 3.03 | 0.41 |
| 15:H:326:ASP:C | 15:H:329:VAL:HG22 | 2.40 | 0.41 |
| 17:J:213:VAL:HG11 | 17:J:233:LEU:CD2 | 2.51 | 0.41 |
| 21:N:87:ASP:OD1 | 21:N:88:ARG:HG2 | 2.20 | 0.41 |
| 21:N:379:LEU:O | 21:N:380:LEU:HD23 | 2.21 | 0.41 |
| 22:O:116:ASN:HB3 | 22:O:127:LEU:CG | 2.50 | 0.41 |
| 22:O:384:MET:CE | 28:U:189:ARG:C | 2.84 | 0.41 |
| 25:R:224:PHE:CE2 | 25:R:328:PHE:CZ | 3.08 | 0.41 |
| 25:R:264:THR:HA | 25:R:267:LYS:HE2 | 2.02 | 0.41 |
| 25:R:304:TYR:HD2 | 25:R:305:PHE:HD1 | 1.69 | 0.41 |
| 26:S:164:ILE:HB | 26:S:165:PRO:CD | 2.51 | 0.41 |
| 28:U:172:GLU:O | 28:U:176:ARG:HG3 | 2.20 | 0.41 |
| 33:Z:763:HIS:CD2 | 33:Z:766:HIS:CE1 | 3.07 | 0.41 |
| 33:Z:888:LEU:CB | 33:Z:901:PHE:HE1 | 2.19 | 0.41 |
| 2:2:3:ILE:HG13 | 2:2:99:ILE:CD1 | 2.50 | 0.41 |
| 7:7:112:GLN:HG2 | 7:7:114:ASN:H | 1.86 | 0.41 |
| 8:A:64:LEU:CD1 | 14:G:157:TRP:HD1 | 2.33 | 0.41 |
| 8:A:91:ARG:HG2 | 14:G:156:TYR:OH | 2.21 | 0.41 |
| 8:A:91:ARG:NH2 | 14:G:113:ASP:OD2 | 2.45 | 0.41 |
| 9:B:211:LEU:CD2 | 9:B:238:LEU:HD12 | 2.47 | 0.41 |
| 12:E:86:ARG:HH12 | 12:E:90:GLU:CB | 2.21 | 0.41 |
| 15:H:161:GLU:HA | 15:H:184:GLU:OE1 | 2.21 | 0.41 |
| 15:H:218:ILE:O | 15:H:222:ARG:HG3 | 2.21 | 0.41 |
| 16:I:214:LYS:NZ | 16:I:318:ASP:O | 2.37 | 0.41 |
| 17:J:28:GLN:HG3 | 26:S:225:HIS:CE1 | 2.56 | 0.41 |
| 17:J:183:LYS:HD2 | 17:J:308:GLY:O | 2.21 | 0.41 |
| 19:L:163:THR:OG1 | 19:L:265:GLU:CG | 2.69 | 0.41 |
| 19:L:283:VAL:HA | 19:L:286:ILE:HG12 | 2.02 | 0.41 |
| 21:N:270:LEU:O | 21:N:274:VAL:HG23 | 2.20 | 0.41 |
| 21:N:535:LEU:O | 21:N:539:MET:HG3 | 2.21 | 0.41 |
| 21:N:771:PHE:HD2 | 21:N:772:GLN:O | 2.04 | 0.41 |
| 22:O:102:LEU:O | 22:O:103:LYS:CG | 2.68 | 0.41 |
| 22:O:211:GLN:HE22 | 22:O:248:TYR:HE2 | 1.69 | 0.41 |
| 27:T:15:PHE:HZ | 27:T:67:LEU:HB3 | 1.77 | 0.41 |
| 28:U:32:ARG:NE | 28:U:94:HIS:HE1 | 2.14 | 0.41 |
| 28:U:77:ASN:HD21 | 28:U:81:LYS:HE3 | 1.85 | 0.41 |
| 32:Y:83:ARG:HB2 | 32:Y:86:ARG:NH2 | 2.35 | 0.41 |
| 33:Z:306:MET:HE2 | 33:Z:310:LEU:HD11 | 2.01 | 0.41 |
| 33:Z:415:MET:HB3 | 33:Z:446:GLU:CB | 2.47 | 0.41 |
| 33:Z:857:LEU:HD21 | 33:Z:908:ILE:CD1 | 2.47 | 0.41 |
| 1:1:-8:LYS:HD3 | 2:2:116:HIS:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:87:TYR:HA | 1:1:116:GLY:O | 2.21 | 0.41 |
| 2:2:36:ARG:NE | 2:2:38:SER:C | 2.74 | 0.41 |
| 2:2:38:SER:HB2 | 2:2:39:PRO:HD2 | 2.02 | 0.41 |
| 4:4:13:ILE:HG21 | 4:4:160:LEU:CD1 | 2.50 | 0.41 |
| 4:4:65:LEU:HD11 | 4:4:69:ARG:NE | 2.36 | 0.41 |
| 4:4:174:ASP:CG | 4:4:176:LYS:NZ | 2.75 | 0.41 |
| 7:7:153:ARG:HG3 | 7:7:155:SER:OG | 2.20 | 0.41 |
| 7:7:180:ASP:OD1 | 7:7:182:ARG:N | 2.41 | 0.41 |
| 8:A:54:ILE:HD12 | 8:A:206:ALA:HB1 | 2.03 | 0.41 |
| 8:A:174:LYS:HG3 | 8:A:214:LEU:HD23 | 2.03 | 0.41 |
| 10:C:13:PHE:HZ | 11:D:127:ARG:HH12 | 1.58 | 0.41 |
| 12:E:15:PHE:CZ | 13:F:126:ARG:CZ | 3.04 | 0.41 |
| 12:E:125:GLU:H | 13:F:124:GLY:HA3 | 1.85 | 0.41 |
| 13:F:105:VAL:HG22 | 13:F:145:LEU:CB | 2.45 | 0.41 |
| 15:H:168:ILE:CD1 | 15:H:187:LEU:HD12 | 2.41 | 0.41 |
| 16:I:136:VAL:HG11 | 16:I:159:VAL:CG1 | 2.50 | 0.41 |
| 16:I:233:ALA:O | 16:I:236:VAL:HG12 | 2.20 | 0.41 |
| 16:I:336:PRO:HA | 16:I:339:ILE:HD12 | 2.02 | 0.41 |
| 18:K:71:GLU:O | 18:K:75:LEU:HG | 2.20 | 0.41 |
| 19:L:214:PRO:HD2 | 19:L:216:LYS:HZ2 | 1.83 | 0.41 |
| 19:L:383:SER:HB3 | 19:L:386:PHE:CD2 | 2.55 | 0.41 |
| 20:M:281:ASP:O | 20:M:282:GLU:HB2 | 2.20 | 0.41 |
| 20:M:290:ARG:NH1 | 20:M:294:GLU:HB3 | 2.35 | 0.41 |
| 20:M:376:TRP:CD2 | 20:M:377:GLN:N | 2.89 | 0.41 |
| 21:N:43:LEU:HD11 | 21:N:69:TYR:CZ | 2.56 | 0.41 |
| 21:N:346:ASN:O | 21:N:350:LYS:HG3 | 2.20 | 0.41 |
| 21:N:572:LEU:O | 21:N:576:VAL:HG23 | 2.21 | 0.41 |
| 21:N:664:LEU:HD21 | 21:N:672:ASN:ND2 | 2.36 | 0.41 |
| 21:N:697:PHE:CZ | 21:N:701:VAL:HG21 | 2.56 | 0.41 |
| 22:O:189:TYR:CE1 | 22:O:193:LEU:HD11 | 2.56 | 0.41 |
| 22:O:304:ASN:HD22 | 28:U:261:LEU:HA | 1.86 | 0.41 |
| 22:O:374:ASN:OD1 | 28:U:200:LEU:HB3 | 2.21 | 0.41 |
| 23:P:392:LYS:HE2 | 24:Q:354:PHE:CE2 | 2.56 | 0.41 |
| 23:P:431:HIS:HE1 | 28:U:137:TYR:HE1 | 1.67 | 0.41 |
| 25:R:102:LEU:HD23 | 25:R:102:LEU:C | 2.41 | 0.41 |
| 25:R:316:LEU:HD11 | 25:R:329:PHE:CZ | 2.52 | 0.41 |
| 26:S:343:LEU:HB3 | 26:S:344:PRO:CD | 2.49 | 0.41 |
| 28:U:48:VAL:HG22 | 28:U:90:ILE:HD11 | 2.02 | 0.41 |
| 29:V:156:PHE:CD1 | 29:V:198:SER:HA | 2.55 | 0.41 |
| 29:V:188:LEU:C | 29:V:188:LEU:CD1 | 2.89 | 0.41 |
| 30:W:8:LEU:HD21 | 30:W:33:VAL:HG22 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:W:20:ASP:CB | 30:W:25:ARG:CZ | 2.92 | 0.41 |
| 31:X:75:TRP:HE1 | 31:X:122:TYR:HA | 1.86 | 0.41 |
| 33:Z:71:LEU:CD2 | 33:Z:118:VAL:HG11 | 2.48 | 0.41 |
| 33:Z:187:SER:CA | 33:Z:201:LEU:HD12 | 2.51 | 0.41 |
| 33:Z:246:CYS:SG | 33:Z:271:ILE:HG22 | 2.50 | 0.41 |
| 33:Z:383:SER:CA | 33:Z:849:ARG:NH1 | 2.84 | 0.41 |
| 33:Z:449:ALA:HB1 | 33:Z:485:ILE:HG23 | 2.03 | 0.41 |
| 7:7:157:ILE:HB | 7:7:158:PRO:HD3 | 2.03 | 0.41 |
| 9:B:184:GLU:CG | 9:B:185:LEU:N | 2.84 | 0.41 |
| 12:E:229:LYS:O | 12:E:231:TYR:CD1 | 2.74 | 0.41 |
| 15:H:147:ILE:CD1 | 15:H:181:TYR:HB3 | 2.43 | 0.41 |
