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

Oct 11, 2021 – 12:37 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2R5H |
| Title | : | Pentamer structure of Major Capsid Protein L1 of Human Papilloma Virus type 16 |
| Authors | : | Bishop, B.; Dasgupta, J.; Chen, X.S. |
| Deposited on | : | 2007-09-03 |
| Resolution | : | 3.70 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

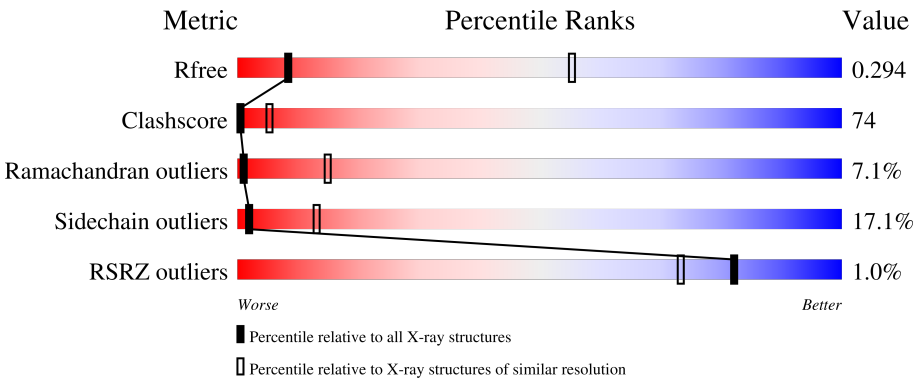
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.23.2 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1049 (3.88-3.52) |
| Clashscore | 141614 | 1027 (3.86-3.54) |
| Ramachandran outliers | 138981 | 1069 (3.88-3.52) |
| Sidechain outliers | 138945 | 1065 (3.88-3.52) |
| RSRZ outliers | 127900 | 1578 (3.90-3.50) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 424 | 15% 36% 37% 11% • |
| 1 | B | 424 | % 12% 36% 42% 9% • |
| 1 | C | 424 | % 11% 42% 36% 10% • |
| 1 | D | 424 | % 9% 39% 41% 9% • |
| 1 | E | 424 | 3% 12% 40% 37% 10% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 424 | .% 13% 39% 35% 12% |
| 1 | G | 424 | .% 12% 37% 39% 11% |
| 1 | H | 424 | .% 11% 39% 37% 12% |
| 1 | I | 424 | .% 12% 36% 42% 8% |
| 1 | J | 424 | 2% 13% 34% 43% 8% |
| 1 | K | 424 | 13% 42% 35% 10% |
| 1 | L | 424 | 16% 34% 40% 8% |
| 1 | M | 424 | 12% 40% 38% 9% |
| 1 | N | 424 | .% 11% 36% 41% 11% |
| 1 | O | 424 | .% 11% 41% 36% 11% |

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 49650 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Late major capsid protein L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | B | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | C | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | D | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | E | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | F | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | G | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | H | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | I | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | J | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | K | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | L | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | M | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | N | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |
| 1 | O | 419 | 3310 | 2108 | 554 | 628 | 20 | 0 | 0 | 0 |

There are 135 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 20 | ALA | - | expression tag | UNP Q81007 |
| A | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| A | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| A | 404 | GLY | - | linker | UNP Q81007 |
| A | 405 | GLY | - | linker | UNP Q81007 |
| A | 406 | SER | - | linker | UNP Q81007 |
| A | 407 | GLY | - | linker | UNP Q81007 |
| A | 408 | GLY | - | linker | UNP Q81007 |
| A | 472 | LEU | - | expression tag | UNP Q81007 |
| B | 20 | ALA | - | expression tag | UNP Q81007 |
| B | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| B | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| B | 404 | GLY | - | linker | UNP Q81007 |
| B | 405 | GLY | - | linker | UNP Q81007 |
| B | 406 | SER | - | linker | UNP Q81007 |
| B | 407 | GLY | - | linker | UNP Q81007 |
| B | 408 | GLY | - | linker | UNP Q81007 |
| B | 472 | LEU | - | expression tag | UNP Q81007 |
| C | 20 | ALA | - | expression tag | UNP Q81007 |
| C | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| C | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| C | 404 | GLY | - | linker | UNP Q81007 |
| C | 405 | GLY | - | linker | UNP Q81007 |
| C | 406 | SER | - | linker | UNP Q81007 |
| C | 407 | GLY | - | linker | UNP Q81007 |
| C | 408 | GLY | - | linker | UNP Q81007 |
| C | 472 | LEU | - | expression tag | UNP Q81007 |
| D | 20 | ALA | - | expression tag | UNP Q81007 |
| D | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| D | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| D | 404 | GLY | - | linker | UNP Q81007 |
| D | 405 | GLY | - | linker | UNP Q81007 |
| D | 406 | SER | - | linker | UNP Q81007 |
| D | 407 | GLY | - | linker | UNP Q81007 |
| D | 408 | GLY | - | linker | UNP Q81007 |
| D | 472 | LEU | - | expression tag | UNP Q81007 |
| E | 20 | ALA | - | expression tag | UNP Q81007 |
| E | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| E | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| E | 404 | GLY | - | linker | UNP Q81007 |
| E | 405 | GLY | - | linker | UNP Q81007 |
| E | 406 | SER | - | linker | UNP Q81007 |
| E | 407 | GLY | - | linker | UNP Q81007 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 408 | GLY | - | linker | UNP Q81007 |
| E | 472 | LEU | - | expression tag | UNP Q81007 |
| F | 20 | ALA | - | expression tag | UNP Q81007 |
| F | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| F | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| F | 404 | GLY | - | linker | UNP Q81007 |
| F | 405 | GLY | - | linker | UNP Q81007 |
| F | 406 | SER | - | linker | UNP Q81007 |
| F | 407 | GLY | - | linker | UNP Q81007 |
| F | 408 | GLY | - | linker | UNP Q81007 |
| F | 472 | LEU | - | expression tag | UNP Q81007 |
| G | 20 | ALA | - | expression tag | UNP Q81007 |
| G | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| G | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| G | 404 | GLY | - | linker | UNP Q81007 |
| G | 405 | GLY | - | linker | UNP Q81007 |
| G | 406 | SER | - | linker | UNP Q81007 |
| G | 407 | GLY | - | linker | UNP Q81007 |
| G | 408 | GLY | - | linker | UNP Q81007 |
| G | 472 | LEU | - | expression tag | UNP Q81007 |
| H | 20 | ALA | - | expression tag | UNP Q81007 |
| H | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| H | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| H | 404 | GLY | - | linker | UNP Q81007 |
| H | 405 | GLY | - | linker | UNP Q81007 |
| H | 406 | SER | - | linker | UNP Q81007 |
| H | 407 | GLY | - | linker | UNP Q81007 |
| H | 408 | GLY | - | linker | UNP Q81007 |
| H | 472 | LEU | - | expression tag | UNP Q81007 |
| I | 20 | ALA | - | expression tag | UNP Q81007 |
| I | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| I | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| I | 404 | GLY | - | linker | UNP Q81007 |
| I | 405 | GLY | - | linker | UNP Q81007 |
| I | 406 | SER | - | linker | UNP Q81007 |
| I | 407 | GLY | - | linker | UNP Q81007 |
| I | 408 | GLY | - | linker | UNP Q81007 |
| I | 472 | LEU | - | expression tag | UNP Q81007 |
| J | 20 | ALA | - | expression tag | UNP Q81007 |
| J | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| J | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| J | 404 | GLY | - | linker | UNP Q81007 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| J | 405 | GLY | - | linker | UNP Q81007 |
| J | 406 | SER | - | linker | UNP Q81007 |
| J | 407 | GLY | - | linker | UNP Q81007 |
| J | 408 | GLY | - | linker | UNP Q81007 |
| J | 472 | LEU | - | expression tag | UNP Q81007 |
| K | 20 | ALA | - | expression tag | UNP Q81007 |
| K | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| K | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| K | 404 | GLY | - | linker | UNP Q81007 |
| K | 405 | GLY | - | linker | UNP Q81007 |
| K | 406 | SER | - | linker | UNP Q81007 |
| K | 407 | GLY | - | linker | UNP Q81007 |
| K | 408 | GLY | - | linker | UNP Q81007 |
| K | 472 | LEU | - | expression tag | UNP Q81007 |
| L | 20 | ALA | - | expression tag | UNP Q81007 |
| L | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| L | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| L | 404 | GLY | - | linker | UNP Q81007 |
| L | 405 | GLY | - | linker | UNP Q81007 |
| L | 406 | SER | - | linker | UNP Q81007 |
| L | 407 | GLY | - | linker | UNP Q81007 |
| L | 408 | GLY | - | linker | UNP Q81007 |
| L | 472 | LEU | - | expression tag | UNP Q81007 |
| M | 20 | ALA | - | expression tag | UNP Q81007 |
| M | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| M | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| M | 404 | GLY | - | linker | UNP Q81007 |
| M | 405 | GLY | - | linker | UNP Q81007 |
| M | 406 | SER | - | linker | UNP Q81007 |
| M | 407 | GLY | - | linker | UNP Q81007 |
| M | 408 | GLY | - | linker | UNP Q81007 |
| M | 472 | LEU | - | expression tag | UNP Q81007 |
| N | 20 | ALA | - | expression tag | UNP Q81007 |
| N | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| N | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| N | 404 | GLY | - | linker | UNP Q81007 |
| N | 405 | GLY | - | linker | UNP Q81007 |
| N | 406 | SER | - | linker | UNP Q81007 |
| N | 407 | GLY | - | linker | UNP Q81007 |
| N | 408 | GLY | - | linker | UNP Q81007 |
| N | 472 | LEU | - | expression tag | UNP Q81007 |
| O | 20 | ALA | - | expression tag | UNP Q81007 |

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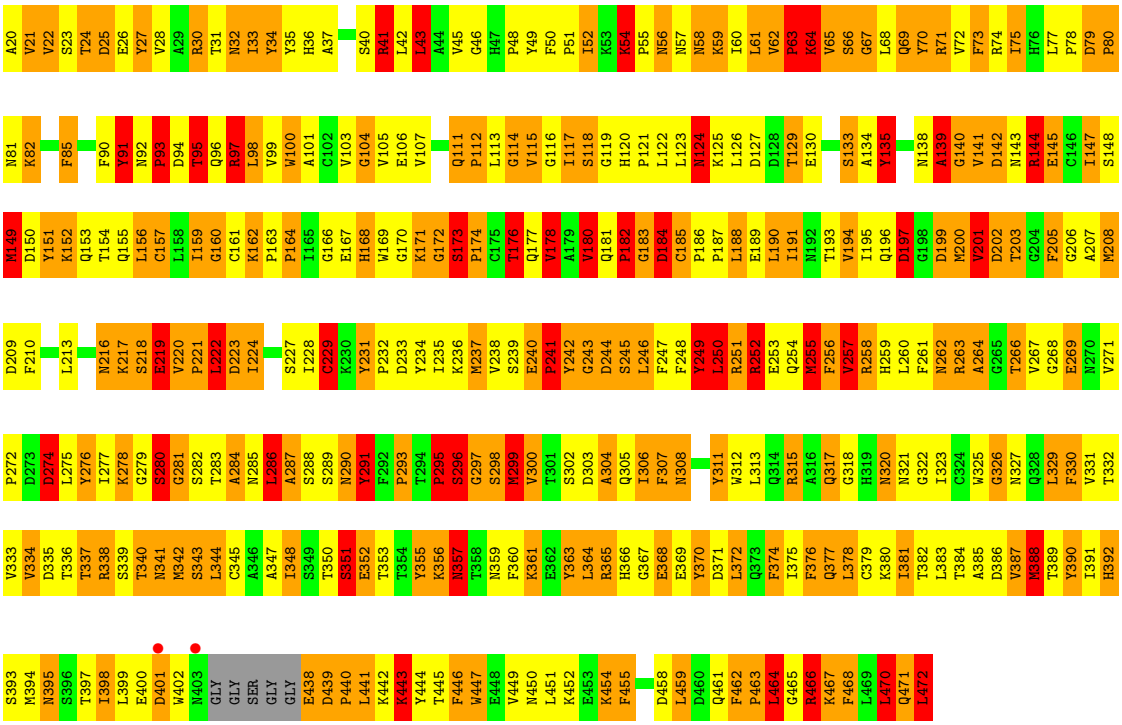
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| O | 177 | GLN | ASN | engineered mutation | UNP Q81007 |
| O | 181 | GLN | ASN | engineered mutation | UNP Q81007 |
| O | 404 | GLY | - | linker | UNP Q81007 |
| O | 405 | GLY | - | linker | UNP Q81007 |
| O | 406 | SER | - | linker | UNP Q81007 |
| O | 407 | GLY | - | linker | UNP Q81007 |
| O | 408 | GLY | - | linker | UNP Q81007 |
| O | 472 | LEU | - | expression tag | UNP Q81007 |

# 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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

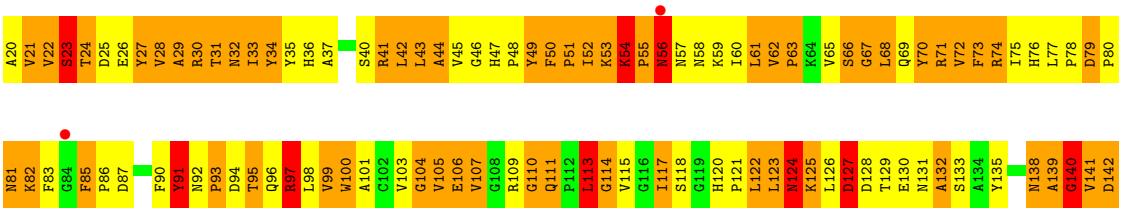
• Molecule 1: Late major capsid protein L1

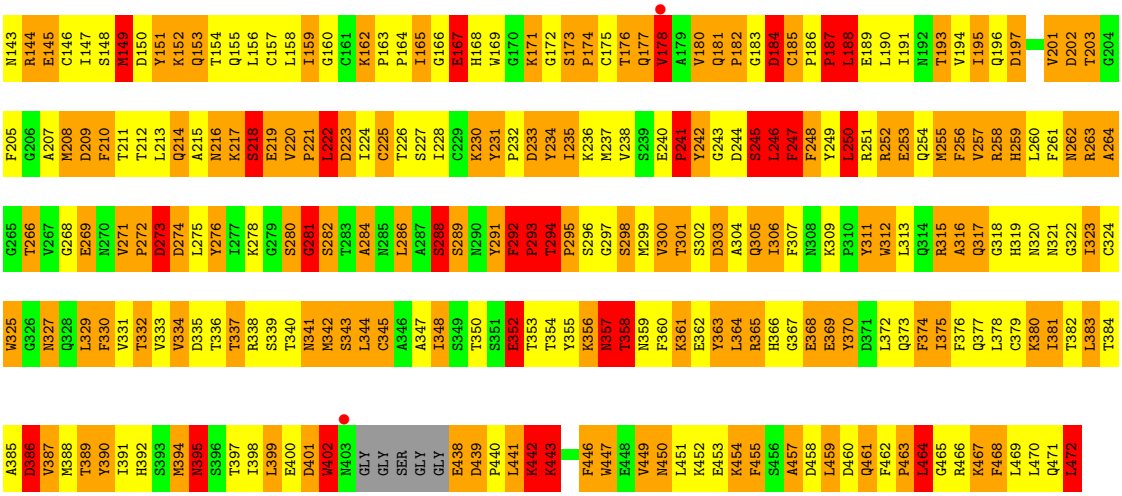
Chain A: 15% 36% 37% 11%



• Molecule 1: Late major capsid protein L1

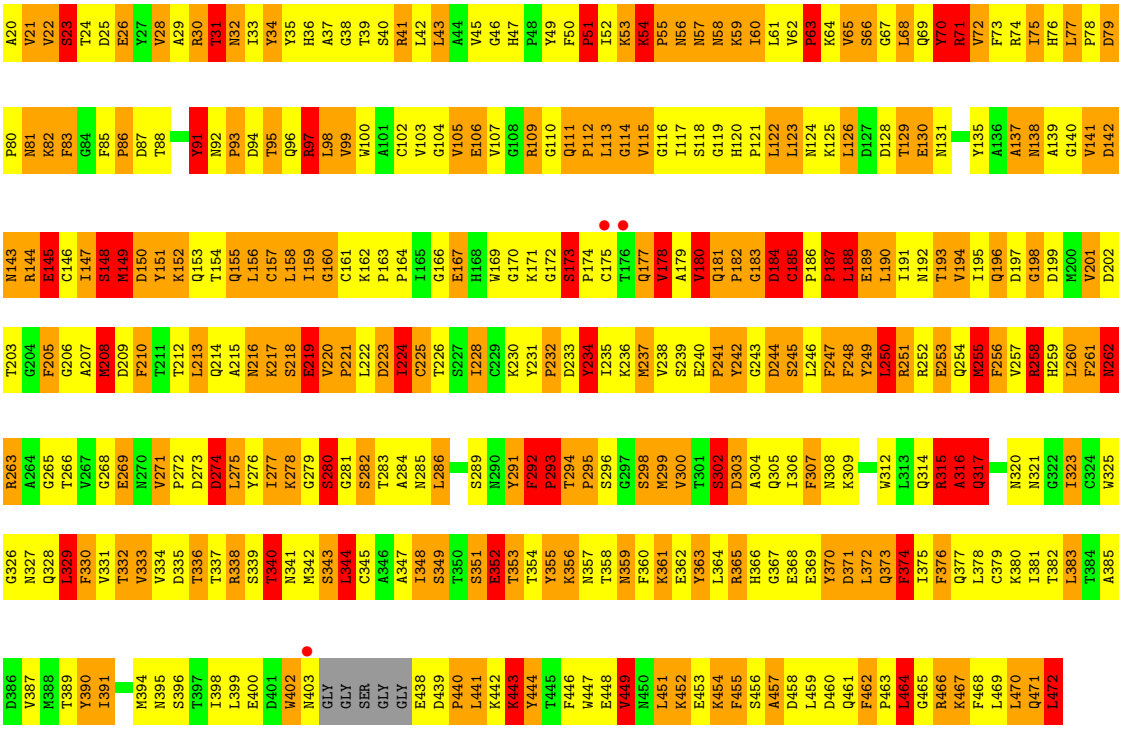
Chain B: % 12% 36% 42% 9%





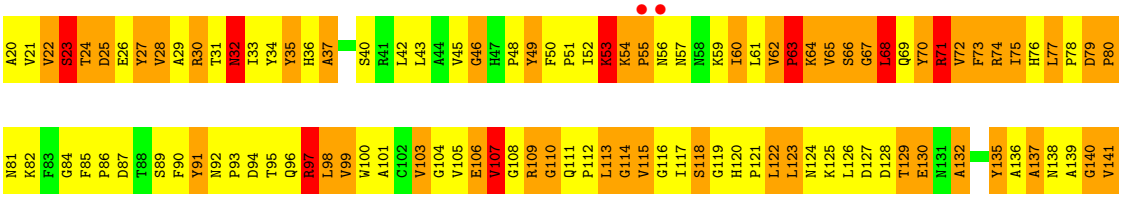
• Molecule 1: Late major capsid protein L1

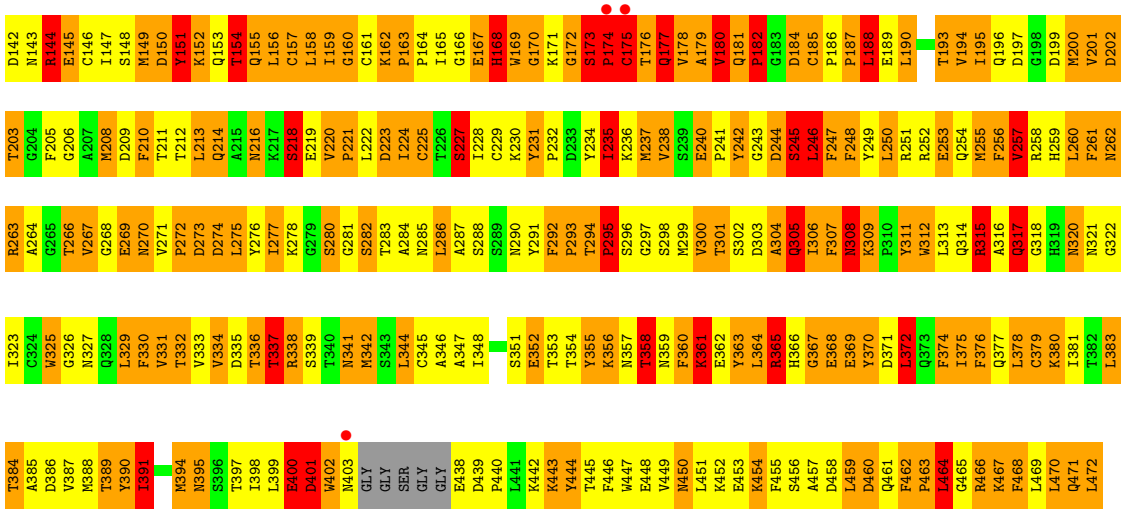
Chain C:



• Molecule 1: Late major capsid protein L1

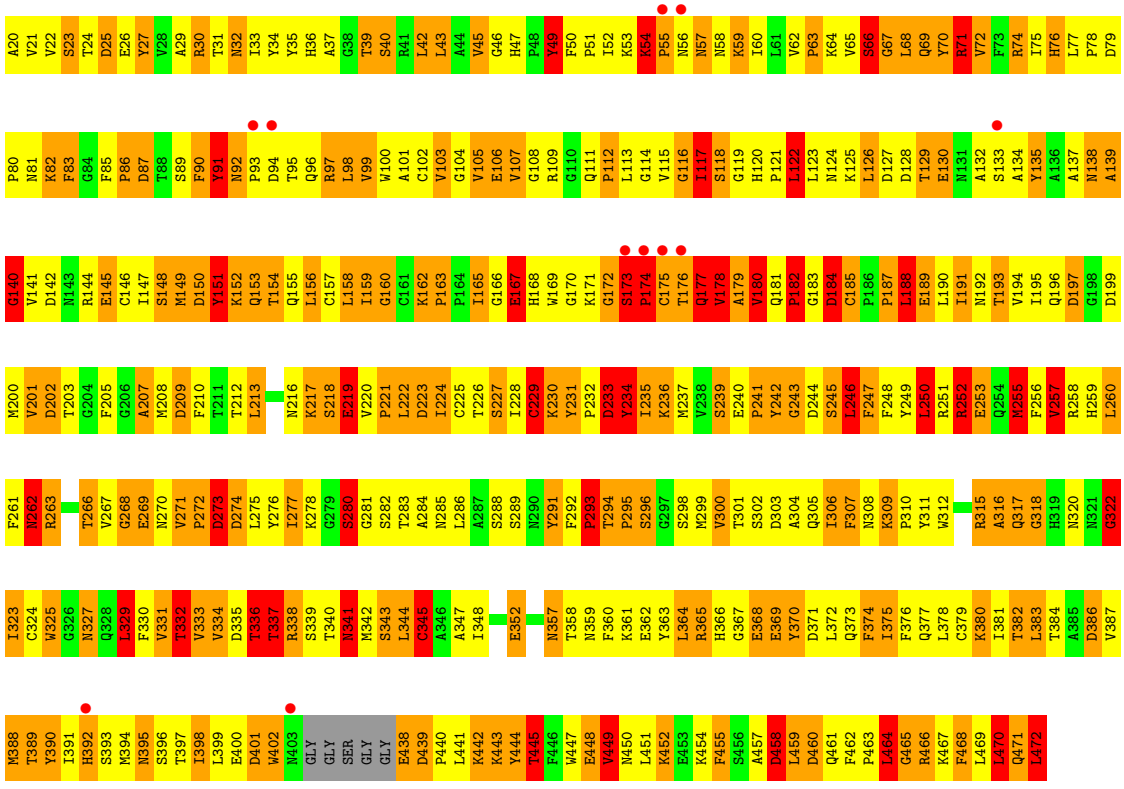
Chain D:





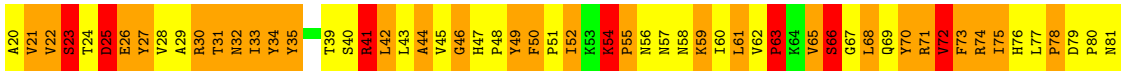
• Molecule 1: Late major capsid protein L1

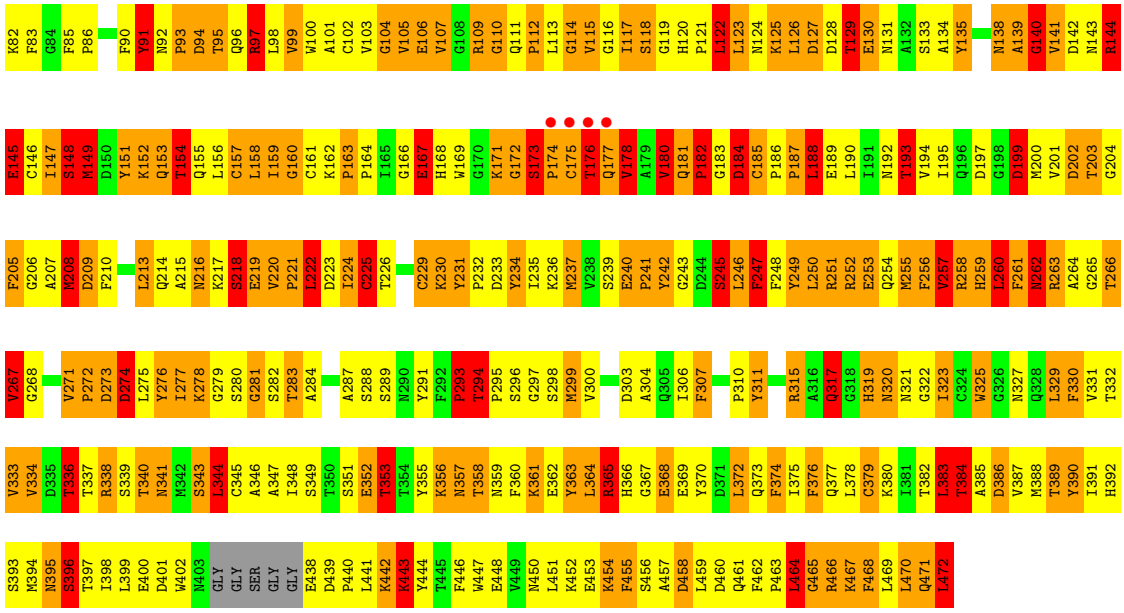
Chain E:



• Molecule 1: Late major capsid protein L1

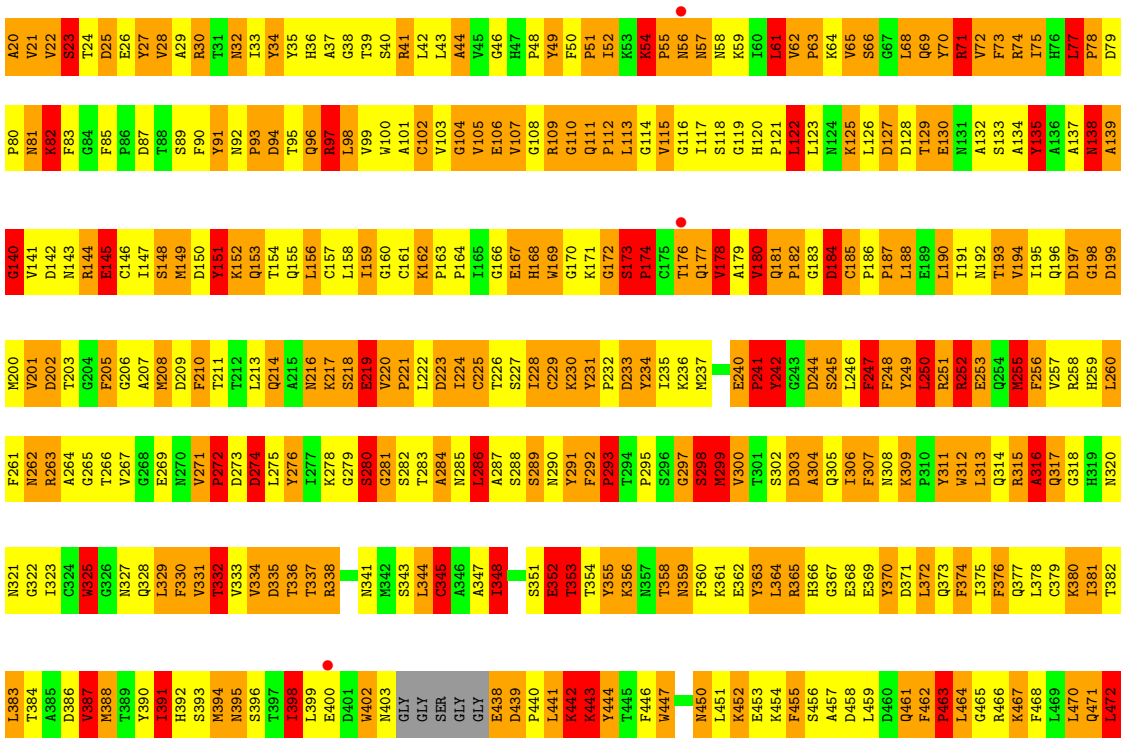
Chain F:





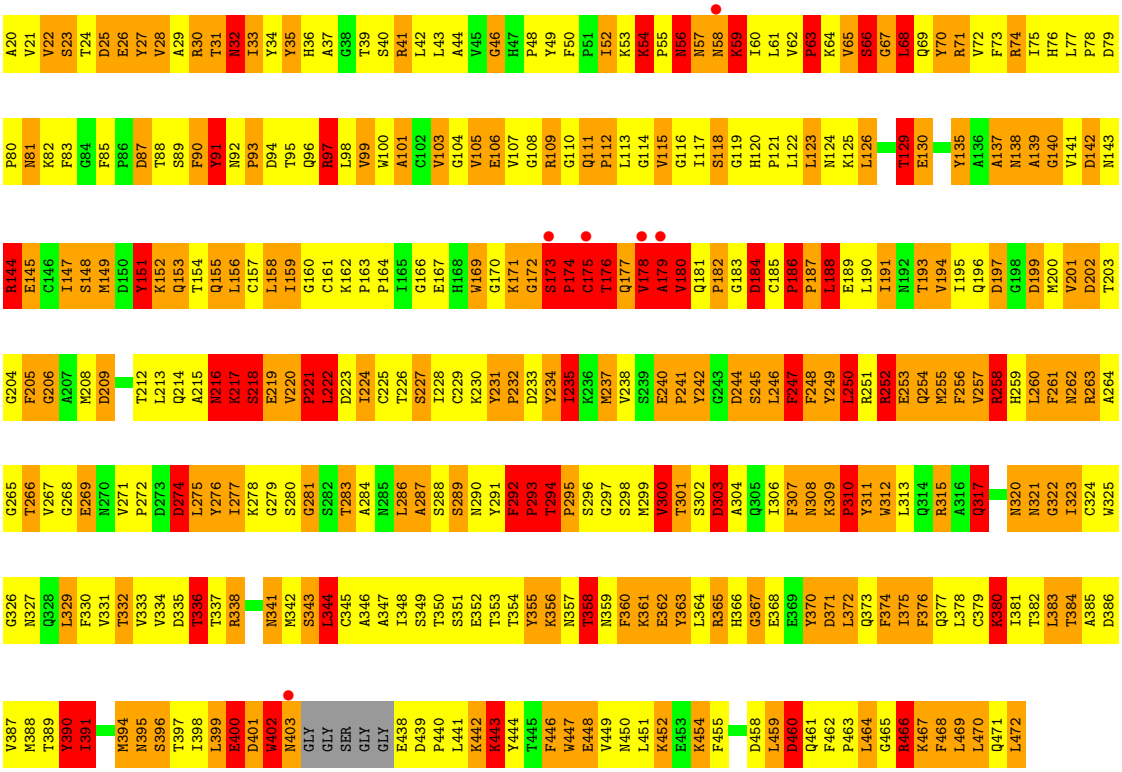

- Molecule 1: Late major capsid protein L1

Chain G: % 12% 37% 39% 11%



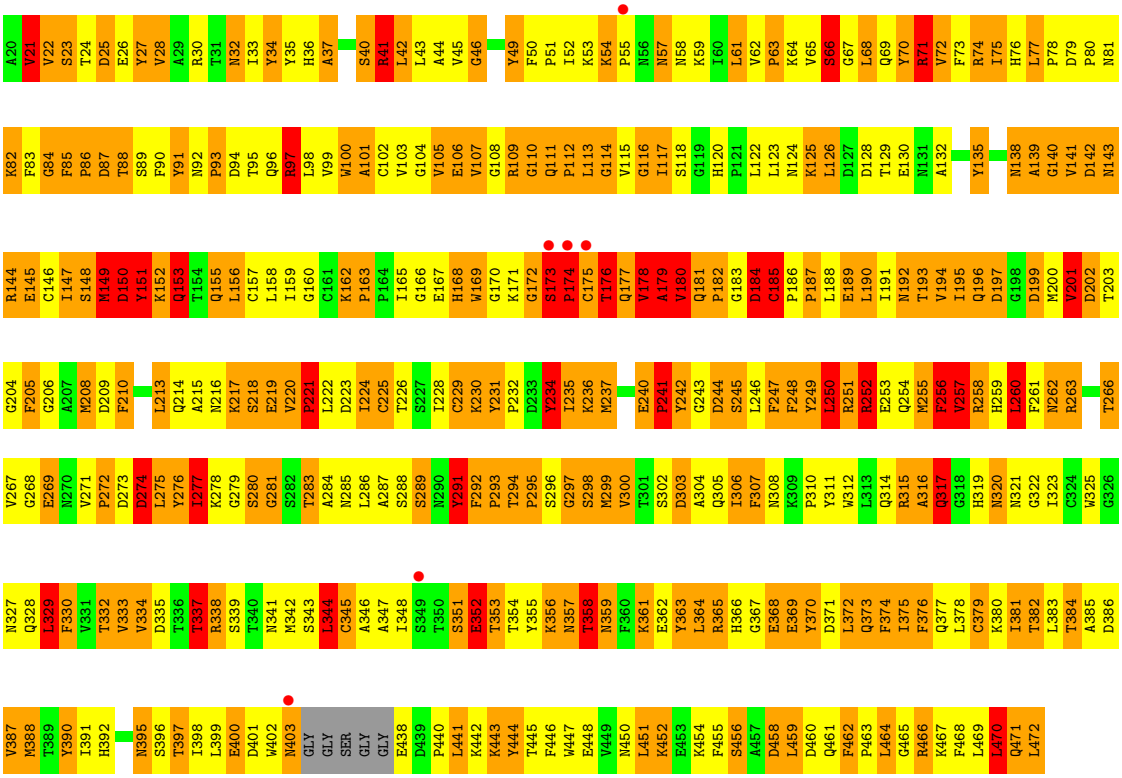

- Molecule 1: Late major capsid protein L1

Chain H: % 11% 39% 37% 12%



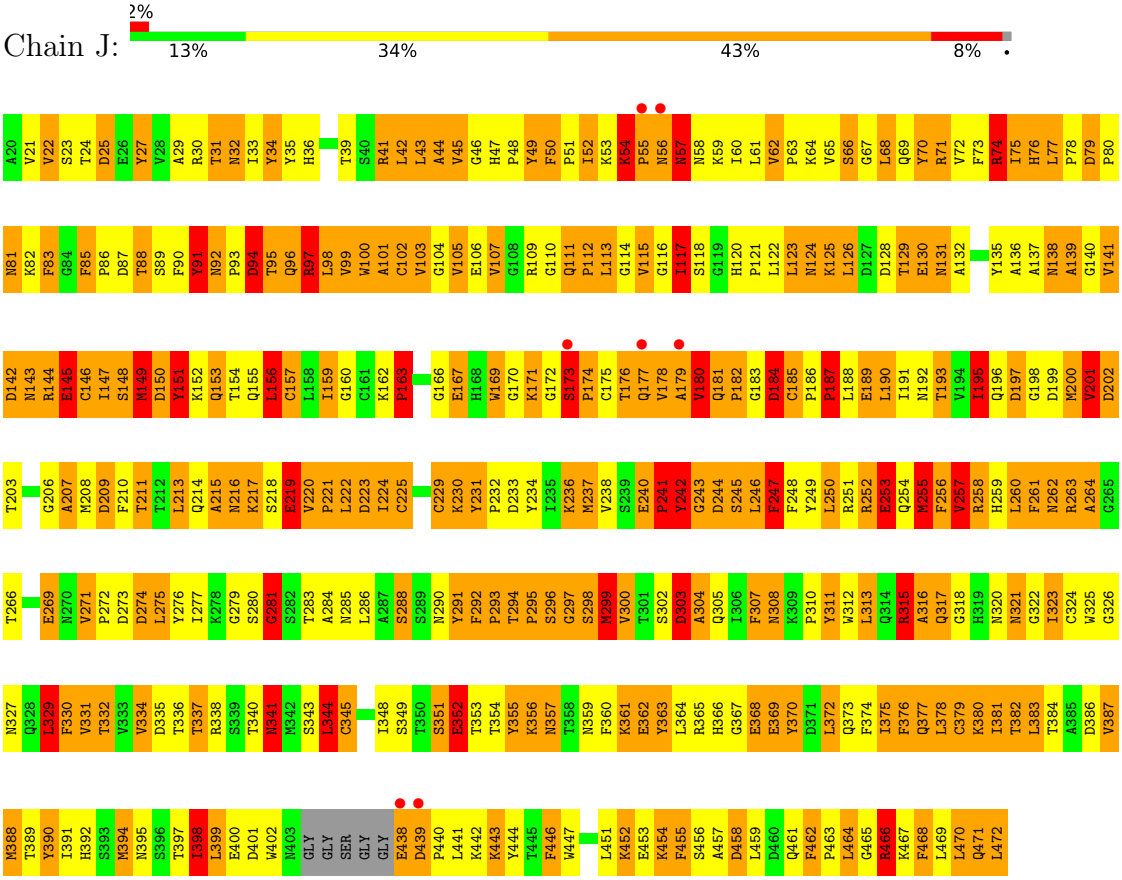
- Molecule 1: Late major capsid protein L1

Chain I:



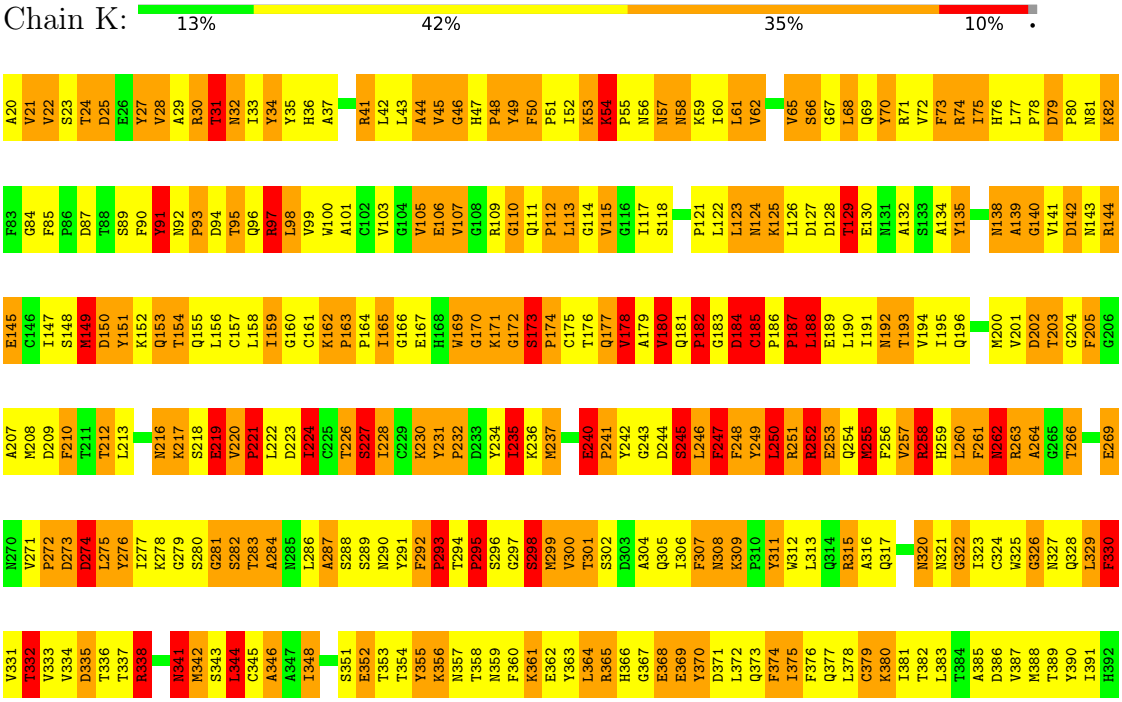
• Molecule 1: Late major capsid protein L1