| 15:H:400:ARG:HH22 | 33:Z:366:LYS:HD2 | 1.85 | 0.41 |
| 18:K:220:THR:CG2 | 18:K:224:LYS:HE3 | 2.51 | 0.41 |
| 18:K:425:ASP:OD1 | 18:K:428:LYS:NZ | 2.52 | 0.41 |
| 20:M:195:GLU:CA | 20:M:199:LEU:HD12 | 2.39 | 0.41 |
| 21:N:9:LEU:HD22 | 21:N:27:SER:HB2 | 2.03 | 0.41 |
| 21:N:23:TYR:HE2 | 27:T:41:ILE:HG23 | 1.86 | 0.41 |
| 21:N:482:ALA:HB1 | 21:N:517:LEU:CD2 | 2.50 | 0.41 |
| 21:N:508:THR:CG2 | 21:N:510:HIS:H | 2.32 | 0.41 |
| 22:O:71:ASP:O | 30:W:18:ASN:CB | 2.64 | 0.41 |
| 22:O:223:LEU:HD22 | 22:O:279:ILE:HB | 2.02 | 0.41 |
| 23:P:239:GLN:HG2 | 23:P:276:LEU:HD11 | 2.03 | 0.41 |
| 24:Q:215:VAL:O | 24:Q:218:LEU:HB2 | 2.21 | 0.41 |
| 24:Q:331:THR:CG2 | 24:Q:335:PHE:CZ | 3.04 | 0.41 |
| 25:R:158:LEU:O | 25:R:161:ALA:HB2 | 2.21 | 0.41 |
| 25:R:237:THR:CG2 | 25:R:275:GLU:OE1 | 2.68 | 0.41 |
| 26:S:201:ILE:HD13 | 26:S:205:ASN:ND2 | 2.35 | 0.41 |
| 26:S:461:PHE:CE1 | 28:U:278:ILE:HA | 2.55 | 0.41 |
| 26:S:461:PHE:CG | 28:U:277:TYR:HB3 | 2.56 | 0.41 |
| 27:T:229:VAL:CG1 | 27:T:230:ASN:H | 2.34 | 0.41 |
| 28:U:65:VAL:HG21 | 30:W:92:GLN:OE1 | 2.21 | 0.41 |
| 30:W:59:PRO:HG2 | 30:W:89:THR:CG2 | 2.51 | 0.41 |
| 33:Z:308:LYS:NZ | 33:Z:919:GLU:OE1 | 2.54 | 0.41 |
| 33:Z:493:LEU:HD21 | 33:Z:497:PHE:HE2 | 1.85 | 0.41 |
| 5:5:17:ASP:OD1 | 5:5:17:ASP:C | 2.59 | 0.40 |
| 5:5:128:CYS:SG | 5:5:140:LEU:CD1 | 3.09 | 0.40 |
| 9:B:94:HIS:CD2 | 9:B:98:LYS:NZ | 2.89 | 0.40 |
| 9:B:190:HIS:CE1 | 24:Q:94:VAL:HG21 | 2.54 | 0.40 |
| 11:D:138:PHE:CE1 | 11:D:215:VAL:HG12 | 2.55 | 0.40 |
| 13:F:43:HIS:CE1 | 13:F:218:LYS:CB | 3.04 | 0.40 |
| 17:J:64:LEU:HD21 | 18:K:121:ARG:NE | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:J:219:VAL:HB | 18:K:281:ARG:HB3 | 2.02 | 0.40 |
| 17:J:277:ASN:ND2 | 17:J:309:ARG:NH2 | 2.67 | 0.40 |
| 21:N:14:ARG:HH21 | 21:N:42:GLU:CD | 2.21 | 0.40 |
| 21:N:130:ASP:OD2 | 21:N:133:LEU:HG | 2.21 | 0.40 |
| 21:N:207:LEU:HD13 | 21:N:232:LEU:HD23 | 2.02 | 0.40 |
| 21:N:300:ASN:O | 21:N:304:LEU:HG | 2.20 | 0.40 |
| 22:O:228:TYR:HA | 22:O:290:LYS:CE | 2.48 | 0.40 |
| 23:P:178:GLN:HA | 23:P:181:LEU:HD12 | 2.01 | 0.40 |
| 24:Q:36:SER:H | 24:Q:46:VAL:HG23 | 1.86 | 0.40 |
| 24:Q:51:ARG:HG2 | 24:Q:85:MET:SD | 2.61 | 0.40 |
| 24:Q:198:LEU:CD2 | 24:Q:225:LEU:HD12 | 2.52 | 0.40 |
| 25:R:63:TYR:HE2 | 25:R:94:PHE:CA | 2.10 | 0.40 |
| 25:R:309:LEU:HD13 | 32:Y:79:ALA:HB2 | 2.03 | 0.40 |
| 26:S:159:ASN:HB3 | 26:S:183:LEU:HD11 | 2.03 | 0.40 |
| 26:S:295:ALA:HA | 26:S:298:ARG:HH21 | 1.85 | 0.40 |
| 28:U:270:ASN:O | 28:U:274:MET:HG3 | 2.20 | 0.40 |
| 33:Z:327:GLN:HE22 | 33:Z:346:LEU:HD11 | 1.84 | 0.40 |
| 33:Z:823:ASN:CG | 33:Z:856:HIS:ND1 | 2.73 | 0.40 |
| 8:A:135:ARG:HH11 | 14:G:124:LEU:CD2 | 2.34 | 0.40 |
| 8:A:170:ALA:HB2 | 8:A:178:ILE:HG21 | 2.01 | 0.40 |
| 9:B:146:SER:HB2 | 9:B:148:TYR:CE2 | 2.56 | 0.40 |
| 10:C:15:PRO:HG3 | 15:H:456:LYS:HZ2 | 1.85 | 0.40 |
| 11:D:70:HIS:CE1 | 11:D:97:ARG:NH2 | 2.87 | 0.40 |
| 13:F:7:ASP:HB3 | 13:F:21:GLN:HE22 | 1.86 | 0.40 |
| 14:G:136:ILE:HG12 | 14:G:149:MET:SD | 2.62 | 0.40 |
| 15:H:200:VAL:HG13 | 15:H:270:THR:HG23 | 2.03 | 0.40 |
| 15:H:327:ASN:O | 15:H:331:ARG:HG3 | 2.21 | 0.40 |
| 17:J:249:GLU:O | 17:J:249:GLU:CG | 2.62 | 0.40 |
| 18:K:89:ILE:HD13 | 29:V:148:LYS:HB3 | 2.03 | 0.40 |
| 18:K:210:LEU:CB | 18:K:334:LEU:HD11 | 2.51 | 0.40 |
| 20:M:197:ILE:HB | 20:M:322:LYS:HE2 | 1.98 | 0.40 |
| 21:N:761:ILE:HD13 | 21:N:768:ILE:HG12 | 2.04 | 0.40 |
| 22:O:99:LEU:HD11 | 22:O:132:GLU:CG | 2.46 | 0.40 |
| 22:O:217:LEU:HD13 | 22:O:238:ILE:HG21 | 2.03 | 0.40 |
| 23:P:98:GLN:OE1 | 23:P:139:VAL:HG23 | 2.22 | 0.40 |
| 23:P:141:LYS:HE3 | 23:P:182:GLU:OE2 | 2.22 | 0.40 |
| 23:P:353:ILE:HG22 | 23:P:402:PHE:CZ | 2.57 | 0.40 |
| 24:Q:51:ARG:CZ | 24:Q:55:GLU:OE2 | 2.69 | 0.40 |
| 26:S:475:TYR:HE1 | 28:U:291:LEU:O | 1.98 | 0.40 |
| 27:T:26:LEU:O | 27:T:30:ILE:HG13 | 2.21 | 0.40 |
| 27:T:158:GLN:OE1 | 27:T:210:PHE:CE1 | 2.74 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:U:190:LEU:HD23 | 28:U:190:LEU:C | 2.41 | 0.40 |
| 33:Z:57:LYS:HG2 | 33:Z:98:ASP:OD2 | 2.21 | 0.40 |
| 33:Z:501:LYS:HD3 | 33:Z:537:THR:HG21 | 2.02 | 0.40 |
| 2:2:86:HIS:O | 2:2:90:TYR:HD2 | 2.04 | 0.40 |
| 7:7:187:PHE:CD2 | 7:7:204:LEU:HB2 | 2.56 | 0.40 |
| 12:E:165:TYR:CG | 12:E:167:TYR:OH | 2.73 | 0.40 |
| 14:G:118:TYR:CE2 | 14:G:131:PHE:HZ | 2.39 | 0.40 |
| 17:J:208:CYS:SG | 17:J:244:ILE:HG12 | 2.60 | 0.40 |
| 21:N:240:GLN:O | 21:N:244:LYS:HG2 | 2.21 | 0.40 |
| 21:N:529:GLN:HB3 | 21:N:530:GLU:OE1 | 2.21 | 0.40 |
| 23:P:170:SER:O | 23:P:173:MET:HE3 | 2.22 | 0.40 |
| 24:Q:302:VAL:HG13 | 24:Q:314:PHE:CD1 | 2.55 | 0.40 |
| 25:R:271:ILE:HB | 25:R:293:THR:HG21 | 2.03 | 0.40 |
| 26:S:234:ILE:HG22 | 26:S:238:LEU:CD1 | 2.50 | 0.40 |
| 26:S:323:LEU:HD23 | 26:S:383:LEU:HD23 | 2.03 | 0.40 |
| 31:X:9:LYS:HE2 | 31:X:34:GLU:OE2 | 2.22 | 0.40 |
| 33:Z:278:LEU:HD22 | 33:Z:297:VAL:CG2 | 2.51 | 0.40 |
| 1:1:12:VAL:HG22 | 1:1:14:LEU:CD1 | 2.50 | 0.40 |
| 3:3:158:ILE:CG2 | 3:3:159:SER:N | 2.85 | 0.40 |
| 4:4:15:ALA:HB1 | 4:4:178:VAL:HG21 | 2.03 | 0.40 |
| 4:4:168:GLU:OE2 | 4:4:177:GLY:N | 2.54 | 0.40 |
| 6:6:138:MET:HB3 | 6:6:139:PRO:HD3 | 2.03 | 0.40 |
| 8:A:34:ALA:C | 8:A:35:THR:HG23 | 2.41 | 0.40 |
| 8:A:43:LEU:C | 8:A:43:LEU:HD12 | 2.42 | 0.40 |
| 8:A:54:ILE:HD13 | 8:A:207:ILE:CG1 | 2.52 | 0.40 |
| 8:A:54:ILE:CD1 | 8:A:206:ALA:HB3 | 2.51 | 0.40 |
| 13:F:120:THR:OG1 | 14:G:129:ARG:NH1 | 2.44 | 0.40 |
| 14:G:243:GLN:O | 14:G:243:GLN:HG3 | 2.20 | 0.40 |
| 15:H:147:ILE:CG1 | 15:H:183:ILE:HD11 | 2.51 | 0.40 |
| 15:H:182:ASN:ND2 | 15:H:184:GLU:OE2 | 2.49 | 0.40 |
| 15:H:455:LYS:O | 15:H:456:LYS:HB2 | 2.22 | 0.40 |
| 16:I:204:HIS:HB3 | 16:I:207:LEU:CG | 2.51 | 0.40 |
| 18:K:105:GLN:HG3 | 18:K:106:ASN:ND2 | 2.37 | 0.40 |
| 18:K:112:SER:HB2 | 18:K:116:MET:O | 2.22 | 0.40 |
| 18:K:132:LYS:N | 18:K:135:MET:SD | 2.94 | 0.40 |
| 21:N:337:GLY:O | 21:N:373:VAL:CG1 | 2.69 | 0.40 |
| 21:N:529:GLN:NE2 | 21:N:558:ALA:O | 2.51 | 0.40 |
| 21:N:729:SER:O | 21:N:733:LEU:HG | 2.22 | 0.40 |
| 22:O:62:TYR:CE2 | 22:O:82:LEU:HD22 | 2.57 | 0.40 |
| 22:O:131:SER:CB | 22:O:135:ARG:HH12 | 2.34 | 0.40 |
| 22:O:301:PHE:HZ | 28:U:234:ASN:HA | 1.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:Q:122:ILE:O | 24:Q:126:LYS:HG3 | 2.22 | 0.40 |
| 24:Q:220:LEU:O | 24:Q:224:ILE:HG13 | 2.21 | 0.40 |
| 25:R:249:ILE:CG2 | 25:R:250:ALA:N | 2.84 | 0.40 |
| 27:T:27:LEU:HB2 | 27:T:28:PRO:HD3 | 2.03 | 0.40 |
| 29:V:161:THR:HB | 29:V:162:GLY:H | 1.65 | 0.40 |
| 31:X:117:LYS:HG2 | 31:X:118:ASP:H | 1.86 | 0.40 |
| 33:Z:574:TYR:OH | 33:Z:584:VAL:HG13 | 2.19 | 0.40 |
| 33:Z:812:ILE:HG22 | 33:Z:847:ILE:HG22 | 2.03 | 0.40 |
| 2:2:8:PHE:HZ | 2:2:11:GLY:HA3 | 1.68 | 0.40 |
| 8:A:92:ASN:ND2 | 14:G:117:GLN:HE22 | 2.19 | 0.40 |
| 8:A:164:VAL:CB | 9:B:61:LEU:CD2 | 2.94 | 0.40 |
| 9:B:123:GLN:NE2 | 10:C:86:ILE:HG13 | 2.35 | 0.40 |
| 15:H:98:GLN:HE21 | 15:H:194:SER:HB3 | 1.85 | 0.40 |
| 16:I:432:LEU:N | 16:I:433:GLU:OE1 | 2.54 | 0.40 |
| 17:J:170:HIS:HB2 | 17:J:173:LEU:HD12 | 2.04 | 0.40 |
| 20:M:376:TRP:CG | 20:M:377:GLN:N | 2.89 | 0.40 |
| 24:Q:4:PRO:CB | 24:Q:50:ARG:HH11 | 2.31 | 0.40 |
| 25:R:209:ARG:NE | 25:R:243:LEU:CD2 | 2.75 | 0.40 |
| 25:R:237:THR:C | 25:R:246:TYR:HE1 | 2.23 | 0.40 |
| 25:R:258:LEU:HD11 | 25:R:288:SER:CA | 2.51 | 0.40 |
| 25:R:262:GLU:HA | 25:R:336:LYS:HZ3 | 1.86 | 0.40 |
| 26:S:176:LEU:HD22 | 26:S:228:GLU:H | 1.87 | 0.40 |
| 26:S:428:ARG:HG3 | 27:T:195:LEU:HD22 | 2.03 | 0.40 |
| 33:Z:108:ASP:HA | 33:Z:109:PRO:HD3 | 1.92 | 0.40 |
| 33:Z:138:ARG:NH1 | 33:Z:157:LEU:HA | 2.37 | 0.40 |
| 33:Z:329:ILE:HG23 | 33:Z:330:ILE:N | 2.37 | 0.40 |
| 33:Z:371:SER:O | 33:Z:372:ALA:HB3 | 2.17 | 0.40 |
| 33:Z:866:VAL:CB | 33:Z:873:LEU:HG | 2.43 | 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 | 1 | 203/215 (94%) | 188 (93%) | 11 (5%) | 4 (2%) | 7 38 |
| 2 | 2 | 221/261 (85%) | 211 (96%) | 10 (4%) | 0 | 100 100 |
| 3 | 3 | 202/205 (98%) | 184 (91%) | 15 (7%) | 3 (2%) | 10 46 |
| 4 | 4 | 196/198 (99%) | 180 (92%) | 13 (7%) | 3 (2%) | 10 46 |
| 5 | 5 | 210/287 (73%) | 197 (94%) | 10 (5%) | 3 (1%) | 11 46 |
| 6 | 6 | 220/241 (91%) | 205 (93%) | 11 (5%) | 4 (2%) | 8 40 |
| 7 | 7 | 231/266 (87%) | 212 (92%) | 17 (7%) | 2 (1%) | 17 57 |
| 8 | A | 241/252 (96%) | 226 (94%) | 12 (5%) | 3 (1%) | 13 50 |
| 9 | B | 248/250 (99%) | 233 (94%) | 12 (5%) | 3 (1%) | 13 50 |
| 10 | C | 243/258 (94%) | 229 (94%) | 11 (4%) | 3 (1%) | 13 50 |
| 11 | D | 240/254 (94%) | 224 (93%) | 14 (6%) | 2 (1%) | 19 60 |
| 12 | E | 241/260 (93%) | 223 (92%) | 14 (6%) | 4 (2%) | 9 42 |
| 13 | F | 231/234 (99%) | 214 (93%) | 12 (5%) | 5 (2%) | 6 35 |
| 14 | G | 243/288 (84%) | 226 (93%) | 13 (5%) | 4 (2%) | 9 44 |
| 15 | H | 353/467 (76%) | 305 (86%) | 27 (8%) | 21 (6%) | 1 17 |
| 16 | I | 358/437 (82%) | 318 (89%) | 29 (8%) | 11 (3%) | 4 27 |
| 17 | J | 369/405 (91%) | 334 (90%) | 26 (7%) | 9 (2%) | 6 33 |
| 18 | K | 377/428 (88%) | 338 (90%) | 32 (8%) | 7 (2%) | 8 38 |
| 19 | L | 359/437 (82%) | 318 (89%) | 36 (10%) | 5 (1%) | 11 46 |
| 20 | M | 363/434 (84%) | 323 (89%) | 29 (8%) | 11 (3%) | 4 28 |
| 21 | N | 843/945 (89%) | 786 (93%) | 49 (6%) | 8 (1%) | 17 57 |
| 22 | O | 385/393 (98%) | 340 (88%) | 31 (8%) | 14 (4%) | 3 25 |
| 23 | P | 413/445 (93%) | 382 (92%) | 19 (5%) | 12 (3%) | 4 29 |
| 24 | Q | 429/434 (99%) | 395 (92%) | 23 (5%) | 11 (3%) | 5 31 |
| 25 | R | 398/429 (93%) | 354 (89%) | 32 (8%) | 12 (3%) | 4 28 |
| 26 | S | 351/523 (67%) | 312 (89%) | 29 (8%) | 10 (3%) | 5 30 |
| 27 | T | 270/274 (98%) | 240 (89%) | 18 (7%) | 12 (4%) | 2 22 |
| 28 | U | 245/338 (72%) | 237 (97%) | 7 (3%) | 1 (0%) | 34 72 |
| 29 | V | 239/306 (78%) | 222 (93%) | 10 (4%) | 7 (3%) | 4 29 |
| 30 | W | 195/268 (73%) | 171 (88%) | 14 (7%) | 10 (5%) | 2 19 |
| 31 | X | 125/156 (80%) | 106 (85%) | 14 (11%) | 5 (4%) | 3 23 |
| 32 | Y | 17/89 (19%) | 17 (100%) | 0 | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 33 | Z | 807/993 (81%) | 722 (90%) | 52 (6%) | 33 (4%) | 3 23 |
| All | All | 10066/11670 (86%) | 9172 (91%) | 652 (6%) | 242 (2%) | 9 33 |