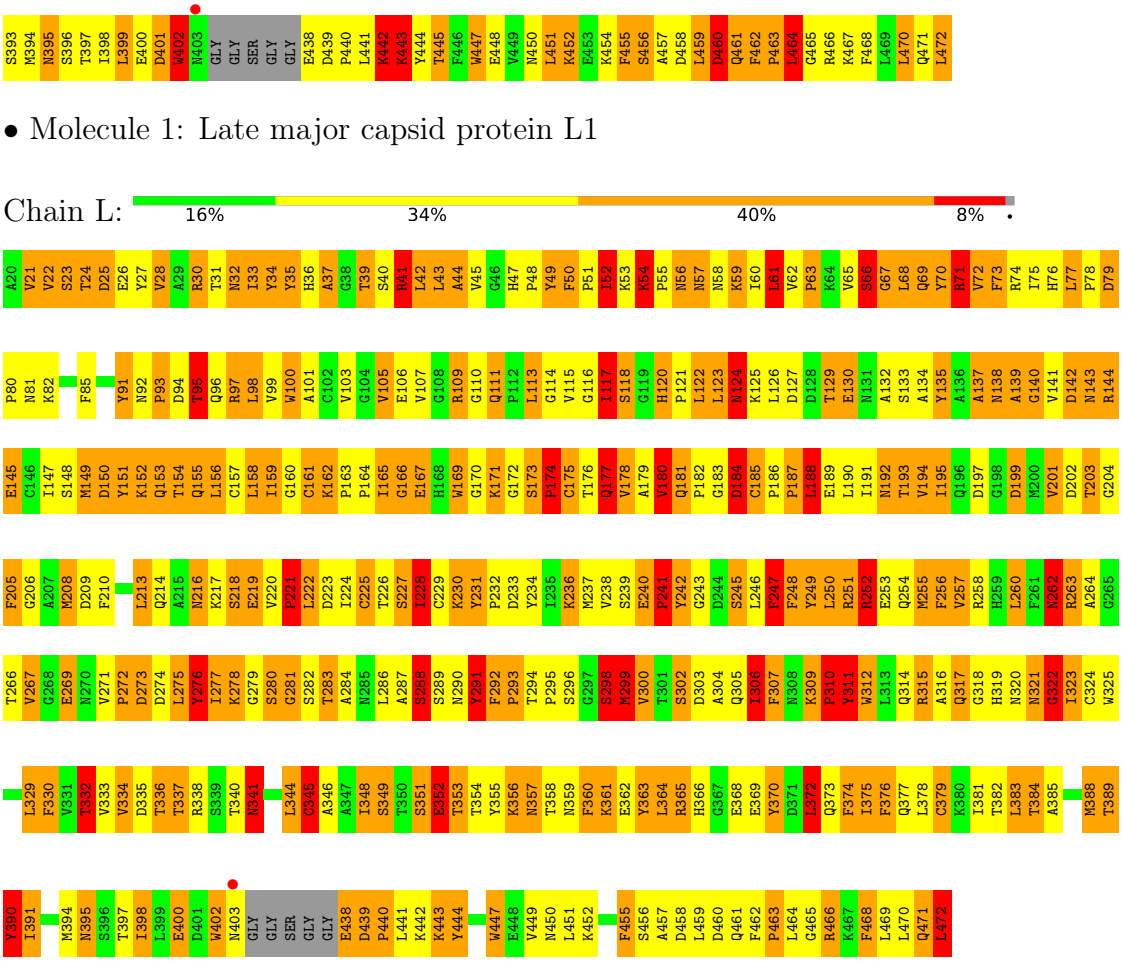
Chain J:




• Molecule 1: Late major capsid protein L1

Chain K:





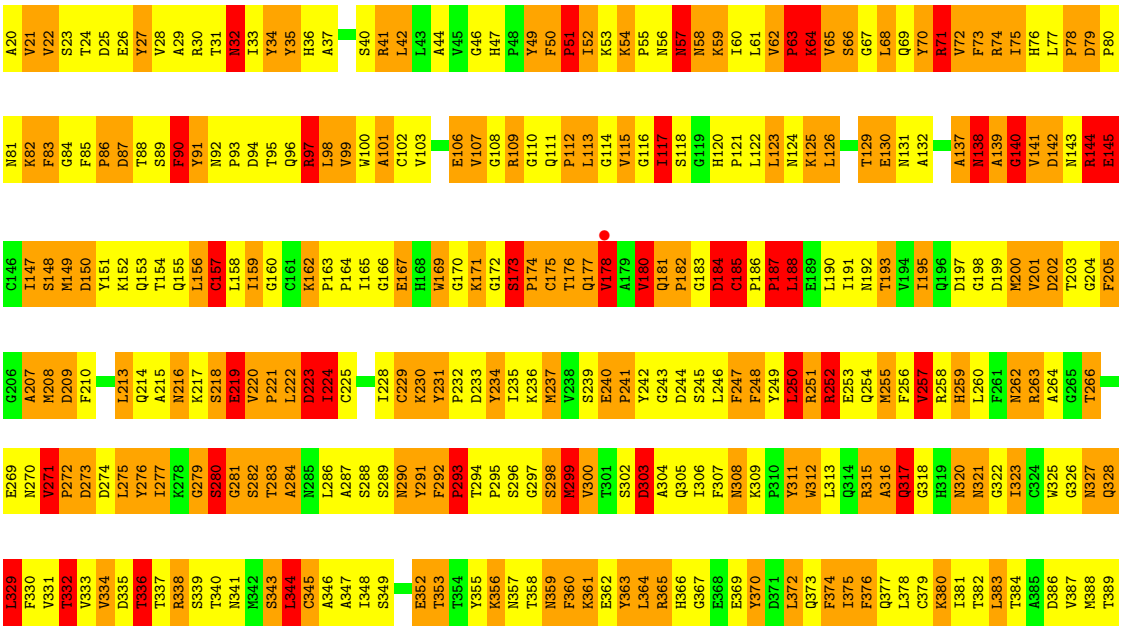

• Molecule 1: Late major capsid protein L1

Chain L: 16% 34% 40% 8%

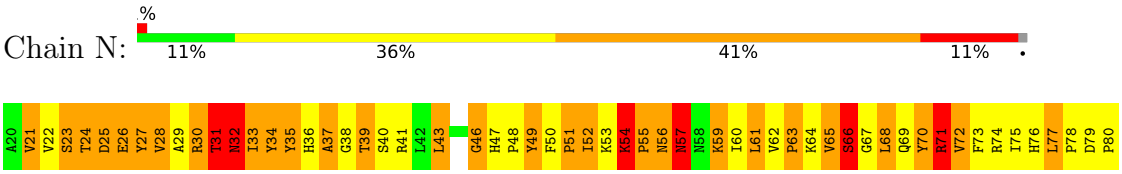



• Molecule 1: Late major capsid protein L1

Chain M: 12% 40% 38% 9%

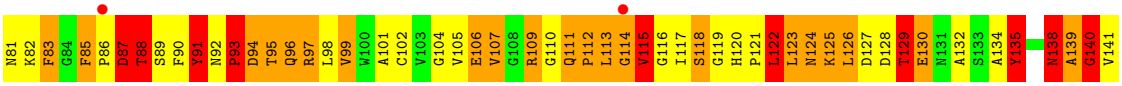


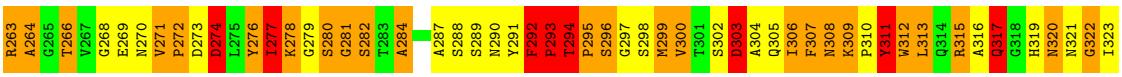
• Molecule 1: Late major capsid protein L1



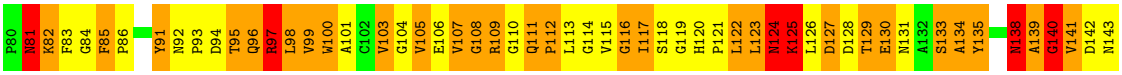


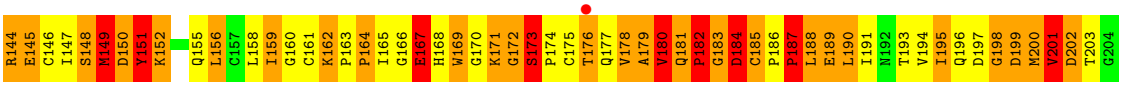


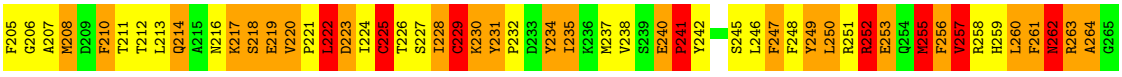


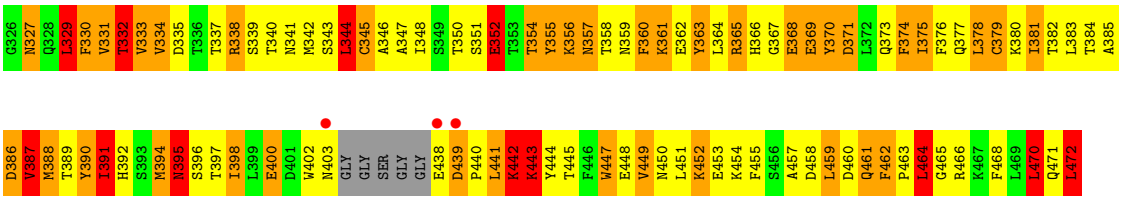


• Molecule 1: Late major capsid protein L1




G326
N327
Q328
L329
F330
V331
T332
V333
V334
D335
T336
T337
R338
S339
T340
N341
M342
S343
L344
C345
A346
A347
I348
S349
T350
S351
E352
T353
T354
Y355
K356
N357
T358
N359
F360
K361
E362
Y363
L364
R365
H366
G367
E368
E369
Y370
D371
L372
Q373
F374
I375
F376
Q377
L378
C379
K380
I381
T382
L383
T384
A385
D386
V387
M388
T389
Y390
I391
H392
S393
M394
N395
S396
T397
I398
L399
E400
D401
W402
N403
GLY
GLY
SER
GLY
GLY
E438
D439
P440
L441
K442
K443
Y444
T445
F446
W447
E448
V449
N450
L451
K452
E453
K454
F455
S456
A457
D458
L459
D460
Q461
F462
P463
L464
G465
R466
K467
F468
L469
L470
Q471
L472

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 105.00Å 159.05Å 413.74Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 3.70<br>14.98 – 3.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 80.5 (15.00-3.70)<br>80.5 (14.98-3.70) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.70 (at 3.66Å) | Xtriage |
| Refinement program | REFMAC 5.2.0019 | Depositor |
| R, $R_{free}$ | 0.247 , 0.305<br>0.241 , 0.294 | Depositor<br>DCC |
| $R_{free}$ test set | 2971 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 92.7 | Xtriage |
| Anisotropy | 0.063 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.20 , 61.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 49650 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 80.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 2.76 | 242/3395 (7.1%) | 2.11 | 115/4616 (2.5%) |
| 1 | B | 2.74 | 260/3395 (7.7%) | 2.03 | 110/4616 (2.4%) |
| 1 | C | 2.76 | 241/3395 (7.1%) | 2.14 | 110/4616 (2.4%) |
| 1 | D | 2.98 | 305/3395 (9.0%) | 2.15 | 130/4616 (2.8%) |
| 1 | E | 2.76 | 244/3395 (7.2%) | 2.02 | 113/4616 (2.4%) |
| 1 | F | 2.85 | 287/3395 (8.5%) | 2.09 | 128/4616 (2.8%) |
| 1 | G | 2.82 | 264/3395 (7.8%) | 2.07 | 121/4616 (2.6%) |
| 1 | H | 2.87 | 287/3395 (8.5%) | 2.09 | 133/4616 (2.9%) |
| 1 | I | 2.82 | 257/3395 (7.6%) | 2.08 | 120/4616 (2.6%) |
| 1 | J | 2.78 | 267/3395 (7.9%) | 2.09 | 123/4616 (2.7%) |
| 1 | K | 2.82 | 258/3395 (7.6%) | 2.04 | 97/4616 (2.1%) |
| 1 | L | 2.82 | 243/3395 (7.2%) | 2.07 | 124/4616 (2.7%) |
| 1 | M | 2.72 | 230/3395 (6.8%) | 2.14 | 129/4616 (2.8%) |
| 1 | N | 2.76 | 269/3395 (7.9%) | 2.12 | 136/4616 (2.9%) |
| 1 | O | 2.73 | 266/3395 (7.8%) | 1.99 | 90/4616 (1.9%) |
| All | All | 2.80 | 3920/50925 (7.7%) | 2.08 | 1779/69240 (2.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | C | 0 | 3 |
| 1 | D | 0 | 1 |
| 1 | E | 0 | 1 |
| 1 | F | 0 | 1 |
| 1 | G | 0 | 1 |
| 1 | L | 0 | 3 |
| 1 | M | 0 | 1 |
| 1 | N | 0 | 1 |
| 1 | O | 0 | 1 |
| All | All | 0 | 13 |