All (242) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | A | 168 | ALA |
| 11 | D | 204 | GLN |
| 13 | F | 41 | ASN |
| 15 | H | 183 | ILE |
| 15 | H | 185 | LEU |
| 15 | H | 188 | PRO |
| 15 | H | 303 | ALA |
| 15 | H | 396 | MET |
| 16 | I | 125 | MET |
| 16 | I | 130 | VAL |
| 17 | J | 134 | VAL |
| 17 | J | 249 | GLU |
| 19 | L | 253 | ASP |
| 20 | M | 256 | ILE |
| 20 | M | 339 | ARG |
| 21 | N | 17 | GLN |
| 22 | O | 15 | ARG |
| 22 | O | 228 | TYR |
| 23 | P | 53 | ALA |
| 23 | P | 130 | ILE |
| 23 | P | 232 | ARG |
| 23 | P | 321 | VAL |
| 23 | P | 333 | ALA |
| 24 | Q | 354 | PHE |
| 24 | Q | 356 | CYS |
| 25 | R | 197 | MET |
| 25 | R | 244 | THR |
| 25 | R | 271 | ILE |
| 26 | S | 151 | GLU |
| 27 | T | 48 | ASN |
| 27 | T | 94 | HIS |
| 27 | T | 243 | ALA |
| 27 | T | 246 | GLU |
| 27 | T | 250 | MET |
| 27 | T | 254 | ASP |
| 28 | U | 43 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | V | 163 | ALA |
| 30 | W | 179 | ARG |
| 31 | X | 78 | ILE |
| 33 | Z | 60 | ASP |
| 33 | Z | 259 | PRO |
| 33 | Z | 318 | LYS |
| 33 | Z | 372 | ALA |
| 33 | Z | 464 | ASP |
| 33 | Z | 482 | ASP |
| 1 | 1 | 19 | ARG |
| 3 | 3 | 31 | PHE |
| 3 | 3 | 93 | PRO |
| 4 | 4 | 175 | PHE |
| 5 | 5 | 145 | LYS |
| 11 | D | 218 | ASP |
| 12 | E | 53 | ARG |
| 13 | F | 202 | ARG |
| 14 | G | 184 | GLU |
| 15 | H | 104 | LYS |
| 15 | H | 167 | ASP |
| 15 | H | 189 | PRO |
| 15 | H | 323 | ALA |
| 15 | H | 370 | ARG |
| 16 | I | 135 | PHE |
| 16 | I | 162 | ASP |
| 16 | I | 298 | GLY |
| 17 | J | 207 | ASP |
| 17 | J | 225 | GLU |
| 18 | K | 248 | GLY |
| 18 | K | 397 | LYS |
| 20 | M | 385 | GLU |
| 20 | M | 423 | GLN |
| 20 | M | 431 | SER |
| 21 | N | 614 | ASN |
| 21 | N | 721 | ASP |
| 22 | O | 82 | LEU |
| 23 | P | 85 | LYS |
| 23 | P | 170 | SER |
| 23 | P | 289 | ASN |
| 23 | P | 290 | LEU |
| 25 | R | 92 | ILE |
| 25 | R | 162 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | R | 241 | ILE |
| 26 | S | 144 | LEU |
| 26 | S | 204 | ASP |
| 26 | S | 452 | TYR |
| 27 | T | 117 | ASN |
| 29 | V | 181 | ASN |
| 30 | W | 47 | ASN |
| 30 | W | 136 | ASN |
| 30 | W | 190 | ILE |
| 31 | X | 38 | ASN |
| 31 | X | 116 | ALA |
| 33 | Z | 80 | SER |
| 33 | Z | 82 | MET |
| 33 | Z | 110 | ASN |
| 33 | Z | 132 | HIS |
| 33 | Z | 442 | VAL |
| 33 | Z | 466 | GLU |
| 33 | Z | 609 | THR |
| 1 | 1 | 92 | ASN |
| 4 | 4 | 111 | ASN |
| 6 | 6 | 10 | ASP |
| 6 | 6 | 157 | GLY |
| 6 | 6 | 211 | LYS |
| 7 | 7 | 221 | GLY |
| 9 | B | 3 | ASP |
| 9 | B | 102 | GLY |
| 9 | B | 215 | GLY |
| 10 | C | 220 | ALA |
| 10 | C | 225 | VAL |
| 12 | E | 122 | ARG |
| 12 | E | 216 | ASN |
| 14 | G | 71 | ARG |
| 15 | H | 164 | SER |
| 15 | H | 325 | GLY |
| 16 | I | 228 | GLY |
| 16 | I | 320 | GLY |
| 17 | J | 194 | GLY |
| 17 | J | 317 | PRO |
| 18 | K | 343 | LEU |
| 18 | K | 427 | TYR |
| 20 | M | 167 | VAL |
| 20 | M | 227 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | M | 282 | GLU |
| 21 | N | 742 | TRP |
| 21 | N | 769 | PRO |
| 21 | N | 781 | ALA |
| 22 | O | 107 | GLN |
| 22 | O | 142 | ASP |
| 22 | O | 247 | ASN |
| 22 | O | 304 | ASN |
| 23 | P | 231 | LYS |
| 24 | Q | 37 | GLN |
| 24 | Q | 48 | ASP |
| 24 | Q | 149 | LYS |
| 24 | Q | 399 | VAL |
| 25 | R | 37 | LYS |
| 26 | S | 199 | GLU |
| 26 | S | 284 | LEU |
| 27 | T | 90 | PHE |
| 29 | V | 194 | ARG |
| 30 | W | 101 | ARG |
| 33 | Z | 184 | SER |
| 33 | Z | 228 | GLU |
| 33 | Z | 338 | HIS |
| 33 | Z | 443 | ASP |
| 33 | Z | 524 | ALA |
| 33 | Z | 920 | GLY |
| 33 | Z | 974 | THR |
| 1 | 1 | -7 | LYS |
| 1 | 1 | 145 | ASN |
| 3 | 3 | 148 | ASN |
| 5 | 5 | 118 | ASP |
| 8 | A | 13 | ASP |
| 8 | A | 198 | SER |
| 13 | F | 222 | PHE |
| 14 | G | 186 | LEU |
| 15 | H | 172 | MET |
| 15 | H | 191 | ILE |
| 18 | K | 278 | ALA |
| 21 | N | 86 | LYS |
| 22 | O | 302 | VAL |
| 22 | O | 358 | ILE |
| 22 | O | 360 | GLY |
| 24 | Q | 38 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | Q | 42 | ALA |
| 25 | R | 326 | ALA |
| 26 | S | 146 | LEU |
| 26 | S | 303 | ASN |
| 27 | T | 244 | ASP |
| 29 | V | 72 | PRO |
| 29 | V | 78 | VAL |
| 30 | W | 57 | ALA |
| 30 | W | 149 | GLN |
| 30 | W | 164 | PRO |
| 30 | W | 169 | SER |
| 33 | Z | 76 | LYS |
| 33 | Z | 142 | ASP |
| 33 | Z | 893 | PHE |
| 5 | 5 | 173 | GLY |
| 6 | 6 | 40 | ASN |
| 13 | F | 69 | HIS |
| 14 | G | 70 | ASP |
| 15 | H | 107 | LYS |
| 15 | H | 143 | ALA |
| 15 | H | 170 | GLU |
| 15 | H | 357 | ARG |
| 16 | I | 165 | ASP |
| 16 | I | 341 | PRO |
| 17 | J | 258 | VAL |
| 18 | K | 160 | VAL |
| 18 | K | 424 | PHE |
| 19 | L | 164 | ASP |
| 20 | M | 425 | ARG |
| 22 | O | 203 | THR |
| 24 | Q | 89 | ALA |
| 24 | Q | 273 | ASN |
| 25 | R | 39 | SER |
| 25 | R | 182 | ASN |
| 25 | R | 222 | ARG |
| 26 | S | 174 | ARG |
| 26 | S | 375 | ASP |
| 27 | T | 73 | PHE |
| 27 | T | 172 | SER |
| 29 | V | 161 | THR |
| 31 | X | 28 | PRO |
| 33 | Z | 75 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | Z | 287 | ARG |
| 33 | Z | 957 | LEU |
| 7 | 7 | 30 | GLY |
| 10 | C | 52 | VAL |
| 12 | E | 190 | SER |
| 13 | F | 103 | LEU |
| 15 | H | 105 | ILE |
| 15 | H | 161 | GLU |
| 16 | I | 205 | PRO |
| 17 | J | 126 | LEU |
| 19 | L | 175 | GLN |
| 19 | L | 183 | ILE |
| 24 | Q | 131 | VAL |
| 25 | R | 198 | ILE |
| 27 | T | 167 | GLY |
| 31 | X | 37 | PRO |
| 33 | Z | 183 | LYS |
| 33 | Z | 919 | GLU |
| 33 | Z | 929 | VAL |
| 33 | Z | 930 | GLY |
| 21 | N | 353 | LEU |
| 23 | P | 396 | PRO |
| 30 | W | 189 | PRO |
| 33 | Z | 469 | PRO |
| 22 | O | 353 | VAL |
| 15 | H | 243 | PRO |
| 19 | L | 287 | GLY |
| 20 | M | 252 | VAL |
| 20 | M | 350 | PRO |
| 22 | O | 164 | PRO |
| 29 | V | 247 | ILE |
| 33 | Z | 578 | GLY |
| 4 | 4 | 149 | PRO |
| 17 | J | 281 | GLY |
| 22 | O | 238 | ILE |
| 23 | P | 211 | PRO |
| 16 | I | 428 | VAL |
| 33 | Z | 462 | 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 | 1 | 169/178 (95%) | 169 (100%) | 0 | 100 | 100 |
| 2 | 2 | 182/214 (85%) | 182 (100%) | 0 | 100 | 100 |
| 3 | 3 | 172/173 (99%) | 172 (100%) | 0 | 100 | 100 |
| 4 | 4 | 175/175 (100%) | 175 (100%) | 0 | 100 | 100 |
| 5 | 5 | 169/235 (72%) | 167 (99%) | 2 (1%) | 71 | 83 |
| 6 | 6 | 185/201 (92%) | 185 (100%) | 0 | 100 | 100 |
| 7 | 7 | 199/224 (89%) | 199 (100%) | 0 | 100 | 100 |
| 8 | A | 207/210 (99%) | 207 (100%) | 0 | 100 | 100 |
| 9 | B | 209/209 (100%) | 209 (100%) | 0 | 100 | 100 |
| 10 | C | 204/216 (94%) | 204 (100%) | 0 | 100 | 100 |
| 11 | D | 214/226 (95%) | 214 (100%) | 0 | 100 | 100 |
| 12 | E | 199/215 (93%) | 199 (100%) | 0 | 100 | 100 |
| 13 | F | 192/193 (100%) | 192 (100%) | 0 | 100 | 100 |
| 14 | G | 201/239 (84%) | 200 (100%) | 1 (0%) | 88 | 93 |
| 15 | H | 303/399 (76%) | 302 (100%) | 1 (0%) | 92 | 95 |
| 16 | I | 319/385 (83%) | 318 (100%) | 1 (0%) | 92 | 95 |
| 17 | J | 325/352 (92%) | 325 (100%) | 0 | 100 | 100 |
| 18 | K | 334/374 (89%) | 333 (100%) | 1 (0%) | 92 | 95 |
| 19 | L | 308/377 (82%) | 307 (100%) | 1 (0%) | 92 | 95 |
| 20 | M | 315/375 (84%) | 315 (100%) | 0 | 100 | 100 |
| 21 | N | 713/797 (90%) | 713 (100%) | 0 | 100 | 100 |
| 22 | O | 363/368 (99%) | 363 (100%) | 0 | 100 | 100 |
| 23 | P | 388/415 (94%) | 387 (100%) | 1 (0%) | 92 | 95 |
| 24 | Q | 388/391 (99%) | 388 (100%) | 0 | 100 | 100 |
| 25 | R | 351/379 (93%) | 351 (100%) | 0 | 100 | 100 |
| 26 | S | 330/489 (68%) | 330 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 27 | T | 254/256 (99%) | 254 (100%) | 0 | 100 100 |
| 28 | U | 234/308 (76%) | 233 (100%) | 1 (0%) | 91 94 |
| 29 | V | 217/268 (81%) | 217 (100%) | 0 | 100 100 |
| 30 | W | 171/230 (74%) | 171 (100%) | 0 | 100 100 |
| 31 | X | 116/144 (81%) | 116 (100%) | 0 | 100 100 |
| 32 | Y | 18/81 (22%) | 18 (100%) | 0 | 100 100 |
| 33 | Z | 692/850 (81%) | 692 (100%) | 0 | 100 100 |
| All | All | 8816/10146 (87%) | 8807 (100%) | 9 (0%) | 93 97 |

All (9) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 5 | 19 | ARG |
| 5 | 5 | 104 | TYR |
| 14 | G | 217 | TRP |
| 15 | H | 164 | SER |
| 16 | I | 257 | LEU |
| 18 | K | 246 | TYR |
| 19 | L | 253 | ASP |
| 23 | P | 31 | ASP |
| 28 | U | 61 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 69 | GLN |
| 1 | 1 | 120 | HIS |
| 1 | 1 | 157 | HIS |
| 2 | 2 | 9 | ASN |
| 3 | 3 | 104 | ASN |
| 3 | 3 | 160 | GLN |
| 4 | 4 | 145 | HIS |
| 4 | 4 | 146 | HIS |
| 4 | 4 | 165 | GLN |
| 5 | 5 | 62 | GLN |
| 5 | 5 | 66 | HIS |
| 5 | 5 | 176 | ASN |
| 5 | 5 | 190 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | 6 | 46 | ASN |
| 6 | 6 | 70 | HIS |
| 6 | 6 | 71 | ASN |
| 7 | 7 | 53 | GLN |
| 7 | 7 | 70 | ASN |
| 7 | 7 | 112 | GLN |
| 7 | 7 | 114 | ASN |
| 8 | A | 36 | ASN |
| 8 | A | 84 | ASN |
| 8 | A | 92 | ASN |
| 9 | B | 20 | GLN |
| 9 | B | 94 | HIS |
| 9 | B | 123 | GLN |
| 9 | B | 180 | ASN |
| 10 | C | 21 | GLN |
| 10 | C | 31 | HIS |
| 10 | C | 96 | GLN |
| 10 | C | 125 | HIS |
| 10 | C | 177 | GLN |
| 11 | D | 19 | GLN |
| 11 | D | 55 | GLN |
| 12 | E | 108 | ASN |
| 12 | E | 114 | GLN |
| 13 | F | 21 | GLN |
| 13 | F | 60 | GLN |
| 13 | F | 91 | GLN |
| 13 | F | 121 | GLN |
| 13 | F | 210 | ASN |
| 14 | G | 11 | ASN |
| 14 | G | 122 | HIS |
| 15 | H | 98 | GLN |
| 15 | H | 217 | GLN |
| 15 | H | 348 | ASN |
| 15 | H | 359 | ASN |
| 16 | I | 102 | ASN |
| 16 | I | 295 | ASN |
| 16 | I | 312 | GLN |
| 17 | J | 156 | GLN |
| 17 | J | 240 | HIS |
| 17 | J | 278 | GLN |
| 17 | J | 331 | HIS |
| 17 | J | 379 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | K | 98 | GLN |
| 18 | K | 106 | ASN |
| 18 | K | 182 | GLN |
| 18 | K | 238 | ASN |
| 18 | K | 414 | GLN |
| 19 | L | 67 | HIS |
| 19 | L | 99 | GLN |
| 19 | L | 133 | ASN |
| 19 | L | 189 | GLN |
| 19 | L | 311 | GLN |
| 20 | M | 81 | ASN |
| 20 | M | 125 | GLN |
| 20 | M | 250 | GLN |
| 20 | M | 311 | GLN |
| 20 | M | 423 | GLN |
| 21 | N | 96 | GLN |
| 21 | N | 176 | GLN |
| 21 | N | 268 | GLN |
| 21 | N | 300 | ASN |
| 21 | N | 306 | ASN |
| 21 | N | 308 | ASN |
| 21 | N | 529 | GLN |
| 21 | N | 614 | ASN |
| 21 | N | 679 | ASN |
| 21 | N | 878 | GLN |
| 21 | N | 900 | ASN |
| 22 | O | 4 | ASN |
| 22 | O | 28 | GLN |
| 22 | O | 105 | GLN |
| 22 | O | 211 | GLN |
| 22 | O | 229 | ASN |
| 22 | O | 235 | HIS |
| 22 | O | 236 | HIS |
| 23 | P | 38 | GLN |
| 23 | P | 48 | GLN |
| 23 | P | 86 | HIS |
| 23 | P | 164 | GLN |
| 23 | P | 277 | GLN |
| 23 | P | 296 | GLN |
| 23 | P | 342 | GLN |
| 23 | P | 366 | ASN |
| 23 | P | 425 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | P | 431 | HIS |
| 24 | Q | 52 | ASN |
| 24 | Q | 405 | GLN |
| 25 | R | 73 | ASN |
| 25 | R | 76 | GLN |
| 25 | R | 89 | ASN |
| 25 | R | 130 | GLN |
| 25 | R | 325 | HIS |
| 25 | R | 340 | GLN |
| 25 | R | 397 | ASN |
| 26 | S | 302 | HIS |
| 26 | S | 317 | HIS |
| 26 | S | 337 | ASN |
| 26 | S | 378 | GLN |
| 26 | S | 417 | GLN |
| 27 | T | 84 | GLN |
| 27 | T | 135 | ASN |
| 27 | T | 158 | GLN |
| 27 | T | 204 | ASN |
| 27 | T | 272 | ASN |
| 28 | U | 21 | HIS |
| 28 | U | 42 | ASN |
| 28 | U | 77 | ASN |
| 28 | U | 84 | ASN |
| 28 | U | 94 | HIS |
| 28 | U | 127 | GLN |
| 28 | U | 230 | GLN |
| 28 | U | 262 | GLN |
| 28 | U | 297 | GLN |
| 29 | V | 109 | HIS |
| 29 | V | 131 | GLN |
| 29 | V | 190 | HIS |
| 29 | V | 291 | ASN |
| 30 | W | 47 | ASN |
| 30 | W | 80 | GLN |
| 30 | W | 95 | GLN |
| 30 | W | 106 | GLN |
| 30 | W | 163 | ASN |
| 31 | X | 38 | ASN |
| 31 | X | 105 | ASN |
| 31 | X | 108 | ASN |
| 32 | Y | 89 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | Z | 214 | HIS |
| 33 | Z | 240 | ASN |
| 33 | Z | 317 | GLN |
| 33 | Z | 327 | GLN |
| 33 | Z | 338 | HIS |
| 33 | Z | 379 | GLN |
| 33 | Z | 387 | ASN |
| 33 | Z | 577 | GLN |
| 33 | Z | 580 | GLN |
| 33 | Z | 766 | HIS |
| 33 | Z | 810 | ASN |
| 33 | Z | 833 | GLN |
| 33 | Z | 852 | GLN |
| 33 | Z | 897 | HIS |
| 33 | Z | 899 | GLN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no monosaccharides in this entry.