All (3920) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 245 | SER | CB-OG | 29.56 | 1.80 | 1.42 |
| 1 | D | 438 | GLU | CD-OE2 | 20.41 | 1.48 | 1.25 |
| 1 | D | 438 | GLU | CD-OE1 | 18.10 | 1.45 | 1.25 |
| 1 | I | 356 | LYS | CE-NZ | 17.09 | 1.91 | 1.49 |
| 1 | D | 178 | VAL | CB-CG2 | 16.71 | 1.88 | 1.52 |
| 1 | L | 161 | CYS | CB-SG | 16.45 | 2.10 | 1.82 |
| 1 | E | 390 | TYR | CE2-CZ | 16.41 | 1.59 | 1.38 |
| 1 | E | 280 | SER | CB-OG | 16.23 | 1.63 | 1.42 |
| 1 | I | 291 | TYR | CE2-CZ | -16.15 | 1.17 | 1.38 |
| 1 | H | 178 | VAL | CB-CG1 | 15.88 | 1.86 | 1.52 |
| 1 | G | 178 | VAL | CB-CG1 | 15.80 | 1.86 | 1.52 |
| 1 | H | 217 | LYS | CE-NZ | 15.74 | 1.88 | 1.49 |
| 1 | H | 157 | CYS | CB-SG | -15.44 | 1.55 | 1.82 |
| 1 | G | 219 | GLU | CD-OE2 | 15.35 | 1.42 | 1.25 |
| 1 | M | 390 | TYR | CD2-CE2 | -15.01 | 1.16 | 1.39 |
| 1 | O | 280 | SER | CB-OG | 14.93 | 1.61 | 1.42 |
| 1 | F | 157 | CYS | CB-SG | -14.55 | 1.57 | 1.82 |
| 1 | M | 230 | LYS | CE-NZ | 14.51 | 1.85 | 1.49 |
| 1 | L | 145 | GLU | CB-CG | -13.99 | 1.25 | 1.52 |
| 1 | D | 100 | TRP | CG-CD1 | -13.96 | 1.17 | 1.36 |
| 1 | F | 175 | CYS | CB-SG | 13.86 | 2.05 | 1.82 |
| 1 | A | 64 | LYS | CD-CE | 13.79 | 1.85 | 1.51 |
| 1 | G | 20 | ALA | CA-CB | 13.74 | 1.81 | 1.52 |
| 1 | I | 179 | ALA | CA-CB | 13.72 | 1.81 | 1.52 |
| 1 | A | 231 | TYR | CD1-CE1 | 13.60 | 1.59 | 1.39 |
| 1 | J | 74 | ARG | CG-CD | 13.48 | 1.85 | 1.51 |
| 1 | B | 70 | TYR | CG-CD2 | -13.23 | 1.22 | 1.39 |
| 1 | F | 40 | SER | CB-OG | 13.15 | 1.59 | 1.42 |
| 1 | E | 368 | GLU | CD-OE1 | 13.02 | 1.40 | 1.25 |
| 1 | L | 59 | LYS | CE-NZ | 13.01 | 1.81 | 1.49 |
| 1 | J | 219 | GLU | CD-OE1 | 12.93 | 1.39 | 1.25 |
| 1 | C | 178 | VAL | CB-CG1 | 12.92 | 1.79 | 1.52 |
| 1 | L | 73 | PHE | CE1-CZ | 12.88 | 1.61 | 1.37 |
| 1 | I | 369 | GLU | CB-CG | 12.86 | 1.76 | 1.52 |
| 1 | G | 219 | GLU | CD-OE1 | 12.85 | 1.39 | 1.25 |
| 1 | F | 207 | ALA | CA-CB | -12.76 | 1.25 | 1.52 |
| 1 | K | 362 | GLU | CD-OE1 | 12.70 | 1.39 | 1.25 |
| 1 | F | 59 | LYS | CE-NZ | 12.70 | 1.80 | 1.49 |
| 1 | G | 280 | SER | CB-OG | 12.68 | 1.58 | 1.42 |
| 1 | F | 139 | ALA | CA-CB | 12.67 | 1.79 | 1.52 |
| 1 | G | 333 | VAL | CB-CG2 | -12.65 | 1.26 | 1.52 |
| 1 | M | 457 | ALA | CA-CB | -12.62 | 1.25 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 201 | VAL | CB-CG1 | -12.61 | 1.26 | 1.52 |
| 1 | H | 301 | THR | CB-CG2 | 12.61 | 1.94 | 1.52 |
| 1 | F | 365 | ARG | CG-CD | 12.56 | 1.83 | 1.51 |
| 1 | B | 225 | CYS | CB-SG | 12.56 | 2.03 | 1.82 |
| 1 | H | 178 | VAL | C-O | 12.48 | 1.47 | 1.23 |
| 1 | J | 453 | GLU | CG-CD | 12.48 | 1.70 | 1.51 |
| 1 | D | 32 | ASN | CB-CG | 12.47 | 1.79 | 1.51 |
| 1 | B | 334 | VAL | CB-CG1 | -12.46 | 1.26 | 1.52 |
| 1 | J | 457 | ALA | CA-CB | -12.46 | 1.26 | 1.52 |
| 1 | N | 207 | ALA | CA-CB | -12.42 | 1.26 | 1.52 |
| 1 | F | 231 | TYR | CD1-CE1 | 12.38 | 1.57 | 1.39 |
| 1 | H | 139 | ALA | CA-CB | 12.37 | 1.78 | 1.52 |
| 1 | J | 180 | VAL | CB-CG2 | 12.35 | 1.78 | 1.52 |
| 1 | D | 181 | GLN | CG-CD | 12.30 | 1.79 | 1.51 |
| 1 | J | 300 | VAL | CB-CG1 | 12.27 | 1.78 | 1.52 |
| 1 | A | 178 | VAL | CB-CG2 | 12.25 | 1.78 | 1.52 |
| 1 | M | 86 | PRO | CA-C | 12.23 | 1.77 | 1.52 |
| 1 | F | 438 | GLU | CG-CD | 12.16 | 1.70 | 1.51 |
| 1 | L | 291 | TYR | CG-CD2 | -12.12 | 1.23 | 1.39 |
| 1 | E | 152 | LYS | CD-CE | 12.12 | 1.81 | 1.51 |
| 1 | G | 105 | VAL | CB-CG2 | 12.08 | 1.78 | 1.52 |
| 1 | M | 137 | ALA | CA-CB | 12.07 | 1.77 | 1.52 |
| 1 | L | 333 | VAL | CB-CG1 | -12.04 | 1.27 | 1.52 |
| 1 | E | 177 | GLN | CG-CD | 12.02 | 1.78 | 1.51 |
| 1 | K | 27 | TYR | CD1-CE1 | 12.01 | 1.57 | 1.39 |
| 1 | E | 189 | GLU | CD-OE1 | 11.99 | 1.38 | 1.25 |
| 1 | K | 27 | TYR | CD2-CE2 | 11.94 | 1.57 | 1.39 |
| 1 | C | 82 | LYS | CE-NZ | 11.89 | 1.78 | 1.49 |
| 1 | M | 178 | VAL | CB-CG1 | 11.87 | 1.77 | 1.52 |
| 1 | L | 169 | TRP | CG-CD1 | -11.83 | 1.20 | 1.36 |
| 1 | F | 145 | GLU | CD-OE1 | 11.82 | 1.38 | 1.25 |
| 1 | K | 178 | VAL | CB-CG1 | 11.81 | 1.77 | 1.52 |
| 1 | I | 257 | VAL | CB-CG1 | -11.81 | 1.28 | 1.52 |
| 1 | D | 137 | ALA | CA-CB | 11.78 | 1.77 | 1.52 |
| 1 | H | 107 | VAL | CB-CG2 | -11.77 | 1.28 | 1.52 |
| 1 | J | 105 | VAL | CB-CG2 | 11.76 | 1.77 | 1.52 |
| 1 | B | 107 | VAL | CB-CG2 | -11.76 | 1.28 | 1.52 |
| 1 | H | 130 | GLU | CD-OE2 | 11.75 | 1.38 | 1.25 |
| 1 | M | 334 | VAL | CB-CG1 | -11.73 | 1.28 | 1.52 |
| 1 | K | 130 | GLU | CD-OE2 | 11.73 | 1.38 | 1.25 |
| 1 | O | 269 | GLU | CB-CG | 11.72 | 1.74 | 1.52 |
| 1 | C | 452 | LYS | CE-NZ | 11.68 | 1.78 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | J | 178 | VAL | CB-CG1 | 11.64 | 1.77 | 1.52 |
| 1 | M | 106 | GLU | CB-CG | 11.64 | 1.74 | 1.52 |
| 1 | F | 362 | GLU | CD-OE2 | 11.60 | 1.38 | 1.25 |
| 1 | A | 368 | GLU | CB-CG | -11.59 | 1.30 | 1.52 |
| 1 | I | 291 | TYR | CE1-CZ | -11.57 | 1.23 | 1.38 |
| 1 | J | 253 | GLU | CD-OE1 | 11.55 | 1.38 | 1.25 |
| 1 | L | 247 | PHE | CE2-CZ | -11.55 | 1.15 | 1.37 |
| 1 | K | 400 | GLU | CD-OE1 | 11.55 | 1.38 | 1.25 |
| 1 | A | 300 | VAL | CB-CG1 | 11.54 | 1.77 | 1.52 |
| 1 | K | 311 | TYR | CD1-CE1 | 11.53 | 1.56 | 1.39 |
| 1 | K | 456 | SER | CB-OG | 11.53 | 1.57 | 1.42 |
| 1 | L | 402 | TRP | C-O | 11.48 | 1.45 | 1.23 |
| 1 | C | 219 | GLU | CD-OE1 | 11.47 | 1.38 | 1.25 |
| 1 | A | 64 | LYS | CE-NZ | 11.46 | 1.77 | 1.49 |
| 1 | H | 32 | ASN | CB-CG | 11.45 | 1.77 | 1.51 |
| 1 | G | 201 | VAL | CB-CG2 | 11.44 | 1.76 | 1.52 |
| 1 | H | 361 | LYS | CG-CD | 11.44 | 1.91 | 1.52 |
| 1 | A | 157 | CYS | CB-SG | -11.42 | 1.62 | 1.82 |
| 1 | B | 369 | GLU | CB-CG | 11.41 | 1.73 | 1.52 |
| 1 | I | 390 | TYR | CE1-CZ | 11.40 | 1.53 | 1.38 |
| 1 | M | 369 | GLU | CD-OE1 | 11.39 | 1.38 | 1.25 |
| 1 | E | 70 | TYR | CE2-CZ | -11.38 | 1.23 | 1.38 |
| 1 | G | 363 | TYR | CD1-CE1 | 11.38 | 1.56 | 1.39 |
| 1 | K | 162 | LYS | CD-CE | 11.38 | 1.79 | 1.51 |
| 1 | E | 236 | LYS | CE-NZ | 11.37 | 1.77 | 1.49 |
| 1 | M | 144 | ARG | CB-CG | 11.36 | 1.83 | 1.52 |
| 1 | O | 130 | GLU | CD-OE2 | 11.35 | 1.38 | 1.25 |
| 1 | F | 467 | LYS | CD-CE | 11.32 | 1.79 | 1.51 |
| 1 | L | 152 | LYS | CD-CE | 11.32 | 1.79 | 1.51 |
| 1 | I | 448 | GLU | CD-OE2 | 11.31 | 1.38 | 1.25 |
| 1 | I | 82 | LYS | CD-CE | 11.28 | 1.79 | 1.51 |
| 1 | D | 468 | PHE | CE2-CZ | 11.27 | 1.58 | 1.37 |
| 1 | M | 331 | VAL | CB-CG2 | -11.23 | 1.29 | 1.52 |
| 1 | M | 82 | LYS | CE-NZ | 11.23 | 1.77 | 1.49 |
| 1 | D | 339 | SER | CB-OG | -11.23 | 1.27 | 1.42 |
| 1 | C | 453 | GLU | CD-OE2 | 11.22 | 1.38 | 1.25 |
| 1 | O | 368 | GLU | CD-OE1 | 11.22 | 1.38 | 1.25 |
| 1 | K | 452 | LYS | CD-CE | 11.21 | 1.79 | 1.51 |
| 1 | G | 27 | TYR | CG-CD2 | 11.20 | 1.53 | 1.39 |
| 1 | K | 185 | CYS | CB-SG | 11.20 | 2.01 | 1.82 |
| 1 | E | 178 | VAL | CB-CG1 | 11.19 | 1.76 | 1.52 |
| 1 | O | 71 | ARG | CZ-NH1 | 11.15 | 1.47 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | L | 72 | VAL | CB-CG2 | -11.14 | 1.29 | 1.52 |
| 1 | E | 201 | VAL | CB-CG1 | -11.12 | 1.29 | 1.52 |
| 1 | C | 135 | TYR | CD1-CE1 | -11.11 | 1.22 | 1.39 |
| 1 | H | 26 | GLU | CD-OE1 | 11.11 | 1.37 | 1.25 |
| 1 | K | 346 | ALA | CA-CB | 11.07 | 1.75 | 1.52 |
| 1 | A | 161 | CYS | CB-SG | 11.06 | 2.01 | 1.82 |
| 1 | M | 32 | ASN | CB-CG | 11.06 | 1.76 | 1.51 |
| 1 | H | 59 | LYS | CE-NZ | 11.06 | 1.76 | 1.49 |
| 1 | K | 289 | SER | CB-OG | 11.05 | 1.56 | 1.42 |
| 1 | M | 145 | GLU | CD-OE2 | 11.01 | 1.37 | 1.25 |
| 1 | J | 145 | GLU | CD-OE2 | 11.01 | 1.37 | 1.25 |
| 1 | G | 400 | GLU | CG-CD | 10.96 | 1.68 | 1.51 |
| 1 | N | 107 | VAL | CB-CG2 | -10.96 | 1.29 | 1.52 |
| 1 | G | 173 | SER | CA-CB | 10.93 | 1.69 | 1.52 |
| 1 | F | 178 | VAL | CB-CG1 | 10.93 | 1.75 | 1.52 |
| 1 | J | 201 | VAL | CB-CG1 | -10.91 | 1.29 | 1.52 |
| 1 | D | 176 | THR | C-O | 10.89 | 1.44 | 1.23 |
| 1 | J | 362 | GLU | CD-OE1 | 10.86 | 1.37 | 1.25 |
| 1 | O | 331 | VAL | CB-CG1 | 10.86 | 1.75 | 1.52 |
| 1 | L | 118 | SER | CB-OG | 10.85 | 1.56 | 1.42 |
| 1 | F | 125 | LYS | C-O | 10.83 | 1.44 | 1.23 |
| 1 | G | 146 | CYS | CB-SG | 10.83 | 2.00 | 1.82 |
| 1 | O | 442 | LYS | CE-NZ | 10.83 | 1.76 | 1.49 |
| 1 | B | 312 | TRP | CG-CD1 | -10.81 | 1.21 | 1.36 |
| 1 | A | 178 | VAL | CB-CG1 | 10.81 | 1.75 | 1.52 |
| 1 | C | 217 | LYS | CD-CE | 10.80 | 1.78 | 1.51 |
| 1 | G | 400 | GLU | CD-OE2 | 10.80 | 1.37 | 1.25 |
| 1 | L | 219 | GLU | CD-OE1 | 10.79 | 1.37 | 1.25 |
| 1 | D | 253 | GLU | CD-OE1 | 10.78 | 1.37 | 1.25 |
| 1 | O | 452 | LYS | CE-NZ | 10.77 | 1.75 | 1.49 |
| 1 | E | 141 | VAL | CB-CG2 | -10.76 | 1.30 | 1.52 |
| 1 | N | 370 | TYR | CD2-CE2 | -10.67 | 1.23 | 1.39 |
| 1 | I | 291 | TYR | CG-CD1 | -10.65 | 1.25 | 1.39 |
| 1 | C | 59 | LYS | CD-CE | 10.64 | 1.77 | 1.51 |
| 1 | D | 65 | VAL | CB-CG1 | -10.64 | 1.30 | 1.52 |
| 1 | I | 361 | LYS | CE-NZ | 10.61 | 1.75 | 1.49 |
| 1 | N | 28 | VAL | CB-CG1 | 10.57 | 1.75 | 1.52 |
| 1 | E | 269 | GLU | CD-OE1 | 10.56 | 1.37 | 1.25 |
| 1 | K | 62 | VAL | CB-CG2 | -10.56 | 1.30 | 1.52 |
| 1 | D | 380 | LYS | CD-CE | 10.54 | 1.77 | 1.51 |
| 1 | E | 100 | TRP | CB-CG | -10.54 | 1.31 | 1.50 |
| 1 | O | 41 | ARG | CZ-NH1 | 10.54 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 280 | SER | CB-OG | 10.54 | 1.55 | 1.42 |
| 1 | O | 256 | PHE | CB-CG | 10.53 | 1.69 | 1.51 |
| 1 | D | 201 | VAL | CB-CG1 | -10.53 | 1.30 | 1.52 |
| 1 | D | 115 | VAL | CB-CG1 | 10.52 | 1.75 | 1.52 |
| 1 | L | 105 | VAL | CB-CG1 | -10.49 | 1.30 | 1.52 |
| 1 | M | 356 | LYS | CE-NZ | 10.47 | 1.75 | 1.49 |
| 1 | I | 333 | VAL | CB-CG1 | -10.47 | 1.30 | 1.52 |
| 1 | D | 100 | TRP | CB-CG | -10.45 | 1.31 | 1.50 |
| 1 | D | 194 | VAL | CB-CG2 | 10.41 | 1.74 | 1.52 |
| 1 | C | 20 | ALA | CA-CB | 10.40 | 1.74 | 1.52 |
| 1 | D | 390 | TYR | CD1-CE1 | 10.40 | 1.54 | 1.39 |
| 1 | J | 206 | GLY | C-O | 10.39 | 1.40 | 1.23 |
| 1 | E | 130 | GLU | CB-CG | -10.39 | 1.32 | 1.52 |
| 1 | G | 316 | ALA | CA-CB | 10.38 | 1.74 | 1.52 |
| 1 | B | 355 | TYR | CD2-CE2 | 10.37 | 1.54 | 1.39 |
| 1 | M | 101 | ALA | CA-CB | -10.36 | 1.30 | 1.52 |
| 1 | H | 256 | PHE | CG-CD1 | -10.33 | 1.23 | 1.38 |
| 1 | H | 54 | LYS | CE-NZ | 10.32 | 1.74 | 1.49 |
| 1 | A | 334 | VAL | CB-CG1 | -10.31 | 1.31 | 1.52 |
| 1 | J | 116 | GLY | C-O | 10.31 | 1.40 | 1.23 |
| 1 | A | 320 | ASN | C-O | -10.30 | 1.03 | 1.23 |
| 1 | C | 207 | ALA | CA-CB | -10.29 | 1.30 | 1.52 |
| 1 | N | 27 | TYR | CD2-CE2 | 10.29 | 1.54 | 1.39 |
| 1 | C | 178 | VAL | CB-CG2 | 10.28 | 1.74 | 1.52 |
| 1 | A | 219 | GLU | CD-OE1 | 10.28 | 1.36 | 1.25 |
| 1 | M | 64 | LYS | CB-CG | 10.25 | 1.80 | 1.52 |
| 1 | M | 117 | ILE | CA-CB | -10.25 | 1.31 | 1.54 |
| 1 | N | 32 | ASN | CB-CG | 10.21 | 1.74 | 1.51 |
| 1 | E | 271 | VAL | CB-CG1 | 10.20 | 1.74 | 1.52 |
| 1 | L | 352 | GLU | CG-CD | 10.20 | 1.67 | 1.51 |
| 1 | J | 438 | GLU | CG-CD | 10.18 | 1.67 | 1.51 |
| 1 | F | 467 | LYS | CG-CD | 10.18 | 1.87 | 1.52 |
| 1 | O | 62 | VAL | CB-CG2 | 10.17 | 1.74 | 1.52 |
| 1 | I | 141 | VAL | CB-CG2 | -10.16 | 1.31 | 1.52 |
| 1 | K | 49 | TYR | CE1-CZ | -10.16 | 1.25 | 1.38 |
| 1 | B | 269 | GLU | CB-CG | 10.15 | 1.71 | 1.52 |
| 1 | G | 362 | GLU | CD-OE1 | 10.14 | 1.36 | 1.25 |
| 1 | F | 362 | GLU | CB-CG | 10.11 | 1.71 | 1.52 |
| 1 | N | 173 | SER | CB-OG | 10.09 | 1.55 | 1.42 |
| 1 | E | 173 | SER | CA-CB | 10.08 | 1.68 | 1.52 |
| 1 | H | 320 | ASN | C-O | -10.08 | 1.04 | 1.23 |
| 1 | N | 181 | GLN | CG-CD | 10.08 | 1.74 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 269 | GLU | CD-OE2 | 10.06 | 1.36 | 1.25 |
| 1 | H | 59 | LYS | CD-CE | 10.05 | 1.76 | 1.51 |
| 1 | H | 91 | TYR | CD2-CE2 | 10.05 | 1.54 | 1.39 |
| 1 | G | 467 | LYS | CE-NZ | 10.04 | 1.74 | 1.49 |
| 1 | D | 257 | VAL | CB-CG2 | 10.04 | 1.74 | 1.52 |
| 1 | G | 363 | TYR | CE1-CZ | 10.03 | 1.51 | 1.38 |
| 1 | A | 368 | GLU | CD-OE2 | 10.03 | 1.36 | 1.25 |
| 1 | I | 170 | GLY | N-CA | 10.03 | 1.61 | 1.46 |
| 1 | C | 369 | GLU | CD-OE2 | 10.03 | 1.36 | 1.25 |
| 1 | D | 20 | ALA | CA-CB | 10.02 | 1.73 | 1.52 |
| 1 | K | 368 | GLU | CD-OE1 | 10.02 | 1.36 | 1.25 |
| 1 | J | 453 | GLU | CD-OE1 | 10.01 | 1.36 | 1.25 |