### 5.6 Ligand geometry

There are no ligands in this entry.

### 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 17 | J | 2 |
| 16 | I | 1 |
| 18 | K | 1 |
| 19 | L | 1 |
| 20 | M | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | J | 218:LEU | C | 219:VAL | N | 3.94 |
| 1 | I | 252:LEU | C | 253:ILE | N | 3.24 |
| 1 | K | 242:PHE | C | 243:VAL | N | 2.17 |
| 1 | J | 224:GLY | C | 225:GLU | N | 1.73 |
| 1 | L | 257:GLY | C | 258:GLU | N | 1.14 |
| 1 | M | 251:LEU | C | 252:VAL | N | 0.84 |

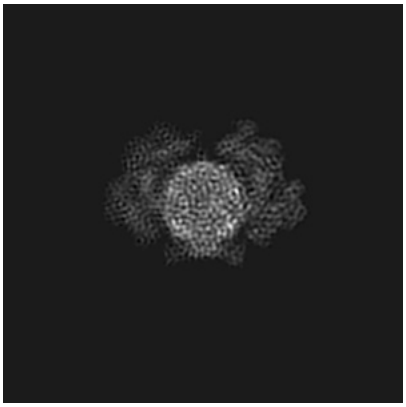
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2594. These allow visual inspection of the internal detail of the map and identification of artifacts.

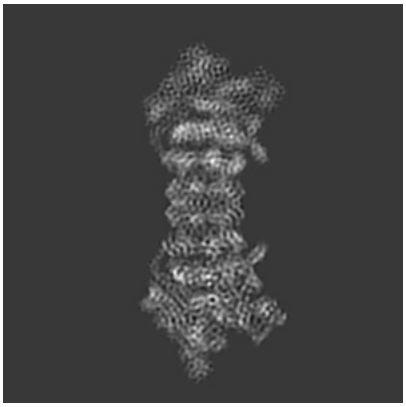
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

### 6.1.1 Primary map



X



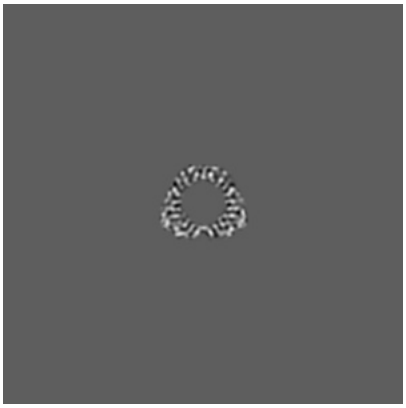
Y

Z

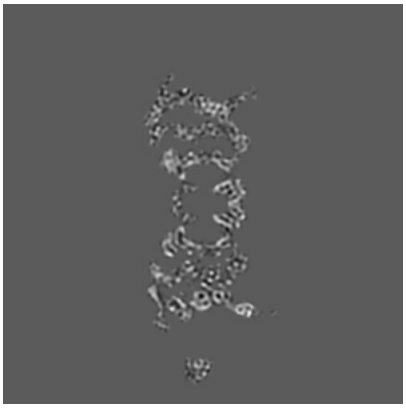
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

### 6.2.1 Primary map



X Index: 140



Y Index: 140

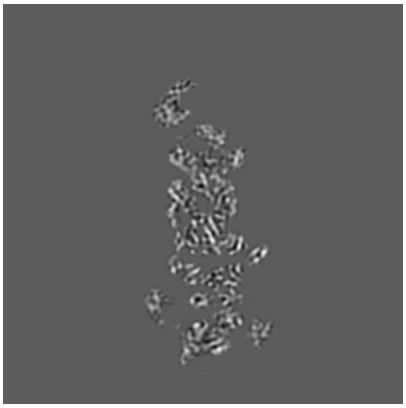
Z Index: 140

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: 72



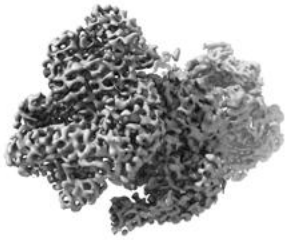
Y Index: 154

Z Index: 139

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

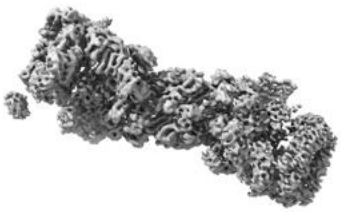
## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.74. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

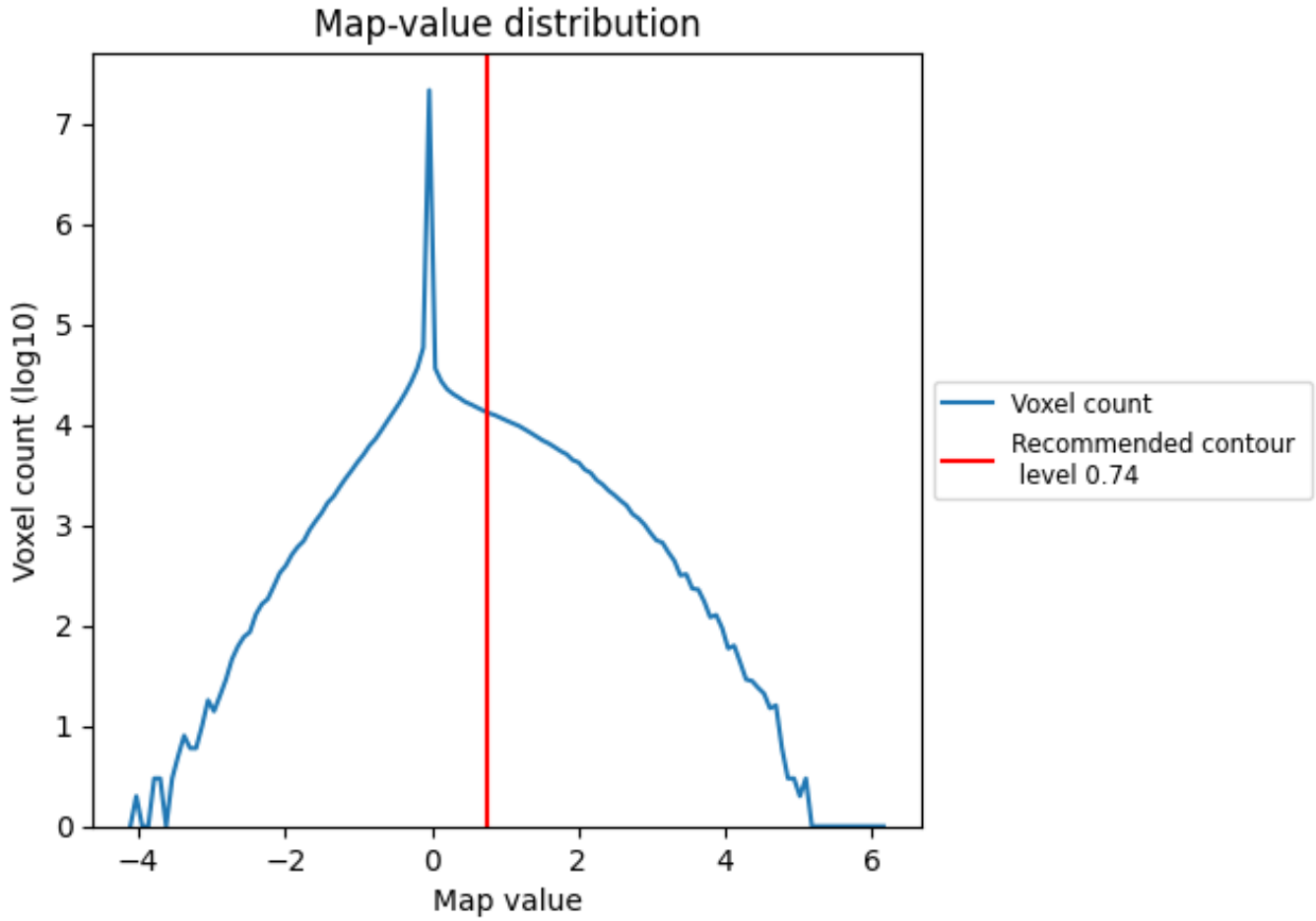
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