| 1 | D | 402 | TRP | CB-CG | 10.00 | 1.68 | 1.50 |
| 1 | O | 230 | LYS | CE-NZ | 10.00 | 1.74 | 1.49 |
| 1 | M | 456 | SER | CB-OG | 9.99 | 1.55 | 1.42 |
| 1 | E | 27 | TYR | CD1-CE1 | 9.98 | 1.54 | 1.39 |
| 1 | C | 400 | GLU | CD-OE2 | 9.97 | 1.36 | 1.25 |
| 1 | A | 356 | LYS | CE-NZ | 9.96 | 1.74 | 1.49 |
| 1 | N | 354 | THR | C-O | 9.96 | 1.42 | 1.23 |
| 1 | I | 256 | PHE | CE2-CZ | -9.96 | 1.18 | 1.37 |
| 1 | D | 361 | LYS | CG-CD | 9.95 | 1.86 | 1.52 |
| 1 | G | 462 | PHE | CB-CG | -9.95 | 1.34 | 1.51 |
| 1 | H | 362 | GLU | CD-OE2 | 9.94 | 1.36 | 1.25 |
| 1 | L | 300 | VAL | CB-CG2 | -9.93 | 1.31 | 1.52 |
| 1 | H | 65 | VAL | CB-CG1 | -9.93 | 1.31 | 1.52 |
| 1 | H | 216 | ASN | C-O | 9.91 | 1.42 | 1.23 |
| 1 | I | 261 | PHE | CD1-CE1 | -9.91 | 1.19 | 1.39 |
| 1 | C | 137 | ALA | CA-CB | 9.91 | 1.73 | 1.52 |
| 1 | E | 352 | GLU | CD-OE2 | 9.90 | 1.36 | 1.25 |
| 1 | N | 453 | GLU | CG-CD | 9.90 | 1.66 | 1.51 |
| 1 | K | 472 | LEU | N-CA | 9.89 | 1.66 | 1.46 |
| 1 | O | 390 | TYR | CD1-CE1 | -9.89 | 1.24 | 1.39 |
| 1 | O | 99 | VAL | CB-CG1 | -9.88 | 1.32 | 1.52 |
| 1 | E | 22 | VAL | CB-CG1 | 9.87 | 1.73 | 1.52 |
| 1 | K | 175 | CYS | CB-SG | 9.86 | 1.99 | 1.82 |
| 1 | C | 316 | ALA | CA-CB | 9.86 | 1.73 | 1.52 |
| 1 | M | 343 | SER | CB-OG | 9.86 | 1.55 | 1.42 |
| 1 | H | 380 | LYS | CD-CE | 9.85 | 1.75 | 1.51 |
| 1 | C | 54 | LYS | CE-NZ | 9.82 | 1.73 | 1.49 |
| 1 | G | 173 | SER | CB-OG | 9.81 | 1.55 | 1.42 |
| 1 | H | 116 | GLY | C-O | 9.81 | 1.39 | 1.23 |
| 1 | D | 116 | GLY | C-O | 9.81 | 1.39 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 206 | GLY | C-O | 9.80 | 1.39 | 1.23 |
| 1 | E | 269 | GLU | CG-CD | 9.79 | 1.66 | 1.51 |
| 1 | K | 130 | GLU | CD-OE1 | 9.79 | 1.36 | 1.25 |
| 1 | B | 169 | TRP | CZ3-CH2 | -9.78 | 1.24 | 1.40 |
| 1 | H | 115 | VAL | CB-CG2 | -9.78 | 1.32 | 1.52 |
| 1 | I | 236 | LYS | CB-CG | 9.78 | 1.78 | 1.52 |
| 1 | J | 362 | GLU | CD-OE2 | 9.78 | 1.36 | 1.25 |
| 1 | I | 114 | GLY | N-CA | 9.77 | 1.60 | 1.46 |
| 1 | N | 73 | PHE | CE2-CZ | 9.76 | 1.55 | 1.37 |
| 1 | B | 70 | TYR | CG-CD1 | -9.75 | 1.26 | 1.39 |
| 1 | A | 370 | TYR | CE2-CZ | -9.75 | 1.25 | 1.38 |
| 1 | A | 115 | VAL | CB-CG2 | -9.75 | 1.32 | 1.52 |
| 1 | J | 249 | TYR | CD2-CE2 | 9.75 | 1.53 | 1.39 |
| 1 | M | 167 | GLU | CD-OE2 | 9.73 | 1.36 | 1.25 |
| 1 | F | 369 | GLU | CB-CG | 9.72 | 1.70 | 1.52 |
| 1 | H | 205 | PHE | CE2-CZ | 9.69 | 1.55 | 1.37 |
| 1 | C | 467 | LYS | CE-NZ | 9.69 | 1.73 | 1.49 |
| 1 | L | 280 | SER | CB-OG | 9.69 | 1.54 | 1.42 |
| 1 | I | 63 | PRO | C-O | 9.69 | 1.42 | 1.23 |
| 1 | A | 379 | CYS | CB-SG | -9.66 | 1.65 | 1.82 |
| 1 | D | 176 | THR | CA-CB | 9.66 | 1.78 | 1.53 |
| 1 | E | 34 | TYR | CG-CD2 | -9.65 | 1.26 | 1.39 |
| 1 | H | 181 | GLN | CG-CD | 9.65 | 1.73 | 1.51 |
| 1 | F | 70 | TYR | CB-CG | -9.65 | 1.37 | 1.51 |
| 1 | L | 114 | GLY | N-CA | 9.65 | 1.60 | 1.46 |
| 1 | L | 449 | VAL | CB-CG1 | -9.64 | 1.32 | 1.52 |
| 1 | L | 309 | LYS | CD-CE | 9.64 | 1.75 | 1.51 |
| 1 | F | 163 | PRO | C-O | 9.64 | 1.42 | 1.23 |
| 1 | G | 21 | VAL | CB-CG1 | 9.64 | 1.73 | 1.52 |
| 1 | O | 167 | GLU | CD-OE2 | 9.63 | 1.36 | 1.25 |
| 1 | B | 176 | THR | CB-CG2 | 9.61 | 1.84 | 1.52 |
| 1 | H | 179 | ALA | C-O | 9.60 | 1.41 | 1.23 |
| 1 | I | 217 | LYS | CE-NZ | 9.59 | 1.73 | 1.49 |
| 1 | N | 139 | ALA | CA-CB | 9.58 | 1.72 | 1.52 |
| 1 | N | 249 | TYR | CG-CD1 | -9.58 | 1.26 | 1.39 |
| 1 | N | 356 | LYS | CE-NZ | 9.58 | 1.73 | 1.49 |
| 1 | F | 138 | ASN | C-O | 9.57 | 1.41 | 1.23 |
| 1 | C | 363 | TYR | CD1-CE1 | 9.57 | 1.53 | 1.39 |
| 1 | D | 402 | TRP | C-O | 9.57 | 1.41 | 1.23 |
| 1 | B | 462 | PHE | CG-CD1 | -9.56 | 1.24 | 1.38 |
| 1 | C | 292 | PHE | CE1-CZ | -9.56 | 1.19 | 1.37 |
| 1 | N | 46 | GLY | C-O | 9.56 | 1.39 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 334 | VAL | CB-CG2 | 9.56 | 1.73 | 1.52 |
| 1 | L | 291 | TYR | CE1-CZ | -9.55 | 1.26 | 1.38 |
| 1 | K | 400 | GLU | CB-CG | 9.53 | 1.70 | 1.52 |
| 1 | C | 370 | TYR | CE1-CZ | 9.53 | 1.50 | 1.38 |
| 1 | D | 269 | GLU | CD-OE1 | -9.52 | 1.15 | 1.25 |
| 1 | F | 249 | TYR | CD1-CE1 | 9.52 | 1.53 | 1.39 |
| 1 | H | 130 | GLU | CB-CG | 9.51 | 1.70 | 1.52 |
| 1 | M | 157 | CYS | CB-SG | -9.51 | 1.66 | 1.82 |
| 1 | G | 438 | GLU | CG-CD | 9.51 | 1.66 | 1.51 |
| 1 | K | 28 | VAL | CB-CG2 | -9.50 | 1.32 | 1.52 |
| 1 | K | 114 | GLY | N-CA | 9.50 | 1.60 | 1.46 |
| 1 | A | 162 | LYS | CE-NZ | 9.50 | 1.72 | 1.49 |
| 1 | B | 21 | VAL | CB-CG1 | -9.50 | 1.32 | 1.52 |
| 1 | A | 242 | TYR | CZ-OH | -9.48 | 1.21 | 1.37 |
| 1 | G | 276 | TYR | CG-CD2 | 9.48 | 1.51 | 1.39 |
| 1 | D | 305 | GLN | CG-CD | 9.48 | 1.72 | 1.51 |
| 1 | D | 118 | SER | CB-OG | 9.47 | 1.54 | 1.42 |
| 1 | C | 457 | ALA | CA-CB | -9.46 | 1.32 | 1.52 |
| 1 | D | 253 | GLU | CD-OE2 | 9.46 | 1.36 | 1.25 |
| 1 | E | 40 | SER | CB-OG | 9.46 | 1.54 | 1.42 |
| 1 | E | 169 | TRP | CG-CD1 | 9.46 | 1.50 | 1.36 |
| 1 | D | 320 | ASN | C-O | -9.46 | 1.05 | 1.23 |
| 1 | O | 347 | ALA | CA-CB | 9.46 | 1.72 | 1.52 |
| 1 | N | 370 | TYR | CD1-CE1 | -9.45 | 1.25 | 1.39 |
| 1 | I | 199 | ASP | CG-OD2 | 9.45 | 1.47 | 1.25 |
| 1 | G | 276 | TYR | CD2-CE2 | -9.43 | 1.25 | 1.39 |
| 1 | O | 26 | GLU | CD-OE2 | 9.42 | 1.36 | 1.25 |
| 1 | M | 438 | GLU | CD-OE2 | 9.42 | 1.36 | 1.25 |
| 1 | A | 304 | ALA | CA-CB | -9.41 | 1.32 | 1.52 |
| 1 | E | 370 | TYR | CD2-CE2 | 9.41 | 1.53 | 1.39 |
| 1 | N | 282 | SER | CB-OG | 9.41 | 1.54 | 1.42 |
| 1 | N | 338 | ARG | CG-CD | 9.39 | 1.75 | 1.51 |
| 1 | B | 264 | ALA | CA-CB | 9.38 | 1.72 | 1.52 |
| 1 | J | 27 | TYR | CE1-CZ | 9.38 | 1.50 | 1.38 |
| 1 | A | 374 | PHE | CE1-CZ | -9.38 | 1.19 | 1.37 |
| 1 | H | 307 | PHE | CE2-CZ | -9.37 | 1.19 | 1.37 |
| 1 | B | 438 | GLU | CG-CD | 9.37 | 1.66 | 1.51 |
| 1 | B | 44 | ALA | CA-CB | 9.36 | 1.72 | 1.52 |
| 1 | H | 361 | LYS | CB-CG | 9.36 | 1.77 | 1.52 |
| 1 | D | 151 | TYR | CD2-CE2 | 9.35 | 1.53 | 1.39 |
| 1 | E | 227 | SER | CB-OG | 9.35 | 1.54 | 1.42 |
| 1 | G | 220 | VAL | CB-CG1 | 9.35 | 1.72 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | L | 276 | TYR | CD2-CE2 | -9.34 | 1.25 | 1.39 |
| 1 | H | 152 | LYS | CE-NZ | 9.34 | 1.72 | 1.49 |
| 1 | L | 35 | TYR | CG-CD1 | -9.33 | 1.27 | 1.39 |
| 1 | A | 264 | ALA | CA-CB | -9.33 | 1.32 | 1.52 |
| 1 | E | 30 | ARG | CZ-NH1 | 9.33 | 1.45 | 1.33 |
| 1 | B | 49 | TYR | CG-CD2 | 9.32 | 1.51 | 1.39 |
| 1 | L | 438 | GLU | CD-OE1 | 9.32 | 1.35 | 1.25 |
| 1 | O | 452 | LYS | CD-CE | 9.29 | 1.74 | 1.51 |
| 1 | M | 173 | SER | CB-OG | 9.29 | 1.54 | 1.42 |
| 1 | L | 272 | PRO | CB-CG | 9.28 | 1.96 | 1.50 |
| 1 | J | 453 | GLU | CD-OE2 | 9.27 | 1.35 | 1.25 |
| 1 | D | 73 | PHE | CB-CG | -9.27 | 1.35 | 1.51 |
| 1 | N | 346 | ALA | CA-CB | 9.27 | 1.72 | 1.52 |
| 1 | A | 368 | GLU | CD-OE1 | 9.27 | 1.35 | 1.25 |
| 1 | L | 166 | GLY | N-CA | -9.26 | 1.32 | 1.46 |
| 1 | D | 297 | GLY | C-O | 9.25 | 1.38 | 1.23 |
| 1 | B | 292 | PHE | CE1-CZ | -9.24 | 1.19 | 1.37 |
| 1 | J | 179 | ALA | CA-CB | 9.23 | 1.71 | 1.52 |
| 1 | O | 173 | SER | CA-CB | 9.22 | 1.66 | 1.52 |
| 1 | D | 177 | GLN | C-O | 9.22 | 1.40 | 1.23 |
| 1 | F | 194 | VAL | CB-CG1 | 9.22 | 1.72 | 1.52 |
| 1 | G | 35 | TYR | CD1-CE1 | -9.20 | 1.25 | 1.39 |
| 1 | M | 62 | VAL | CB-CG1 | 9.19 | 1.72 | 1.52 |
| 1 | F | 352 | GLU | CD-OE1 | 9.19 | 1.35 | 1.25 |
| 1 | K | 107 | VAL | C-O | -9.17 | 1.05 | 1.23 |
| 1 | C | 248 | PHE | CE2-CZ | 9.17 | 1.54 | 1.37 |
| 1 | I | 175 | CYS | CB-SG | 9.16 | 1.97 | 1.82 |
| 1 | K | 30 | ARG | CG-CD | 9.16 | 1.74 | 1.51 |
| 1 | E | 178 | VAL | C-O | 9.16 | 1.40 | 1.23 |
| 1 | J | 96 | GLN | CA-C | 9.16 | 1.76 | 1.52 |
| 1 | D | 449 | VAL | CB-CG1 | -9.15 | 1.33 | 1.52 |
| 1 | C | 269 | GLU | CG-CD | 9.15 | 1.65 | 1.51 |
| 1 | G | 248 | PHE | CE2-CZ | 9.15 | 1.54 | 1.37 |
| 1 | J | 103 | VAL | CB-CG2 | 9.15 | 1.72 | 1.52 |
| 1 | D | 355 | TYR | CG-CD1 | -9.14 | 1.27 | 1.39 |
| 1 | G | 216 | ASN | CG-OD1 | 9.14 | 1.44 | 1.24 |
| 1 | G | 40 | SER | CB-OG | 9.14 | 1.54 | 1.42 |
| 1 | L | 462 | PHE | CB-CG | -9.14 | 1.35 | 1.51 |
| 1 | I | 72 | VAL | CB-CG1 | -9.14 | 1.33 | 1.52 |
| 1 | E | 269 | GLU | CD-OE2 | 9.12 | 1.35 | 1.25 |
| 1 | G | 180 | VAL | C-O | 9.12 | 1.40 | 1.23 |
| 1 | I | 89 | SER | CB-OG | 9.11 | 1.54 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 376 | PHE | CG-CD2 | 9.11 | 1.52 | 1.38 |
| 1 | O | 210 | PHE | CD2-CE2 | -9.10 | 1.21 | 1.39 |
| 1 | G | 73 | PHE | CE2-CZ | 9.09 | 1.54 | 1.37 |
| 1 | A | 133 | SER | CB-OG | 9.09 | 1.54 | 1.42 |
| 1 | H | 443 | LYS | CD-CE | 9.09 | 1.74 | 1.51 |
| 1 | J | 368 | GLU | CD-OE1 | 9.08 | 1.35 | 1.25 |
| 1 | I | 151 | TYR | CZ-OH | -9.07 | 1.22 | 1.37 |
| 1 | H | 26 | GLU | CG-CD | 9.07 | 1.65 | 1.51 |
| 1 | G | 138 | ASN | C-O | 9.05 | 1.40 | 1.23 |
| 1 | O | 172 | GLY | C-O | 9.04 | 1.38 | 1.23 |
| 1 | C | 453 | GLU | CG-CD | 9.03 | 1.65 | 1.51 |
| 1 | B | 70 | TYR | CE2-CZ | -9.03 | 1.26 | 1.38 |
| 1 | C | 330 | PHE | CE1-CZ | 9.03 | 1.54 | 1.37 |
| 1 | D | 438 | GLU | CG-CD | 9.03 | 1.65 | 1.51 |
| 1 | J | 356 | LYS | C-O | -9.02 | 1.06 | 1.23 |
| 1 | J | 454 | LYS | CE-NZ | 9.02 | 1.71 | 1.49 |
| 1 | C | 21 | VAL | CB-CG1 | -9.02 | 1.33 | 1.52 |
| 1 | F | 438 | GLU | CD-OE1 | 9.01 | 1.35 | 1.25 |
| 1 | C | 269 | GLU | CB-CG | 9.01 | 1.69 | 1.52 |
| 1 | K | 360 | PHE | CE1-CZ | -9.01 | 1.20 | 1.37 |
| 1 | B | 178 | VAL | CB-CG1 | 9.00 | 1.71 | 1.52 |
| 1 | B | 70 | TYR | CB-CG | -9.00 | 1.38 | 1.51 |
| 1 | C | 232 | PRO | CG-CD | -9.00 | 1.21 | 1.50 |
| 1 | I | 178 | VAL | CA-CB | 9.00 | 1.73 | 1.54 |
| 1 | D | 356 | LYS | CE-NZ | 8.99 | 1.71 | 1.49 |
| 1 | I | 240 | GLU | CD-OE1 | 8.99 | 1.35 | 1.25 |
| 1 | H | 151 | TYR | CD2-CE2 | 8.98 | 1.52 | 1.39 |
| 1 | M | 280 | SER | CB-OG | 8.98 | 1.53 | 1.42 |
| 1 | A | 438 | GLU | CD-OE2 | 8.98 | 1.35 | 1.25 |
| 1 | C | 106 | GLU | CD-OE2 | 8.97 | 1.35 | 1.25 |
| 1 | I | 292 | PHE | CE2-CZ | 8.97 | 1.54 | 1.37 |
| 1 | M | 349 | SER | CB-OG | 8.96 | 1.53 | 1.42 |
| 1 | C | 196 | GLN | C-O | -8.96 | 1.06 | 1.23 |
| 1 | F | 390 | TYR | CE1-CZ | 8.95 | 1.50 | 1.38 |
| 1 | N | 106 | GLU | CD-OE2 | 8.95 | 1.35 | 1.25 |
| 1 | F | 448 | GLU | CG-CD | 8.95 | 1.65 | 1.51 |
| 1 | L | 37 | ALA | CA-CB | -8.95 | 1.33 | 1.52 |
| 1 | N | 152 | LYS | CE-NZ | -8.95 | 1.26 | 1.49 |
| 1 | D | 325 | TRP | CE3-CZ3 | 8.94 | 1.53 | 1.38 |
| 1 | G | 300 | VAL | CB-CG2 | -8.94 | 1.34 | 1.52 |
| 1 | I | 294 | THR | CB-CG2 | -8.94 | 1.22 | 1.52 |
| 1 | D | 64 | LYS | CB-CG | 8.93 | 1.76 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 113 | LEU | C-O | 8.93 | 1.40 | 1.23 |
| 1 | L | 471 | GLN | CB-CG | -8.93 | 1.28 | 1.52 |
| 1 | D | 454 | LYS | CE-NZ | 8.92 | 1.71 | 1.49 |
| 1 | M | 249 | TYR | CD2-CE2 | 8.91 | 1.52 | 1.39 |
| 1 | C | 396 | SER | CB-OG | 8.91 | 1.53 | 1.42 |
| 1 | A | 449 | VAL | CB-CG2 | -8.90 | 1.34 | 1.52 |
| 1 | O | 444 | TYR | CD2-CE2 | 8.90 | 1.52 | 1.39 |
| 1 | M | 73 | PHE | CE2-CZ | -8.90 | 1.20 | 1.37 |
| 1 | I | 261 | PHE | CE1-CZ | -8.89 | 1.20 | 1.37 |
| 1 | D | 73 | PHE | CG-CD1 | -8.88 | 1.25 | 1.38 |
| 1 | E | 83 | PHE | CG-CD1 | 8.88 | 1.52 | 1.38 |
| 1 | G | 22 | VAL | CA-CB | -8.88 | 1.36 | 1.54 |
| 1 | G | 249 | TYR | CD2-CE2 | 8.87 | 1.52 | 1.39 |
| 1 | J | 331 | VAL | CB-CG2 | -8.87 | 1.34 | 1.52 |
| 1 | I | 361 | LYS | CD-CE | 8.87 | 1.73 | 1.51 |
| 1 | G | 292 | PHE | CE2-CZ | -8.86 | 1.20 | 1.37 |
| 1 | D | 188 | LEU | C-O | -8.86 | 1.06 | 1.23 |
| 1 | K | 362 | GLU | CB-CG | -8.85 | 1.35 | 1.52 |
| 1 | M | 291 | TYR | CD1-CE1 | -8.85 | 1.26 | 1.39 |
| 1 | B | 132 | ALA | CA-CB | -8.84 | 1.33 | 1.52 |
| 1 | D | 66 | SER | CB-OG | 8.84 | 1.53 | 1.42 |
| 1 | G | 207 | ALA | CA-CB | -8.84 | 1.33 | 1.52 |
| 1 | O | 177 | GLN | CG-CD | 8.84 | 1.71 | 1.51 |
| 1 | K | 370 | TYR | CG-CD2 | -8.84 | 1.27 | 1.39 |
| 1 | I | 444 | TYR | CD1-CE1 | 8.83 | 1.52 | 1.39 |
| 1 | N | 169 | TRP | CB-CG | -8.82 | 1.34 | 1.50 |
| 1 | L | 139 | ALA | CA-CB | 8.82 | 1.71 | 1.52 |
| 1 | O | 72 | VAL | CB-CG1 | -8.82 | 1.34 | 1.52 |
| 1 | A | 63 | PRO | C-O | 8.80 | 1.40 | 1.23 |