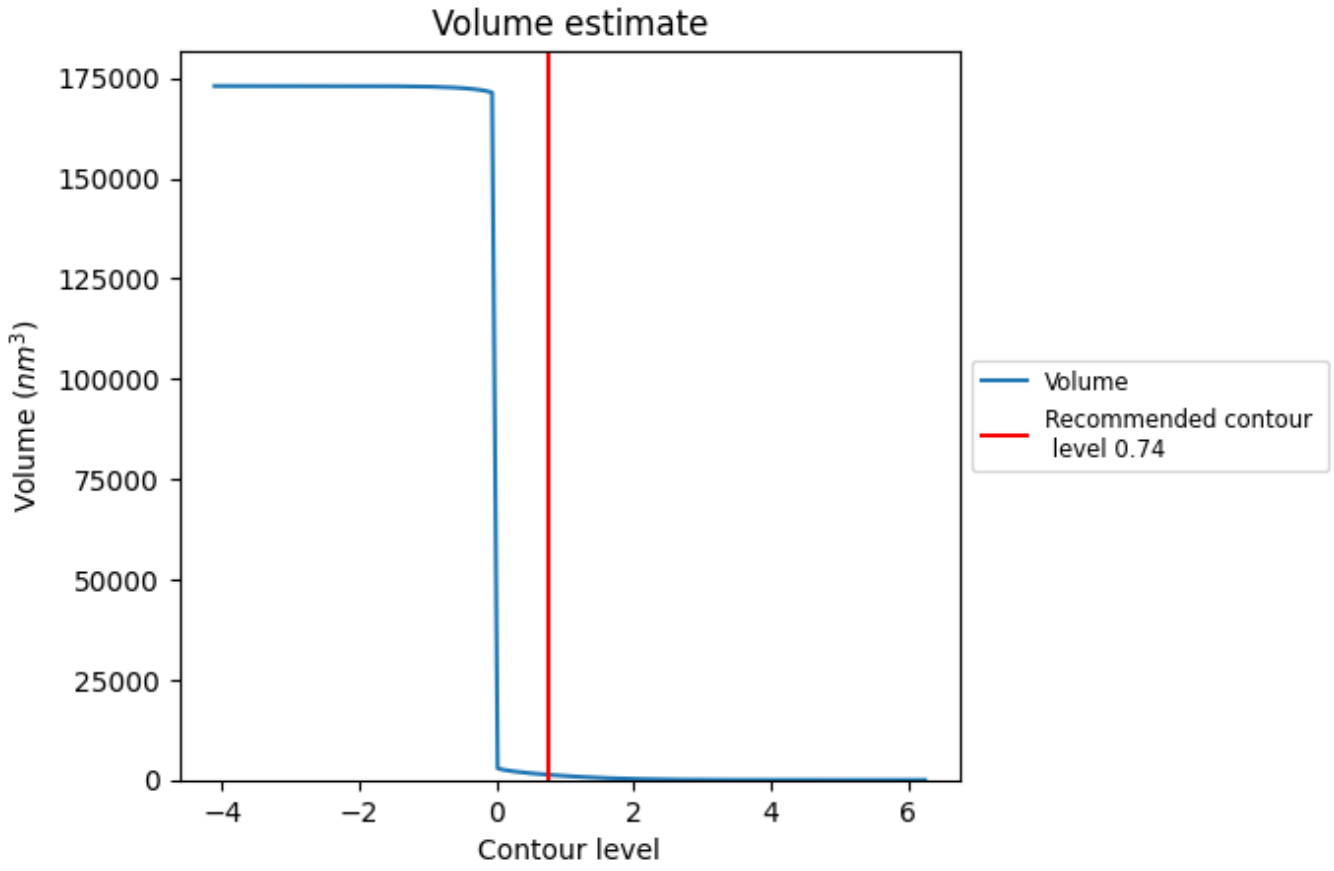
This section contains the results of statistical analysis of the map.

## 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.

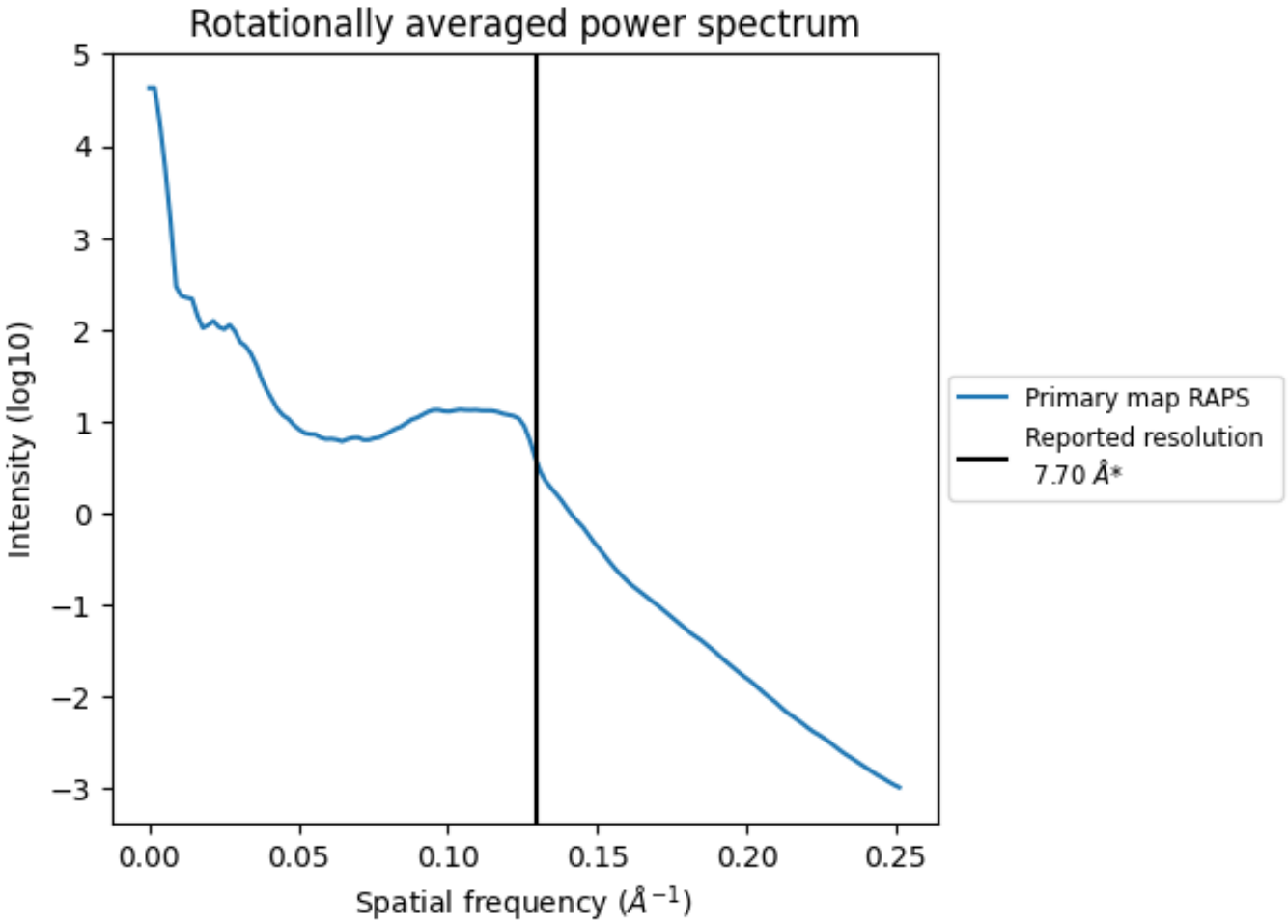
## 7.2 Volume estimate




The volume at the recommended contour level is 1311 $nm^3$; this corresponds to an approximate mass of 1184 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 0.130 Å$^{-1}$

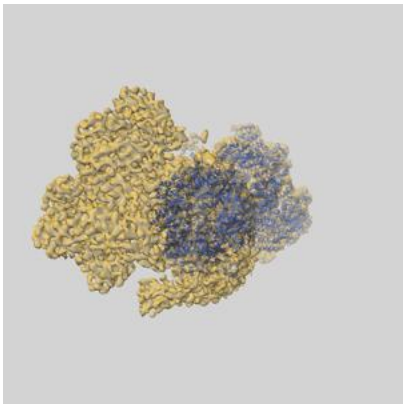
# 8 Fourier-Shell correlation

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

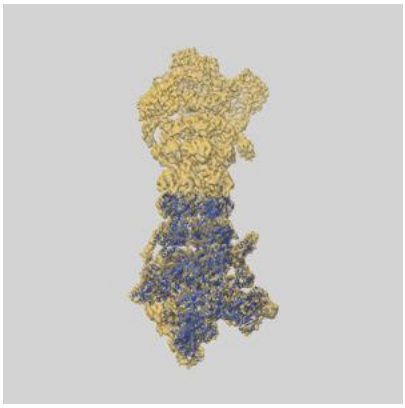
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2594 and PDB model 4CR2. Per-residue inclusion information can be found in section 3 on page 9.