| 1 | G | 256 | PHE | CE2-CZ | -8.80 | 1.20 | 1.37 |
| 1 | D | 370 | TYR | CE2-CZ | -8.79 | 1.27 | 1.38 |
| 1 | A | 26 | GLU | CG-CD | 8.79 | 1.65 | 1.51 |
| 1 | F | 220 | VAL | C-O | -8.79 | 1.06 | 1.23 |
| 1 | L | 456 | SER | CB-OG | 8.79 | 1.53 | 1.42 |
| 1 | K | 100 | TRP | CG-CD1 | -8.78 | 1.24 | 1.36 |
| 1 | L | 152 | LYS | CE-NZ | 8.77 | 1.71 | 1.49 |
| 1 | L | 201 | VAL | CB-CG2 | -8.77 | 1.34 | 1.52 |
| 1 | N | 472 | LEU | N-CA | 8.77 | 1.63 | 1.46 |
| 1 | A | 161 | CYS | C-O | 8.76 | 1.40 | 1.23 |
| 1 | H | 376 | PHE | CD2-CE2 | -8.75 | 1.21 | 1.39 |
| 1 | A | 249 | TYR | CZ-OH | 8.75 | 1.52 | 1.37 |
| 1 | C | 300 | VAL | CB-CG2 | -8.75 | 1.34 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 70 | TYR | CG-CD2 | -8.75 | 1.27 | 1.39 |
| 1 | C | 471 | GLN | C-O | 8.75 | 1.40 | 1.23 |
| 1 | D | 307 | PHE | CG-CD1 | -8.75 | 1.25 | 1.38 |
| 1 | E | 368 | GLU | CD-OE2 | 8.75 | 1.35 | 1.25 |
| 1 | N | 317 | GLN | CG-CD | 8.75 | 1.71 | 1.51 |
| 1 | G | 64 | LYS | C-O | 8.74 | 1.40 | 1.23 |
| 1 | H | 370 | TYR | CB-CG | -8.74 | 1.38 | 1.51 |
| 1 | L | 178 | VAL | CB-CG2 | 8.74 | 1.71 | 1.52 |
| 1 | N | 157 | CYS | CB-SG | -8.74 | 1.67 | 1.82 |
| 1 | N | 363 | TYR | CD2-CE2 | 8.74 | 1.52 | 1.39 |
| 1 | E | 352 | GLU | CD-OE1 | 8.73 | 1.35 | 1.25 |
| 1 | I | 210 | PHE | CE1-CZ | 8.73 | 1.53 | 1.37 |
| 1 | B | 472 | LEU | N-CA | 8.73 | 1.63 | 1.46 |
| 1 | F | 376 | PHE | CD2-CE2 | -8.73 | 1.21 | 1.39 |
| 1 | A | 152 | LYS | CE-NZ | 8.72 | 1.70 | 1.49 |
| 1 | C | 464 | LEU | CG-CD1 | 8.72 | 1.84 | 1.51 |
| 1 | D | 206 | GLY | C-O | 8.72 | 1.37 | 1.23 |
| 1 | F | 253 | GLU | CD-OE2 | 8.72 | 1.35 | 1.25 |
| 1 | J | 438 | GLU | CD-OE2 | 8.71 | 1.35 | 1.25 |
| 1 | L | 70 | TYR | CG-CD1 | -8.71 | 1.27 | 1.39 |
| 1 | N | 26 | GLU | CB-CG | -8.71 | 1.35 | 1.52 |
| 1 | F | 32 | ASN | CB-CG | 8.70 | 1.71 | 1.51 |
| 1 | F | 103 | VAL | CB-CG2 | 8.69 | 1.71 | 1.52 |
| 1 | J | 92 | ASN | CB-CG | 8.68 | 1.71 | 1.51 |
| 1 | K | 231 | TYR | CD1-CE1 | 8.68 | 1.52 | 1.39 |
| 1 | J | 264 | ALA | CA-CB | -8.67 | 1.34 | 1.52 |
| 1 | M | 291 | TYR | CE1-CZ | -8.66 | 1.27 | 1.38 |
| 1 | A | 296 | SER | CB-OG | 8.66 | 1.53 | 1.42 |
| 1 | B | 49 | TYR | CE2-CZ | -8.65 | 1.27 | 1.38 |
| 1 | B | 347 | ALA | C-O | 8.65 | 1.39 | 1.23 |
| 1 | G | 180 | VAL | CB-CG2 | 8.63 | 1.71 | 1.52 |
| 1 | K | 294 | THR | CB-CG2 | -8.62 | 1.23 | 1.52 |
| 1 | C | 374 | PHE | CG-CD1 | 8.62 | 1.51 | 1.38 |
| 1 | D | 152 | LYS | CE-NZ | 8.61 | 1.70 | 1.49 |
| 1 | B | 256 | PHE | CG-CD2 | 8.61 | 1.51 | 1.38 |
| 1 | L | 361 | LYS | CE-NZ | 8.60 | 1.70 | 1.49 |
| 1 | O | 352 | GLU | CD-OE2 | 8.59 | 1.35 | 1.25 |
| 1 | B | 123 | LEU | CG-CD2 | 8.59 | 1.83 | 1.51 |
| 1 | E | 176 | THR | C-O | 8.59 | 1.39 | 1.23 |
| 1 | A | 64 | LYS | CB-CG | 8.58 | 1.75 | 1.52 |
| 1 | D | 159 | ILE | CA-CB | -8.58 | 1.35 | 1.54 |
| 1 | L | 349 | SER | CB-OG | 8.58 | 1.53 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 40 | SER | CB-OG | 8.57 | 1.53 | 1.42 |
| 1 | N | 293 | PRO | CA-CB | -8.57 | 1.36 | 1.53 |
| 1 | L | 234 | TYR | CG-CD2 | 8.57 | 1.50 | 1.39 |
| 1 | O | 217 | LYS | CE-NZ | 8.56 | 1.70 | 1.49 |
| 1 | A | 205 | PHE | CE1-CZ | -8.56 | 1.21 | 1.37 |
| 1 | L | 103 | VAL | CB-CG2 | -8.56 | 1.34 | 1.52 |
| 1 | C | 441 | LEU | CG-CD2 | 8.55 | 1.83 | 1.51 |
| 1 | E | 172 | GLY | C-O | 8.55 | 1.37 | 1.23 |
| 1 | E | 269 | GLU | CB-CG | 8.55 | 1.68 | 1.52 |
| 1 | H | 231 | TYR | CE2-CZ | 8.55 | 1.49 | 1.38 |
| 1 | G | 374 | PHE | CE2-CZ | 8.54 | 1.53 | 1.37 |
| 1 | L | 275 | LEU | CG-CD2 | 8.54 | 1.83 | 1.51 |
| 1 | C | 360 | PHE | CE2-CZ | -8.54 | 1.21 | 1.37 |
| 1 | A | 380 | LYS | CD-CE | 8.54 | 1.72 | 1.51 |
| 1 | D | 225 | CYS | CB-SG | 8.54 | 1.96 | 1.82 |
| 1 | I | 194 | VAL | CB-CG1 | 8.54 | 1.70 | 1.52 |
| 1 | A | 278 | LYS | CE-NZ | 8.53 | 1.70 | 1.49 |
| 1 | G | 151 | TYR | CD2-CE2 | 8.53 | 1.52 | 1.39 |
| 1 | D | 285 | ASN | C-O | 8.53 | 1.39 | 1.23 |
| 1 | L | 155 | GLN | CB-CG | -8.52 | 1.29 | 1.52 |
| 1 | I | 37 | ALA | CA-CB | 8.52 | 1.70 | 1.52 |
| 1 | K | 70 | TYR | CE2-CZ | -8.52 | 1.27 | 1.38 |
| 1 | J | 330 | PHE | CE1-CZ | 8.51 | 1.53 | 1.37 |
| 1 | L | 379 | CYS | CB-SG | -8.51 | 1.67 | 1.82 |
| 1 | A | 43 | LEU | C-O | -8.51 | 1.07 | 1.23 |
| 1 | A | 311 | TYR | CD1-CE1 | 8.51 | 1.52 | 1.39 |
| 1 | B | 362 | GLU | CB-CG | 8.51 | 1.68 | 1.52 |
| 1 | I | 27 | TYR | CG-CD2 | 8.51 | 1.50 | 1.39 |
| 1 | J | 62 | VAL | CB-CG1 | -8.51 | 1.34 | 1.52 |
| 1 | C | 291 | TYR | CG-CD1 | -8.51 | 1.28 | 1.39 |
| 1 | B | 300 | VAL | CB-CG1 | 8.50 | 1.70 | 1.52 |
| 1 | J | 315 | ARG | CZ-NH2 | 8.50 | 1.44 | 1.33 |
| 1 | F | 197 | ASP | C-O | -8.49 | 1.07 | 1.23 |
| 1 | G | 362 | GLU | C-O | 8.48 | 1.39 | 1.23 |
| 1 | L | 315 | ARG | CG-CD | 8.48 | 1.73 | 1.51 |
| 1 | K | 205 | PHE | CE1-CZ | -8.48 | 1.21 | 1.37 |
| 1 | C | 51 | PRO | CB-CG | 8.47 | 1.92 | 1.50 |
| 1 | D | 53 | LYS | CB-CG | 8.47 | 1.75 | 1.52 |
| 1 | G | 102 | CYS | CB-SG | 8.47 | 1.96 | 1.82 |
| 1 | E | 173 | SER | CB-OG | 8.47 | 1.53 | 1.42 |
| 1 | L | 35 | TYR | CB-CG | -8.46 | 1.39 | 1.51 |
| 1 | O | 256 | PHE | CE1-CZ | -8.46 | 1.21 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 263 | ARG | CZ-NH2 | -8.46 | 1.22 | 1.33 |
| 1 | G | 240 | GLU | CD-OE1 | 8.46 | 1.34 | 1.25 |
| 1 | K | 47 | HIS | C-O | -8.45 | 1.07 | 1.23 |
| 1 | G | 330 | PHE | CG-CD2 | 8.45 | 1.51 | 1.38 |
| 1 | H | 180 | VAL | CB-CG2 | 8.45 | 1.70 | 1.52 |
| 1 | L | 291 | TYR | CD1-CE1 | -8.45 | 1.26 | 1.39 |
| 1 | H | 400 | GLU | CD-OE2 | 8.45 | 1.34 | 1.25 |
| 1 | M | 287 | ALA | CA-CB | 8.45 | 1.70 | 1.52 |
| 1 | L | 241 | PRO | CB-CG | 8.44 | 1.92 | 1.50 |
| 1 | C | 161 | CYS | CB-SG | -8.44 | 1.67 | 1.82 |
| 1 | C | 115 | VAL | C-O | 8.44 | 1.39 | 1.23 |
| 1 | G | 369 | GLU | CD-OE2 | 8.44 | 1.34 | 1.25 |
| 1 | M | 455 | PHE | CB-CG | -8.43 | 1.37 | 1.51 |
| 1 | E | 209 | ASP | C-O | 8.42 | 1.39 | 1.23 |
| 1 | N | 387 | VAL | CB-CG1 | 8.42 | 1.70 | 1.52 |
| 1 | B | 442 | LYS | CD-CE | 8.42 | 1.72 | 1.51 |
| 1 | I | 249 | TYR | CD2-CE2 | 8.42 | 1.51 | 1.39 |
| 1 | I | 330 | PHE | CG-CD2 | 8.41 | 1.51 | 1.38 |
| 1 | E | 291 | TYR | CG-CD2 | -8.41 | 1.28 | 1.39 |
| 1 | F | 204 | GLY | C-O | -8.41 | 1.10 | 1.23 |
| 1 | L | 352 | GLU | CD-OE1 | 8.41 | 1.34 | 1.25 |
| 1 | J | 88 | THR | CB-CG2 | 8.41 | 1.80 | 1.52 |
| 1 | K | 472 | LEU | C-OXT | 8.41 | 1.39 | 1.23 |
| 1 | J | 171 | LYS | C-O | 8.40 | 1.39 | 1.23 |
| 1 | B | 133 | SER | CB-OG | 8.40 | 1.53 | 1.42 |
| 1 | N | 186 | PRO | C-O | -8.40 | 1.06 | 1.23 |
| 1 | E | 72 | VAL | CB-CG2 | -8.39 | 1.35 | 1.52 |
| 1 | N | 83 | PHE | CD1-CE1 | 8.39 | 1.56 | 1.39 |
| 1 | N | 87 | ASP | CG-OD2 | 8.39 | 1.44 | 1.25 |
| 1 | B | 83 | PHE | C-O | 8.39 | 1.39 | 1.23 |
| 1 | F | 206 | GLY | C-O | 8.38 | 1.37 | 1.23 |
| 1 | K | 360 | PHE | CG-CD1 | -8.38 | 1.26 | 1.38 |
| 1 | D | 282 | SER | CB-OG | 8.37 | 1.53 | 1.42 |
| 1 | I | 46 | GLY | C-O | 8.38 | 1.37 | 1.23 |
| 1 | F | 49 | TYR | C-O | 8.37 | 1.39 | 1.23 |
| 1 | D | 347 | ALA | C-O | 8.37 | 1.39 | 1.23 |
| 1 | J | 231 | TYR | CD1-CE1 | 8.37 | 1.51 | 1.39 |
| 1 | L | 263 | ARG | CZ-NH2 | -8.37 | 1.22 | 1.33 |
| 1 | M | 390 | TYR | CD1-CE1 | -8.37 | 1.26 | 1.39 |
| 1 | B | 82 | LYS | CB-CG | 8.36 | 1.75 | 1.52 |
| 1 | H | 161 | CYS | CB-SG | 8.36 | 1.96 | 1.82 |
| 1 | L | 374 | PHE | CD1-CE1 | 8.36 | 1.55 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 309 | LYS | CD-CE | 8.36 | 1.72 | 1.51 |
| 1 | N | 54 | LYS | CD-CE | 8.36 | 1.72 | 1.51 |
| 1 | D | 374 | PHE | CE1-CZ | 8.35 | 1.53 | 1.37 |
| 1 | L | 267 | VAL | CA-CB | -8.35 | 1.37 | 1.54 |
| 1 | E | 276 | TYR | CE1-CZ | -8.34 | 1.27 | 1.38 |
| 1 | N | 247 | PHE | CE1-CZ | 8.33 | 1.53 | 1.37 |
| 1 | C | 20 | ALA | N-CA | 8.33 | 1.63 | 1.46 |
| 1 | N | 112 | PRO | CG-CD | 8.32 | 1.78 | 1.50 |
| 1 | O | 333 | VAL | C-O | 8.32 | 1.39 | 1.23 |
| 1 | C | 194 | VAL | CB-CG2 | 8.32 | 1.70 | 1.52 |
| 1 | F | 50 | PHE | CD1-CE1 | -8.32 | 1.22 | 1.39 |
| 1 | J | 379 | CYS | CB-SG | -8.32 | 1.68 | 1.82 |
| 1 | O | 219 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | C | 467 | LYS | CG-CD | 8.31 | 1.80 | 1.52 |
| 1 | D | 291 | TYR | CD2-CE2 | 8.31 | 1.51 | 1.39 |
| 1 | I | 471 | GLN | CG-CD | 8.31 | 1.70 | 1.51 |
| 1 | F | 442 | LYS | CD-CE | 8.31 | 1.72 | 1.51 |
| 1 | D | 169 | TRP | CE3-CZ3 | -8.31 | 1.24 | 1.38 |
| 1 | H | 374 | PHE | CE2-CZ | 8.30 | 1.53 | 1.37 |
| 1 | J | 368 | GLU | CD-OE2 | 8.30 | 1.34 | 1.25 |
| 1 | H | 27 | TYR | CD2-CE2 | 8.30 | 1.51 | 1.39 |
| 1 | B | 284 | ALA | CA-CB | -8.29 | 1.35 | 1.52 |
| 1 | E | 116 | GLY | C-O | 8.29 | 1.36 | 1.23 |
| 1 | A | 472 | LEU | N-CA | 8.29 | 1.62 | 1.46 |
| 1 | J | 157 | CYS | CB-SG | -8.29 | 1.68 | 1.82 |
| 1 | C | 238 | VAL | CB-CG1 | -8.27 | 1.35 | 1.52 |
| 1 | I | 217 | LYS | CD-CE | 8.27 | 1.72 | 1.51 |
| 1 | G | 442 | LYS | CE-NZ | 8.26 | 1.69 | 1.49 |
| 1 | J | 369 | GLU | CB-CG | 8.26 | 1.67 | 1.52 |
| 1 | K | 231 | TYR | CD2-CE2 | 8.26 | 1.51 | 1.39 |
| 1 | L | 26 | GLU | CD-OE2 | 8.26 | 1.34 | 1.25 |
| 1 | D | 312 | TRP | CG-CD1 | -8.26 | 1.25 | 1.36 |
| 1 | N | 123 | LEU | CG-CD2 | 8.26 | 1.82 | 1.51 |
| 1 | M | 370 | TYR | CB-CG | -8.25 | 1.39 | 1.51 |
| 1 | F | 70 | TYR | CE2-CZ | -8.25 | 1.27 | 1.38 |
| 1 | D | 167 | GLU | CG-CD | -8.24 | 1.39 | 1.51 |
| 1 | L | 132 | ALA | CA-CB | -8.24 | 1.35 | 1.52 |
| 1 | K | 278 | LYS | C-O | 8.23 | 1.39 | 1.23 |
| 1 | L | 26 | GLU | CD-OE1 | 8.23 | 1.34 | 1.25 |
| 1 | E | 438 | GLU | CD-OE2 | 8.23 | 1.34 | 1.25 |
| 1 | B | 390 | TYR | CG-CD1 | 8.22 | 1.49 | 1.39 |
| 1 | C | 387 | VAL | CB-CG2 | 8.22 | 1.70 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 276 | TYR | CD2-CE2 | 8.22 | 1.51 | 1.39 |
| 1 | C | 167 | GLU | CG-CD | 8.22 | 1.64 | 1.51 |
| 1 | G | 333 | VAL | C-O | 8.21 | 1.39 | 1.23 |
| 1 | E | 103 | VAL | CB-CG1 | -8.21 | 1.35 | 1.52 |
| 1 | K | 20 | ALA | CA-CB | 8.20 | 1.69 | 1.52 |
| 1 | C | 70 | TYR | CG-CD2 | -8.19 | 1.28 | 1.39 |
| 1 | H | 237 | MET | CG-SD | 8.19 | 2.02 | 1.81 |
| 1 | M | 49 | TYR | CG-CD1 | -8.19 | 1.28 | 1.39 |
| 1 | I | 346 | ALA | CA-CB | 8.18 | 1.69 | 1.52 |
| 1 | C | 362 | GLU | C-O | 8.18 | 1.38 | 1.23 |
| 1 | M | 207 | ALA | CA-CB | -8.18 | 1.35 | 1.52 |
| 1 | C | 362 | GLU | CG-CD | -8.18 | 1.39 | 1.51 |
| 1 | I | 276 | TYR | CE1-CZ | -8.18 | 1.27 | 1.38 |
| 1 | L | 231 | TYR | CD1-CE1 | 8.18 | 1.51 | 1.39 |
| 1 | D | 276 | TYR | CG-CD2 | -8.18 | 1.28 | 1.39 |
| 1 | O | 100 | TRP | CZ3-CH2 | 8.17 | 1.53 | 1.40 |
| 1 | E | 438 | GLU | CB-CG | 8.17 | 1.67 | 1.52 |
| 1 | O | 234 | TYR | CE2-CZ | -8.17 | 1.27 | 1.38 |
| 1 | C | 355 | TYR | CD2-CE2 | -8.17 | 1.27 | 1.39 |
| 1 | B | 380 | LYS | CD-CE | 8.16 | 1.71 | 1.51 |
| 1 | E | 239 | SER | CB-OG | 8.16 | 1.52 | 1.42 |
| 1 | G | 77 | LEU | C-O | 8.16 | 1.38 | 1.23 |
| 1 | I | 113 | LEU | C-O | 8.16 | 1.38 | 1.23 |
| 1 | F | 256 | PHE | CG-CD2 | 8.15 | 1.50 | 1.38 |
| 1 | C | 56 | ASN | CB-CG | 8.15 | 1.69 | 1.51 |
| 1 | C | 64 | LYS | CD-CE | 8.15 | 1.71 | 1.51 |
| 1 | D | 46 | GLY | C-O | 8.15 | 1.36 | 1.23 |
| 1 | H | 219 | GLU | CB-CG | 8.15 | 1.67 | 1.52 |
| 1 | N | 70 | TYR | CG-CD1 | -8.14 | 1.28 | 1.39 |
| 1 | D | 159 | ILE | CB-CG2 | -8.13 | 1.27 | 1.52 |
| 1 | O | 72 | VAL | CB-CG2 | -8.13 | 1.35 | 1.52 |
| 1 | O | 460 | ASP | CB-CG | 8.13 | 1.68 | 1.51 |
| 1 | H | 144 | ARG | CD-NE | -8.13 | 1.32 | 1.46 |
| 1 | I | 63 | PRO | N-CD | 8.12 | 1.59 | 1.47 |
| 1 | J | 462 | PHE | CG-CD2 | -8.12 | 1.26 | 1.38 |
| 1 | I | 234 | TYR | CE2-CZ | -8.12 | 1.28 | 1.38 |
| 1 | M | 257 | VAL | CB-CG2 | 8.12 | 1.69 | 1.52 |
| 1 | C | 349 | SER | CB-OG | 8.11 | 1.52 | 1.42 |
| 1 | L | 247 | PHE | CG-CD1 | -8.11 | 1.26 | 1.38 |
| 1 | H | 173 | SER | CA-CB | 8.11 | 1.65 | 1.52 |
| 1 | I | 138 | ASN | C-O | 8.11 | 1.38 | 1.23 |
| 1 | B | 245 | SER | CB-OG | 8.10 | 1.52 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 90 | PHE | CE1-CZ | 8.10 | 1.52 | 1.37 |
| 1 | N | 444 | TYR | CD1-CE1 | 8.10 | 1.51 | 1.39 |
| 1 | A | 276 | TYR | CE2-CZ | 8.09 | 1.49 | 1.38 |
| 1 | A | 454 | LYS | CE-NZ | 8.09 | 1.69 | 1.49 |
| 1 | F | 384 | THR | N-CA | 8.09 | 1.62 | 1.46 |
| 1 | G | 151 | TYR | CD1-CE1 | 8.09 | 1.51 | 1.39 |
| 1 | O | 325 | TRP | CZ3-CH2 | 8.09 | 1.52 | 1.40 |
| 1 | K | 387 | VAL | CB-CG1 | 8.09 | 1.69 | 1.52 |
| 1 | G | 227 | SER | C-O | 8.09 | 1.38 | 1.23 |
| 1 | N | 73 | PHE | CB-CG | -8.09 | 1.37 | 1.51 |
| 1 | O | 179 | ALA | C-O | 8.09 | 1.38 | 1.23 |
| 1 | B | 110 | GLY | C-O | 8.08 | 1.36 | 1.23 |
| 1 | D | 138 | ASN | CG-ND2 | 8.08 | 1.53 | 1.32 |
| 1 | K | 139 | ALA | CA-CB | 8.08 | 1.69 | 1.52 |
| 1 | F | 34 | TYR | CD2-CE2 | -8.08 | 1.27 | 1.39 |
| 1 | I | 291 | TYR | CD1-CE1 | -8.08 | 1.27 | 1.39 |
| 1 | H | 224 | ILE | CB-CG2 | -8.07 | 1.27 | 1.52 |
| 1 | A | 347 | ALA | CA-CB | 8.07 | 1.69 | 1.52 |
| 1 | A | 70 | TYR | CE2-CZ | -8.07 | 1.28 | 1.38 |
| 1 | M | 72 | VAL | C-O | -8.07 | 1.08 | 1.23 |
| 1 | F | 164 | PRO | CG-CD | -8.07 | 1.24 | 1.50 |
| 1 | A | 468 | PHE | CG-CD1 | -8.06 | 1.26 | 1.38 |
| 1 | J | 352 | GLU | CD-OE2 | 8.06 | 1.34 | 1.25 |
| 1 | G | 309 | LYS | CE-NZ | 8.06 | 1.69 | 1.49 |
| 1 | H | 205 | PHE | CD1-CE1 | 8.06 | 1.55 | 1.39 |
| 1 | L | 318 | GLY | C-O | -8.06 | 1.10 | 1.23 |
| 1 | F | 471 | GLN | CG-CD | 8.06 | 1.69 | 1.51 |
| 1 | G | 32 | ASN | CB-CG | 8.06 | 1.69 | 1.51 |
| 1 | M | 276 | TYR | CE1-CZ | -8.06 | 1.28 | 1.38 |
| 1 | L | 169 | TRP | CD2-CE2 | -8.05 | 1.31 | 1.41 |
| 1 | C | 265 | GLY | C-O | 8.05 | 1.36 | 1.23 |
| 1 | C | 185 | CYS | CB-SG | 8.04 | 1.96 | 1.82 |
| 1 | G | 234 | TYR | CD1-CE1 | 8.04 | 1.51 | 1.39 |
| 1 | K | 130 | GLU | CB-CG | 8.04 | 1.67 | 1.52 |
| 1 | K | 400 | GLU | CG-CD | 8.04 | 1.64 | 1.51 |
| 1 | A | 219 | GLU | CB-CG | -8.04 | 1.36 | 1.52 |
| 1 | L | 390 | TYR | CE1-CZ | 8.04 | 1.49 | 1.38 |
| 1 | G | 91 | TYR | CG-CD2 | 8.04 | 1.49 | 1.39 |
| 1 | H | 265 | GLY | C-O | 8.02 | 1.36 | 1.23 |
| 1 | J | 462 | PHE | CB-CG | -8.02 | 1.37 | 1.51 |
| 1 | O | 139 | ALA | CA-CB | 8.02 | 1.69 | 1.52 |
| 1 | A | 343 | SER | CB-OG | 8.02 | 1.52 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 271 | VAL | CB-CG1 | -8.02 | 1.36 | 1.52 |
| 1 | M | 291 | TYR | CG-CD2 | -8.02 | 1.28 | 1.39 |
| 1 | O | 164 | PRO | CG-CD | 8.02 | 1.77 | 1.50 |
| 1 | H | 91 | TYR | CD1-CE1 | 8.02 | 1.51 | 1.39 |
| 1 | N | 185 | CYS | CB-SG | 8.02 | 1.95 | 1.82 |
| 1 | A | 159 | ILE | CB-CG2 | -8.01 | 1.28 | 1.52 |
| 1 | N | 249 | TYR | CD2-CE2 | 8.01 | 1.51 | 1.39 |
| 1 | J | 117 | ILE | CA-CB | -8.00 | 1.36 | 1.54 |
| 1 | I | 185 | CYS | C-O | 8.00 | 1.38 | 1.23 |
| 1 | K | 338 | ARG | CB-CG | 8.00 | 1.74 | 1.52 |
| 1 | F | 234 | TYR | CG-CD2 | 8.00 | 1.49 | 1.39 |
| 1 | J | 107 | VAL | CB-CG1 | -8.00 | 1.36 | 1.52 |
| 1 | D | 210 | PHE | CE1-CZ | 8.00 | 1.52 | 1.37 |
| 1 | F | 28 | VAL | CB-CG1 | 7.99 | 1.69 | 1.52 |
| 1 | B | 231 | TYR | CE2-CZ | 7.99 | 1.49 | 1.38 |
| 1 | D | 244 | ASP | CB-CG | 7.99 | 1.68 | 1.51 |
| 1 | E | 343 | SER | CA-CB | 7.99 | 1.65 | 1.52 |
| 1 | N | 261 | PHE | CG-CD2 | -7.99 | 1.26 | 1.38 |
| 1 | N | 173 | SER | CA-CB | 7.98 | 1.65 | 1.52 |
| 1 | K | 70 | TYR | CD1-CE1 | 7.98 | 1.51 | 1.39 |
| 1 | L | 442 | LYS | CB-CG | 7.98 | 1.74 | 1.52 |
| 1 | J | 236 | LYS | CG-CD | 7.97 | 1.79 | 1.52 |
| 1 | O | 459 | LEU | C-O | -7.97 | 1.08 | 1.23 |
| 1 | F | 140 | GLY | C-O | 7.97 | 1.36 | 1.23 |
| 1 | L | 151 | TYR | CG-CD1 | 7.97 | 1.49 | 1.39 |
| 1 | K | 362 | GLU | CD-OE2 | 7.96 | 1.34 | 1.25 |
| 1 | A | 381 | ILE | CB-CG2 | 7.96 | 1.77 | 1.52 |
| 1 | E | 231 | TYR | CD1-CE1 | 7.96 | 1.51 | 1.39 |
| 1 | M | 444 | TYR | CD1-CE1 | 7.96 | 1.51 | 1.39 |
| 1 | N | 355 | TYR | CZ-OH | 7.96 | 1.51 | 1.37 |
| 1 | H | 311 | TYR | C-O | 7.96 | 1.38 | 1.23 |
| 1 | N | 313 | LEU | CG-CD2 | 7.95 | 1.81 | 1.51 |
| 1 | D | 231 | TYR | CD1-CE1 | 7.95 | 1.51 | 1.39 |
| 1 | J | 334 | VAL | CB-CG1 | -7.95 | 1.36 | 1.52 |
| 1 | L | 111 | GLN | CG-CD | 7.95 | 1.69 | 1.51 |
| 1 | H | 177 | GLN | CB-CG | -7.94 | 1.31 | 1.52 |
| 1 | J | 220 | VAL | CB-CG2 | -7.94 | 1.36 | 1.52 |
| 1 | M | 224 | ILE | CB-CG2 | -7.94 | 1.28 | 1.52 |
| 1 | G | 51 | PRO | CB-CG | 7.93 | 1.89 | 1.50 |
| 1 | G | 151 | TYR | CB-CG | -7.93 | 1.39 | 1.51 |
| 1 | M | 311 | TYR | CE2-CZ | 7.93 | 1.48 | 1.38 |
| 1 | C | 106 | GLU | CD-OE1 | 7.92 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 26 | GLU | CD-OE2 | 7.92 | 1.34 | 1.25 |
| 1 | I | 116 | GLY | C-O | 7.92 | 1.36 | 1.23 |
| 1 | H | 446 | PHE | CD2-CE2 | 7.91 | 1.55 | 1.39 |
| 1 | J | 106 | GLU | CD-OE2 | 7.91 | 1.34 | 1.25 |
| 1 | A | 82 | LYS | CE-NZ | 7.91 | 1.68 | 1.49 |
| 1 | H | 70 | TYR | CD2-CE2 | -7.90 | 1.27 | 1.39 |
| 1 | K | 50 | PHE | CD2-CE2 | -7.90 | 1.23 | 1.39 |
| 1 | D | 157 | CYS | CB-SG | -7.90 | 1.68 | 1.82 |
| 1 | N | 229 | CYS | CB-SG | -7.90 | 1.68 | 1.82 |
| 1 | I | 287 | ALA | C-O | 7.90 | 1.38 | 1.23 |
| 1 | I | 315 | ARG | CG-CD | 7.90 | 1.71 | 1.51 |
| 1 | A | 355 | TYR | CZ-OH | 7.90 | 1.51 | 1.37 |
| 1 | B | 442 | LYS | CE-NZ | 7.90 | 1.68 | 1.49 |
| 1 | N | 312 | TRP | CD2-CE2 | 7.90 | 1.50 | 1.41 |
| 1 | O | 453 | GLU | CG-CD | 7.89 | 1.63 | 1.51 |
| 1 | F | 172 | GLY | C-O | 7.89 | 1.36 | 1.23 |
| 1 | D | 268 | GLY | C-O | 7.89 | 1.36 | 1.23 |
| 1 | D | 249 | TYR | CD1-CE1 | -7.88 | 1.27 | 1.39 |
| 1 | L | 195 | ILE | C-O | -7.88 | 1.08 | 1.23 |
| 1 | B | 216 | ASN | C-O | -7.88 | 1.08 | 1.23 |
| 1 | N | 382 | THR | CB-CG2 | 7.88 | 1.78 | 1.52 |
| 1 | F | 20 | ALA | N-CA | 7.87 | 1.62 | 1.46 |
| 1 | I | 151 | TYR | CD2-CE2 | -7.86 | 1.27 | 1.39 |
| 1 | A | 297 | GLY | N-CA | 7.86 | 1.57 | 1.46 |
| 1 | B | 467 | LYS | CG-CD | 7.86 | 1.79 | 1.52 |
| 1 | F | 139 | ALA | CA-C | 7.86 | 1.73 | 1.52 |
| 1 | H | 297 | GLY | C-O | 7.85 | 1.36 | 1.23 |
| 1 | D | 80 | PRO | CG-CD | 7.85 | 1.76 | 1.50 |
| 1 | D | 49 | TYR | CE2-CZ | 7.84 | 1.48 | 1.38 |
| 1 | H | 50 | PHE | CE1-CZ | -7.84 | 1.22 | 1.37 |
| 1 | G | 355 | TYR | CE2-CZ | -7.84 | 1.28 | 1.38 |
| 1 | K | 125 | LYS | CD-CE | 7.84 | 1.70 | 1.51 |
| 1 | E | 444 | TYR | CE2-CZ | 7.83 | 1.48 | 1.38 |
| 1 | A | 206 | GLY | C-O | 7.83 | 1.36 | 1.23 |
| 1 | K | 309 | LYS | CD-CE | 7.82 | 1.70 | 1.51 |
| 1 | L | 447 | TRP | CB-CG | 7.82 | 1.64 | 1.50 |
| 1 | O | 291 | TYR | CE1-CZ | -7.82 | 1.28 | 1.38 |
| 1 | J | 35 | TYR | CE1-CZ | -7.82 | 1.28 | 1.38 |
| 1 | E | 177 | GLN | CA-CB | 7.82 | 1.71 | 1.53 |
| 1 | A | 464 | LEU | CG-CD2 | -7.81 | 1.23 | 1.51 |
| 1 | E | 335 | ASP | C-O | 7.81 | 1.38 | 1.23 |
| 1 | E | 347 | ALA | C-O | 7.81 | 1.38 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 137 | ALA | CA-CB | 7.81 | 1.68 | 1.52 |
| 1 | L | 365 | ARG | CZ-NH2 | -7.81 | 1.23 | 1.33 |
| 1 | B | 49 | TYR | CG-CD1 | -7.80 | 1.29 | 1.39 |
| 1 | D | 139 | ALA | CA-CB | 7.80 | 1.68 | 1.52 |
| 1 | L | 306 | ILE | CB-CG2 | -7.80 | 1.28 | 1.52 |
| 1 | G | 91 | TYR | CG-CD1 | 7.80 | 1.49 | 1.39 |
| 1 | A | 240 | GLU | CB-CG | 7.80 | 1.67 | 1.52 |
| 1 | G | 35 | TYR | CD2-CE2 | -7.80 | 1.27 | 1.39 |
| 1 | H | 469 | LEU | CG-CD2 | 7.80 | 1.80 | 1.51 |
| 1 | I | 352 | GLU | CG-CD | 7.80 | 1.63 | 1.51 |
| 1 | K | 355 | TYR | CD1-CE1 | 7.79 | 1.51 | 1.39 |
| 1 | L | 247 | PHE | CE1-CZ | 7.79 | 1.52 | 1.37 |
| 1 | O | 48 | PRO | CG-CD | -7.79 | 1.25 | 1.50 |
| 1 | E | 291 | TYR | CE1-CZ | -7.79 | 1.28 | 1.38 |
| 1 | J | 247 | PHE | CE1-CZ | 7.79 | 1.52 | 1.37 |
| 1 | J | 35 | TYR | CG-CD1 | -7.79 | 1.29 | 1.39 |
| 1 | H | 100 | TRP | CZ3-CH2 | -7.78 | 1.27 | 1.40 |
| 1 | B | 311 | TYR | CD1-CE1 | 7.78 | 1.51 | 1.39 |
| 1 | I | 101 | ALA | CA-CB | -7.78 | 1.36 | 1.52 |
| 1 | G | 169 | TRP | CE3-CZ3 | -7.77 | 1.25 | 1.38 |
| 1 | I | 456 | SER | C-O | 7.77 | 1.38 | 1.23 |
| 1 | H | 91 | TYR | CE1-CZ | 7.77 | 1.48 | 1.38 |
| 1 | J | 438 | GLU | CD-OE1 | 7.76 | 1.34 | 1.25 |
| 1 | E | 252 | ARG | CG-CD | 7.76 | 1.71 | 1.51 |
| 1 | F | 360 | PHE | CB-CG | -7.76 | 1.38 | 1.51 |
| 1 | H | 355 | TYR | CE1-CZ | 7.76 | 1.48 | 1.38 |
| 1 | I | 135 | TYR | CB-CG | 7.76 | 1.63 | 1.51 |
| 1 | F | 205 | PHE | CD1-CE1 | -7.75 | 1.23 | 1.39 |
| 1 | E | 334 | VAL | CB-CG2 | -7.74 | 1.36 | 1.52 |
| 1 | A | 217 | LYS | CD-CE | 7.74 | 1.70 | 1.51 |
| 1 | H | 347 | ALA | C-O | 7.74 | 1.38 | 1.23 |
| 1 | F | 154 | THR | CB-CG2 | 7.73 | 1.77 | 1.52 |
| 1 | H | 148 | SER | CB-OG | 7.73 | 1.52 | 1.42 |
| 1 | C | 256 | PHE | CE2-CZ | -7.73 | 1.22 | 1.37 |
| 1 | M | 167 | GLU | CG-CD | 7.72 | 1.63 | 1.51 |
| 1 | B | 441 | LEU | CG-CD2 | 7.72 | 1.80 | 1.51 |
| 1 | N | 203 | THR | N-CA | 7.72 | 1.61 | 1.46 |
| 1 | O | 312 | TRP | CE2-CZ2 | -7.72 | 1.26 | 1.39 |
| 1 | A | 70 | TYR | CG-CD2 | -7.72 | 1.29 | 1.39 |
| 1 | F | 44 | ALA | CA-CB | 7.71 | 1.68 | 1.52 |
| 1 | G | 181 | GLN | CG-CD | 7.71 | 1.68 | 1.51 |
| 1 | K | 248 | PHE | CE1-CZ | -7.71 | 1.22 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 181 | GLN | CG-CD | 7.71 | 1.68 | 1.51 |
| 1 | E | 323 | ILE | CB-CG2 | 7.71 | 1.76 | 1.52 |
| 1 | F | 54 | LYS | CE-NZ | 7.71 | 1.68 | 1.49 |
| 1 | N | 49 | TYR | CD1-CE1 | 7.71 | 1.50 | 1.39 |
| 1 | J | 357 | ASN | C-O | 7.70 | 1.38 | 1.23 |
| 1 | A | 463 | PRO | CA-C | -7.70 | 1.37 | 1.52 |
| 1 | G | 336 | THR | C-O | -7.70 | 1.08 | 1.23 |
| 1 | N | 311 | TYR | CE1-CZ | -7.70 | 1.28 | 1.38 |
| 1 | D | 261 | PHE | CE1-CZ | -7.70 | 1.22 | 1.37 |
| 1 | B | 261 | PHE | CE2-CZ | -7.69 | 1.22 | 1.37 |
| 1 | D | 312 | TRP | CD2-CE3 | -7.69 | 1.28 | 1.40 |
| 1 | K | 49 | TYR | CE2-CZ | -7.69 | 1.28 | 1.38 |
| 1 | C | 28 | VAL | CB-CG1 | 7.68 | 1.69 | 1.52 |
| 1 | O | 324 | CYS | CB-SG | 7.68 | 1.95 | 1.82 |
| 1 | D | 468 | PHE | CE1-CZ | -7.68 | 1.22 | 1.37 |
| 1 | A | 443 | LYS | CE-NZ | 7.68 | 1.68 | 1.49 |
| 1 | K | 100 | TRP | CB-CG | -7.68 | 1.36 | 1.50 |
| 1 | N | 276 | TYR | CD1-CE1 | 7.68 | 1.50 | 1.39 |
| 1 | N | 291 | TYR | CB-CG | -7.68 | 1.40 | 1.51 |
| 1 | E | 72 | VAL | CA-CB | -7.68 | 1.38 | 1.54 |
| 1 | G | 438 | GLU | CD-OE2 | 7.68 | 1.34 | 1.25 |
| 1 | G | 44 | ALA | CA-CB | 7.67 | 1.68 | 1.52 |
| 1 | L | 249 | TYR | CD1-CE1 | -7.67 | 1.27 | 1.39 |
| 1 | I | 458 | ASP | CG-OD2 | 7.67 | 1.43 | 1.25 |
| 1 | H | 444 | TYR | CD1-CE1 | 7.66 | 1.50 | 1.39 |
| 1 | E | 438 | GLU | CD-OE1 | 7.66 | 1.34 | 1.25 |
| 1 | I | 317 | GLN | CG-CD | 7.66 | 1.68 | 1.51 |
| 1 | D | 100 | TRP | CD2-CE2 | -7.65 | 1.32 | 1.41 |
| 1 | D | 248 | PHE | CB-CG | -7.65 | 1.38 | 1.51 |
| 1 | I | 241 | PRO | N-CA | 7.65 | 1.60 | 1.47 |
| 1 | G | 69 | GLN | C-O | 7.65 | 1.37 | 1.23 |
| 1 | H | 178 | VAL | CB-CG2 | 7.64 | 1.69 | 1.52 |
| 1 | K | 230 | LYS | CG-CD | 7.64 | 1.78 | 1.52 |
| 1 | A | 28 | VAL | CB-CG1 | 7.64 | 1.68 | 1.52 |
| 1 | H | 360 | PHE | CD2-CE2 | 7.64 | 1.54 | 1.39 |
| 1 | I | 317 | GLN | CB-CG | 7.64 | 1.73 | 1.52 |
| 1 | C | 86 | PRO | CA-C | 7.64 | 1.68 | 1.52 |
| 1 | O | 333 | VAL | CB-CG2 | -7.64 | 1.36 | 1.52 |
| 1 | C | 400 | GLU | CG-CD | 7.64 | 1.63 | 1.51 |
| 1 | F | 83 | PHE | CE1-CZ | 7.64 | 1.51 | 1.37 |
| 1 | J | 256 | PHE | CE2-CZ | -7.63 | 1.22 | 1.37 |
| 1 | I | 84 | GLY | CA-C | 7.63 | 1.64 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 165 | ILE | C-O | 7.63 | 1.37 | 1.23 |
| 1 | C | 356 | LYS | CE-NZ | 7.62 | 1.68 | 1.49 |
| 1 | H | 194 | VAL | CB-CG1 | 7.62 | 1.68 | 1.52 |
| 1 | C | 280 | SER | CB-OG | 7.62 | 1.52 | 1.42 |
| 1 | H | 217 | LYS | CD-CE | 7.61 | 1.70 | 1.51 |
| 1 | I | 376 | PHE | CD2-CE2 | -7.61 | 1.24 | 1.39 |
| 1 | N | 189 | GLU | CD-OE2 | 7.61 | 1.34 | 1.25 |
| 1 | O | 317 | GLN | CG-CD | 7.61 | 1.68 | 1.51 |
| 1 | N | 138 | ASN | CB-CG | 7.61 | 1.68 | 1.51 |
| 1 | B | 305 | GLN | CB-CG | -7.61 | 1.32 | 1.52 |
| 1 | E | 362 | GLU | CD-OE1 | 7.61 | 1.34 | 1.25 |
| 1 | I | 291 | TYR | CG-CD2 | -7.60 | 1.29 | 1.39 |
| 1 | I | 97 | ARG | CZ-NH1 | 7.60 | 1.43 | 1.33 |
| 1 | L | 291 | TYR | CG-CD1 | -7.60 | 1.29 | 1.39 |
| 1 | C | 353 | THR | CB-CG2 | 7.60 | 1.77 | 1.52 |
| 1 | I | 280 | SER | C-O | 7.59 | 1.37 | 1.23 |
| 1 | O | 107 | VAL | CB-CG1 | -7.59 | 1.36 | 1.52 |
| 1 | G | 217 | LYS | CE-NZ | 7.59 | 1.68 | 1.49 |
| 1 | N | 456 | SER | CB-OG | 7.59 | 1.52 | 1.42 |
| 1 | D | 267 | VAL | CB-CG2 | 7.59 | 1.68 | 1.52 |
| 1 | F | 472 | LEU | N-CA | 7.59 | 1.61 | 1.46 |
| 1 | N | 189 | GLU | CG-CD | 7.59 | 1.63 | 1.51 |