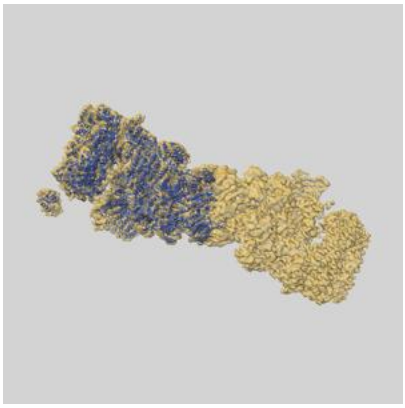
## 9.1 Map-model overlay



X



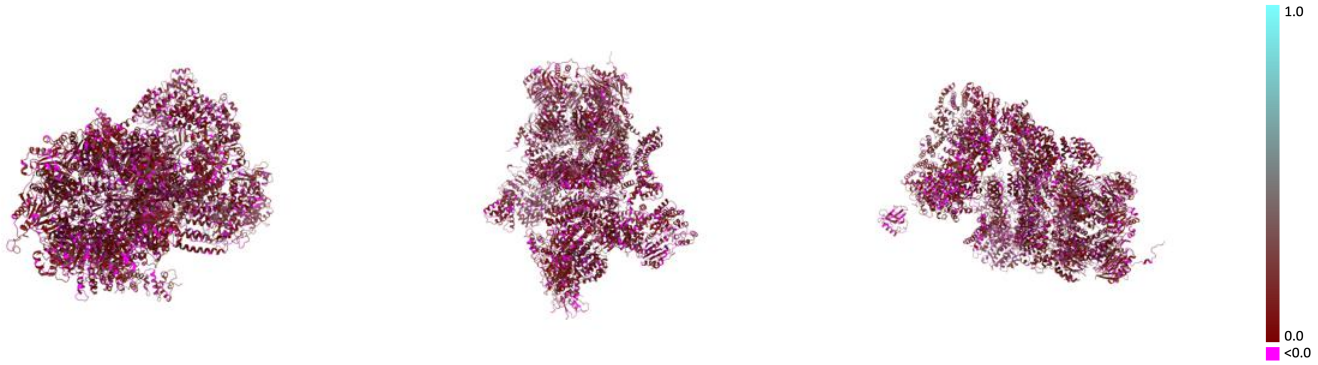
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.74 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.

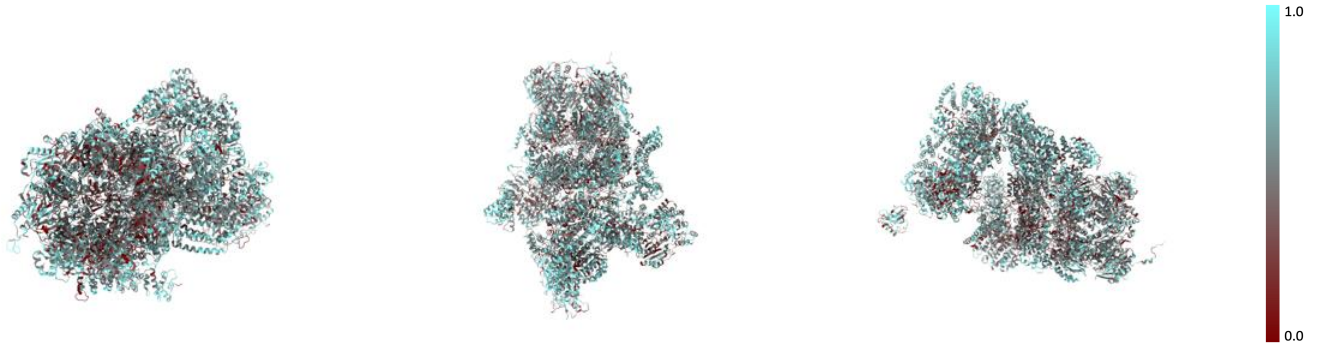
## 9.2 Q-score mapped to coordinate model (i)




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.

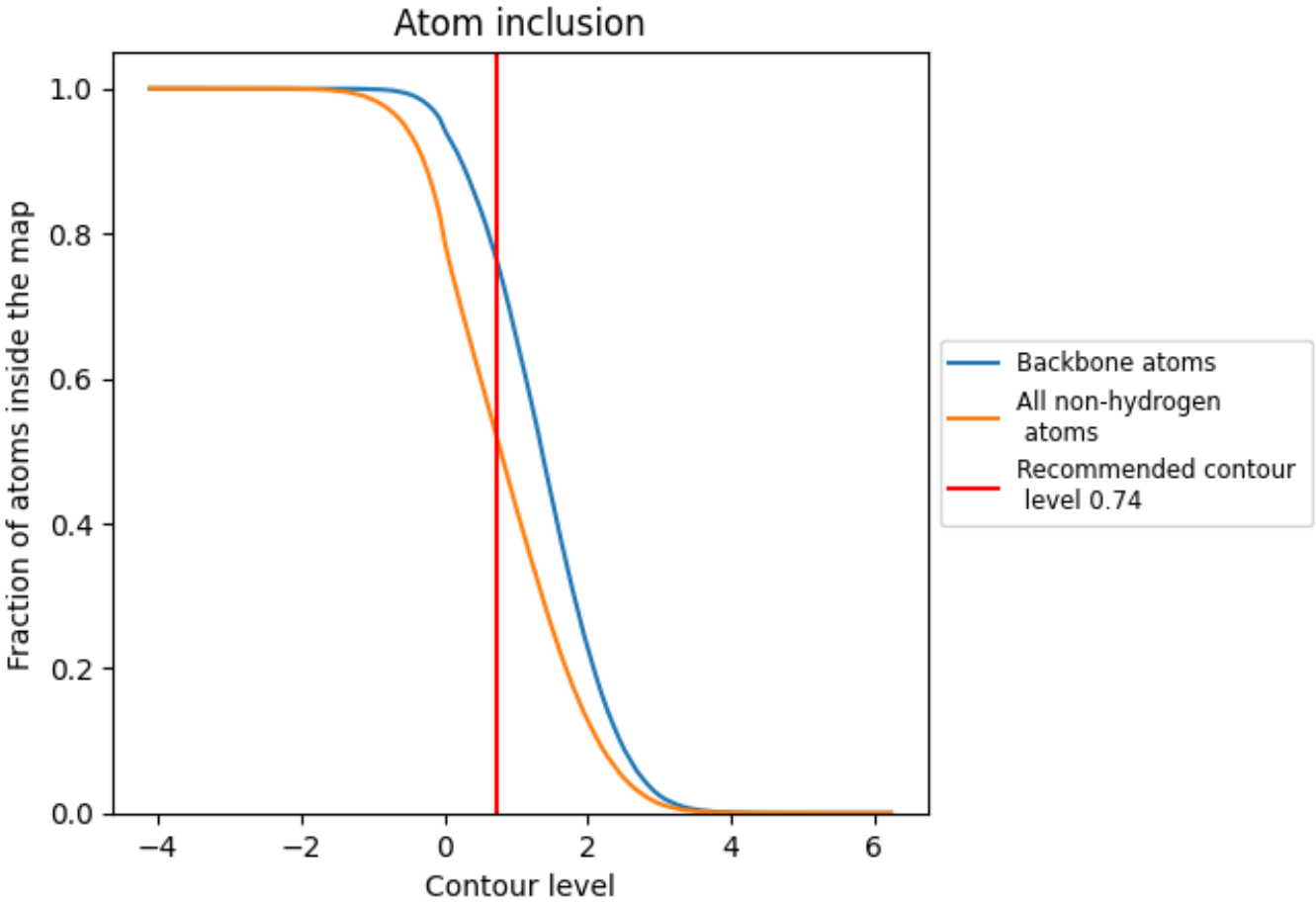
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.74).

## 9.4 Atom inclusion (i)




At the recommended contour level, 76% of all backbone atoms, 52% 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 (0.74) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5165 | 0.1040 |
| 1 | 0.4942 | 0.0930 |
| 2 | 0.5135 | 0.1150 |
| 3 | 0.4717 | 0.1080 |
| 4 | 0.5406 | 0.1090 |
| 5 | 0.5531 | 0.1140 |
| 6 | 0.5221 | 0.1110 |
| 7 | 0.5159 | 0.1070 |
| A | 0.4828 | 0.1150 |
| B | 0.4499 | 0.1020 |
| C | 0.4947 | 0.1170 |
| D | 0.4997 | 0.1100 |
| E | 0.4932 | 0.1110 |
| F | 0.5151 | 0.1200 |
| G | 0.4610 | 0.1070 |
| H | 0.4422 | 0.0870 |
| I | 0.4461 | 0.0960 |
| J | 0.4925 | 0.1020 |
| K | 0.4596 | 0.1050 |
| L | 0.4869 | 0.1020 |
| M | 0.4828 | 0.1080 |
| N | 0.5624 | 0.1190 |
| O | 0.5631 | 0.0940 |
| P | 0.6246 | 0.1070 |
| Q | 0.5850 | 0.1010 |
| R | 0.5544 | 0.0930 |
| S | 0.4814 | 0.0970 |
| T | 0.6074 | 0.1120 |
| U | 0.5486 | 0.1200 |
| V | 0.5172 | 0.1040 |
| W | 0.4583 | 0.0710 |
| X | 0.4906 | 0.0420 |
| Y | 0.5951 | 0.1020 |
| Z | 0.5172 | 0.0930 |