| 1 | G | 230 | LYS | CE-NZ | 7.58 | 1.68 | 1.49 |
| 1 | G | 374 | PHE | CG-CD1 | 7.58 | 1.50 | 1.38 |
| 1 | K | 292 | PHE | CD2-CE2 | 7.58 | 1.54 | 1.39 |
| 1 | D | 296 | SER | CB-OG | -7.58 | 1.32 | 1.42 |
| 1 | O | 176 | THR | CB-CG2 | 7.58 | 1.77 | 1.52 |
| 1 | L | 97 | ARG | CG-CD | 7.57 | 1.70 | 1.51 |
| 1 | J | 54 | LYS | C-O | 7.57 | 1.37 | 1.23 |
| 1 | C | 230 | LYS | CB-CG | 7.57 | 1.73 | 1.52 |
| 1 | D | 453 | GLU | CG-CD | 7.57 | 1.63 | 1.51 |
| 1 | G | 450 | ASN | CG-ND2 | 7.57 | 1.51 | 1.32 |
| 1 | K | 266 | THR | CB-CG2 | 7.56 | 1.77 | 1.52 |
| 1 | K | 300 | VAL | CB-CG1 | 7.56 | 1.68 | 1.52 |
| 1 | D | 178 | VAL | CB-CG1 | 7.56 | 1.68 | 1.52 |
| 1 | F | 117 | ILE | CA-CB | -7.56 | 1.37 | 1.54 |
| 1 | F | 114 | GLY | N-CA | 7.55 | 1.57 | 1.46 |
| 1 | N | 53 | LYS | CB-CG | 7.55 | 1.73 | 1.52 |
| 1 | D | 172 | GLY | C-O | 7.55 | 1.35 | 1.23 |
| 1 | I | 147 | ILE | C-O | 7.55 | 1.37 | 1.23 |
| 1 | H | 248 | PHE | C-O | 7.55 | 1.37 | 1.23 |
| 1 | N | 87 | ASP | CG-OD1 | 7.55 | 1.42 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 165 | ILE | CA-CB | -7.55 | 1.37 | 1.54 |
| 1 | K | 292 | PHE | CD1-CE1 | 7.54 | 1.54 | 1.39 |
| 1 | N | 231 | TYR | CE2-CZ | 7.54 | 1.48 | 1.38 |
| 1 | A | 338 | ARG | CG-CD | 7.54 | 1.70 | 1.51 |
| 1 | I | 84 | GLY | C-O | 7.54 | 1.35 | 1.23 |
| 1 | L | 362 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 1 | A | 30 | ARG | C-O | -7.54 | 1.09 | 1.23 |
| 1 | E | 118 | SER | CB-OG | 7.54 | 1.52 | 1.42 |
| 1 | C | 115 | VAL | CB-CG2 | -7.54 | 1.37 | 1.52 |
| 1 | L | 456 | SER | C-O | 7.54 | 1.37 | 1.23 |
| 1 | E | 135 | TYR | CD1-CE1 | -7.54 | 1.28 | 1.39 |
| 1 | K | 210 | PHE | CD2-CE2 | -7.53 | 1.24 | 1.39 |
| 1 | O | 335 | ASP | C-O | 7.53 | 1.37 | 1.23 |
| 1 | L | 375 | ILE | C-O | 7.53 | 1.37 | 1.23 |
| 1 | L | 272 | PRO | N-CD | 7.53 | 1.58 | 1.47 |
| 1 | D | 360 | PHE | CE2-CZ | -7.52 | 1.23 | 1.37 |
| 1 | E | 449 | VAL | CA-CB | 7.52 | 1.70 | 1.54 |
| 1 | N | 292 | PHE | CD1-CE1 | -7.52 | 1.24 | 1.39 |
| 1 | J | 44 | ALA | CA-CB | 7.52 | 1.68 | 1.52 |
| 1 | K | 330 | PHE | CD2-CE2 | -7.52 | 1.24 | 1.39 |
| 1 | B | 263 | ARG | CZ-NH2 | -7.51 | 1.23 | 1.33 |
| 1 | I | 263 | ARG | CZ-NH1 | -7.51 | 1.23 | 1.33 |
| 1 | J | 240 | GLU | CG-CD | 7.51 | 1.63 | 1.51 |
| 1 | J | 472 | LEU | N-CA | 7.51 | 1.61 | 1.46 |
| 1 | D | 40 | SER | CB-OG | 7.51 | 1.52 | 1.42 |
| 1 | J | 106 | GLU | CG-CD | 7.51 | 1.63 | 1.51 |
| 1 | L | 311 | TYR | CG-CD2 | 7.51 | 1.49 | 1.39 |
| 1 | G | 176 | THR | CA-CB | 7.50 | 1.72 | 1.53 |
| 1 | H | 256 | PHE | CB-CG | -7.50 | 1.38 | 1.51 |
| 1 | J | 390 | TYR | CB-CG | -7.50 | 1.40 | 1.51 |
| 1 | E | 236 | LYS | CD-CE | 7.50 | 1.70 | 1.51 |
| 1 | F | 468 | PHE | CG-CD1 | 7.50 | 1.50 | 1.38 |
| 1 | G | 362 | GLU | CD-OE2 | 7.50 | 1.33 | 1.25 |
| 1 | I | 364 | LEU | C-O | 7.50 | 1.37 | 1.23 |
| 1 | L | 230 | LYS | CE-NZ | 7.50 | 1.67 | 1.49 |
| 1 | F | 28 | VAL | C-O | 7.49 | 1.37 | 1.23 |
| 1 | J | 263 | ARG | CG-CD | -7.49 | 1.33 | 1.51 |
| 1 | O | 352 | GLU | CG-CD | 7.49 | 1.63 | 1.51 |
| 1 | O | 210 | PHE | CE1-CZ | 7.49 | 1.51 | 1.37 |
| 1 | C | 355 | TYR | CD1-CE1 | -7.49 | 1.28 | 1.39 |
| 1 | J | 115 | VAL | CB-CG2 | -7.49 | 1.37 | 1.52 |
| 1 | O | 249 | TYR | CZ-OH | 7.49 | 1.50 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | M | 140 | GLY | N-CA | 7.48 | 1.57 | 1.46 |
| 1 | A | 242 | TYR | CE1-CZ | -7.48 | 1.28 | 1.38 |
| 1 | I | 375 | ILE | C-O | 7.48 | 1.37 | 1.23 |
| 1 | I | 458 | ASP | CG-OD1 | 7.47 | 1.42 | 1.25 |
| 1 | F | 97 | ARG | CG-CD | 7.47 | 1.70 | 1.51 |
| 1 | H | 356 | LYS | C-O | -7.47 | 1.09 | 1.23 |
| 1 | I | 379 | CYS | CB-SG | 7.47 | 1.95 | 1.82 |
| 1 | C | 307 | PHE | CE1-CZ | 7.46 | 1.51 | 1.37 |
| 1 | H | 220 | VAL | CB-CG1 | -7.46 | 1.37 | 1.52 |
| 1 | H | 261 | PHE | CE1-CZ | -7.46 | 1.23 | 1.37 |
| 1 | G | 263 | ARG | CG-CD | -7.46 | 1.33 | 1.51 |
| 1 | L | 49 | TYR | CD2-CE2 | -7.46 | 1.28 | 1.39 |
| 1 | L | 177 | GLN | CG-CD | 7.46 | 1.68 | 1.51 |
| 1 | D | 257 | VAL | CA-CB | 7.45 | 1.70 | 1.54 |
| 1 | O | 173 | SER | CB-OG | 7.45 | 1.51 | 1.42 |
| 1 | D | 245 | SER | CB-OG | 7.45 | 1.51 | 1.42 |
| 1 | I | 242 | TYR | CD1-CE1 | 7.45 | 1.50 | 1.39 |
| 1 | I | 205 | PHE | CG-CD2 | 7.44 | 1.50 | 1.38 |
| 1 | K | 210 | PHE | CD1-CE1 | -7.44 | 1.24 | 1.39 |
| 1 | E | 343 | SER | CB-OG | 7.43 | 1.51 | 1.42 |
| 1 | J | 382 | THR | C-O | 7.43 | 1.37 | 1.23 |
| 1 | N | 219 | GLU | CB-CG | 7.43 | 1.66 | 1.52 |
| 1 | C | 70 | TYR | CE2-CZ | -7.43 | 1.28 | 1.38 |
| 1 | J | 338 | ARG | CZ-NH1 | 7.43 | 1.42 | 1.33 |
| 1 | N | 138 | ASN | C-O | 7.43 | 1.37 | 1.23 |
| 1 | K | 444 | TYR | CD1-CE1 | -7.43 | 1.28 | 1.39 |
| 1 | K | 49 | TYR | CB-CG | 7.42 | 1.62 | 1.51 |
| 1 | N | 40 | SER | CB-OG | 7.42 | 1.51 | 1.42 |
| 1 | H | 20 | ALA | CA-CB | 7.42 | 1.68 | 1.52 |
| 1 | D | 256 | PHE | CE2-CZ | -7.42 | 1.23 | 1.37 |
| 1 | M | 70 | TYR | CG-CD2 | -7.42 | 1.29 | 1.39 |
| 1 | O | 27 | TYR | CG-CD2 | 7.42 | 1.48 | 1.39 |
| 1 | F | 139 | ALA | C-N | 7.41 | 1.46 | 1.33 |
| 1 | J | 360 | PHE | CE1-CZ | -7.41 | 1.23 | 1.37 |
| 1 | O | 344 | LEU | C-O | 7.41 | 1.37 | 1.23 |
| 1 | B | 169 | TRP | CD2-CE2 | -7.41 | 1.32 | 1.41 |
| 1 | O | 22 | VAL | CB-CG1 | 7.41 | 1.68 | 1.52 |
| 1 | D | 258 | ARG | CZ-NH2 | -7.41 | 1.23 | 1.33 |
| 1 | H | 391 | ILE | CA-CB | -7.41 | 1.37 | 1.54 |
| 1 | I | 90 | PHE | CE1-CZ | 7.41 | 1.51 | 1.37 |
| 1 | I | 390 | TYR | CD2-CE2 | -7.41 | 1.28 | 1.39 |
| 1 | M | 132 | ALA | CA-CB | 7.41 | 1.68 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 276 | TYR | CD2-CE2 | 7.40 | 1.50 | 1.39 |
| 1 | M | 249 | TYR | CD1-CE1 | 7.40 | 1.50 | 1.39 |
| 1 | I | 225 | CYS | CB-SG | 7.40 | 1.94 | 1.82 |
| 1 | K | 462 | PHE | CB-CG | -7.40 | 1.38 | 1.51 |
| 1 | I | 28 | VAL | CB-CG2 | -7.40 | 1.37 | 1.52 |
| 1 | C | 453 | GLU | CD-OE1 | 7.39 | 1.33 | 1.25 |
| 1 | F | 448 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | L | 205 | PHE | CG-CD2 | 7.39 | 1.49 | 1.38 |
| 1 | J | 32 | ASN | CB-CG | 7.39 | 1.68 | 1.51 |
| 1 | C | 333 | VAL | CB-CG2 | -7.38 | 1.37 | 1.52 |
| 1 | F | 126 | LEU | C-O | 7.38 | 1.37 | 1.23 |
| 1 | N | 454 | LYS | CE-NZ | 7.38 | 1.67 | 1.49 |
| 1 | B | 67 | GLY | CA-C | 7.38 | 1.63 | 1.51 |
| 1 | D | 115 | VAL | C-O | 7.38 | 1.37 | 1.23 |
| 1 | K | 287 | ALA | CA-CB | 7.37 | 1.68 | 1.52 |
| 1 | C | 77 | LEU | CG-CD2 | 7.37 | 1.79 | 1.51 |
| 1 | B | 217 | LYS | CD-CE | 7.36 | 1.69 | 1.51 |
| 1 | B | 276 | TYR | CG-CD1 | -7.36 | 1.29 | 1.39 |
| 1 | I | 174 | PRO | C-O | 7.36 | 1.38 | 1.23 |
| 1 | J | 271 | VAL | CB-CG2 | -7.36 | 1.37 | 1.52 |
| 1 | N | 27 | TYR | C-O | 7.36 | 1.37 | 1.23 |
| 1 | J | 455 | PHE | CE2-CZ | 7.36 | 1.51 | 1.37 |
| 1 | O | 220 | VAL | CB-CG1 | 7.35 | 1.68 | 1.52 |
| 1 | D | 249 | TYR | CG-CD1 | -7.35 | 1.29 | 1.39 |
| 1 | D | 294 | THR | CB-CG2 | -7.35 | 1.28 | 1.52 |
| 1 | E | 291 | TYR | CB-CG | -7.35 | 1.40 | 1.51 |
| 1 | M | 253 | GLU | CD-OE2 | -7.35 | 1.17 | 1.25 |
| 1 | E | 376 | PHE | CD2-CE2 | -7.35 | 1.24 | 1.39 |
| 1 | H | 360 | PHE | CE2-CZ | -7.35 | 1.23 | 1.37 |
| 1 | N | 272 | PRO | CA-C | -7.35 | 1.38 | 1.52 |
| 1 | B | 258 | ARG | C-O | 7.35 | 1.37 | 1.23 |
| 1 | H | 333 | VAL | C-O | 7.35 | 1.37 | 1.23 |
| 1 | K | 311 | TYR | C-O | 7.34 | 1.37 | 1.23 |
| 1 | C | 59 | LYS | CE-NZ | 7.34 | 1.67 | 1.49 |
| 1 | M | 369 | GLU | CD-OE2 | 7.34 | 1.33 | 1.25 |
| 1 | D | 165 | ILE | CA-CB | -7.34 | 1.38 | 1.54 |
| 1 | D | 370 | TYR | CB-CG | -7.33 | 1.40 | 1.51 |
| 1 | F | 106 | GLU | CG-CD | 7.33 | 1.62 | 1.51 |
| 1 | D | 115 | VAL | CA-CB | -7.32 | 1.39 | 1.54 |
| 1 | K | 151 | TYR | CD2-CE2 | 7.32 | 1.50 | 1.39 |
| 1 | J | 376 | PHE | CE1-CZ | 7.32 | 1.51 | 1.37 |
| 1 | J | 292 | PHE | CG-CD2 | 7.32 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 269 | GLU | CG-CD | 7.32 | 1.62 | 1.51 |
| 1 | C | 23 | SER | CB-OG | 7.31 | 1.51 | 1.42 |
| 1 | F | 442 | LYS | C-O | 7.31 | 1.37 | 1.23 |
| 1 | L | 360 | PHE | CB-CG | -7.31 | 1.39 | 1.51 |
| 1 | H | 361 | LYS | CE-NZ | 7.30 | 1.67 | 1.49 |
| 1 | M | 155 | GLN | CB-CG | -7.30 | 1.32 | 1.52 |
| 1 | H | 249 | TYR | N-CA | 7.30 | 1.60 | 1.46 |
| 1 | N | 89 | SER | C-O | 7.30 | 1.37 | 1.23 |
| 1 | H | 175 | CYS | CB-SG | 7.30 | 1.94 | 1.82 |
| 1 | M | 35 | TYR | CG-CD1 | -7.30 | 1.29 | 1.39 |
| 1 | H | 311 | TYR | CE1-CZ | -7.29 | 1.29 | 1.38 |
| 1 | E | 151 | TYR | CG-CD2 | 7.29 | 1.48 | 1.39 |
| 1 | F | 181 | GLN | CG-CD | 7.29 | 1.67 | 1.51 |
| 1 | E | 35 | TYR | CD1-CE1 | -7.29 | 1.28 | 1.39 |
| 1 | H | 309 | LYS | CD-CE | 7.29 | 1.69 | 1.51 |
| 1 | F | 315 | ARG | CG-CD | 7.29 | 1.70 | 1.51 |
| 1 | A | 268 | GLY | C-O | 7.29 | 1.35 | 1.23 |
| 1 | E | 468 | PHE | CE2-CZ | 7.29 | 1.51 | 1.37 |
| 1 | N | 258 | ARG | CB-CG | -7.29 | 1.32 | 1.52 |
| 1 | D | 189 | GLU | CG-CD | 7.28 | 1.62 | 1.51 |
| 1 | C | 374 | PHE | CE1-CZ | 7.28 | 1.51 | 1.37 |
| 1 | E | 234 | TYR | CD2-CE2 | 7.28 | 1.50 | 1.39 |
| 1 | M | 269 | GLU | CD-OE1 | -7.28 | 1.17 | 1.25 |
| 1 | M | 347 | ALA | C-O | 7.28 | 1.37 | 1.23 |
| 1 | H | 276 | TYR | CD2-CE2 | 7.28 | 1.50 | 1.39 |
| 1 | O | 187 | PRO | CG-CD | 7.28 | 1.74 | 1.50 |
| 1 | B | 355 | TYR | CZ-OH | 7.27 | 1.50 | 1.37 |
| 1 | C | 376 | PHE | CE2-CZ | 7.27 | 1.51 | 1.37 |
| 1 | H | 109 | ARG | NE-CZ | 7.27 | 1.42 | 1.33 |
| 1 | J | 377 | GLN | CG-CD | 7.27 | 1.67 | 1.51 |
| 1 | E | 382 | THR | C-O | 7.26 | 1.37 | 1.23 |
| 1 | G | 178 | VAL | CB-CG2 | 7.26 | 1.68 | 1.52 |
| 1 | N | 72 | VAL | N-CA | 7.26 | 1.60 | 1.46 |
| 1 | B | 234 | TYR | CE2-CZ | -7.26 | 1.29 | 1.38 |
| 1 | H | 347 | ALA | CA-CB | 7.26 | 1.67 | 1.52 |
| 1 | F | 27 | TYR | CE1-CZ | 7.26 | 1.48 | 1.38 |
| 1 | F | 189 | GLU | CG-CD | 7.26 | 1.62 | 1.51 |
| 1 | F | 383 | LEU | CG-CD2 | 7.26 | 1.78 | 1.51 |
| 1 | G | 148 | SER | CB-OG | 7.26 | 1.51 | 1.42 |
| 1 | J | 243 | GLY | C-O | 7.26 | 1.35 | 1.23 |
| 1 | M | 298 | SER | CB-OG | 7.26 | 1.51 | 1.42 |
| 1 | B | 362 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 163 | PRO | CA-CB | -7.25 | 1.39 | 1.53 |
| 1 | B | 201 | VAL | CB-CG1 | -7.25 | 1.37 | 1.52 |
| 1 | K | 48 | PRO | C-O | 7.25 | 1.37 | 1.23 |
| 1 | D | 110 | GLY | C-O | -7.25 | 1.12 | 1.23 |
| 1 | J | 173 | SER | CB-OG | 7.24 | 1.51 | 1.42 |
| 1 | H | 130 | GLU | CG-CD | 7.24 | 1.62 | 1.51 |
| 1 | C | 253 | GLU | CD-OE2 | -7.24 | 1.17 | 1.25 |
| 1 | E | 66 | SER | C-O | 7.24 | 1.37 | 1.23 |
| 1 | I | 204 | GLY | C-O | 7.24 | 1.35 | 1.23 |
| 1 | C | 249 | TYR | CE1-CZ | -7.23 | 1.29 | 1.38 |
| 1 | N | 21 | VAL | CB-CG2 | 7.23 | 1.68 | 1.52 |
| 1 | F | 438 | GLU | CD-OE2 | 7.23 | 1.33 | 1.25 |
| 1 | O | 74 | ARG | CZ-NH1 | 7.23 | 1.42 | 1.33 |
| 1 | H | 50 | PHE | CD2-CE2 | -7.23 | 1.24 | 1.39 |
| 1 | H | 346 | ALA | CA-CB | 7.22 | 1.67 | 1.52 |
| 1 | L | 181 | GLN | CG-CD | 7.22 | 1.67 | 1.51 |
| 1 | A | 54 | LYS | CE-NZ | 7.22 | 1.67 | 1.49 |
| 1 | D | 176 | THR | N-CA | 7.22 | 1.60 | 1.46 |
| 1 | A | 67 | GLY | CA-C | 7.22 | 1.63 | 1.51 |
| 1 | A | 361 | LYS | CD-CE | 7.22 | 1.69 | 1.51 |
| 1 | K | 43 | LEU | C-O | -7.22 | 1.09 | 1.23 |
| 1 | J | 363 | TYR | CE2-CZ | 7.22 | 1.48 | 1.38 |
| 1 | B | 203 | THR | CA-CB | -7.21 | 1.34 | 1.53 |
| 1 | E | 331 | VAL | CB-CG1 | 7.21 | 1.68 | 1.52 |
| 1 | G | 35 | TYR | CE1-CZ | -7.21 | 1.29 | 1.38 |
| 1 | L | 469 | LEU | C-O | -7.21 | 1.09 | 1.23 |
| 1 | A | 103 | VAL | CB-CG1 | -7.21 | 1.37 | 1.52 |
| 1 | M | 138 | ASN | C-O | 7.21 | 1.37 | 1.23 |
| 1 | A | 227 | SER | CB-OG | 7.21 | 1.51 | 1.42 |
| 1 | B | 145 | GLU | CD-OE1 | 7.21 | 1.33 | 1.25 |
| 1 | K | 185 | CYS | C-O | 7.21 | 1.37 | 1.23 |
| 1 | B | 230 | LYS | CE-NZ | 7.20 | 1.67 | 1.49 |
| 1 | E | 282 | SER | CB-OG | 7.20 | 1.51 | 1.42 |
| 1 | I | 247 | PHE | CE1-CZ | 7.20 | 1.51 | 1.37 |
| 1 | J | 370 | TYR | C-O | 7.20 | 1.37 | 1.23 |
| 1 | L | 227 | SER | CB-OG | 7.20 | 1.51 | 1.42 |
| 1 | L | 236 | LYS | CB-CG | 7.20 | 1.72 | 1.52 |
| 1 | B | 91 | TYR | CG-CD1 | 7.20 | 1.48 | 1.39 |
| 1 | O | 360 | PHE | CG-CD1 | -7.19 | 1.27 | 1.38 |
| 1 | I | 172 | GLY | C-O | 7.19 | 1.35 | 1.23 |
| 1 | K | 219 | GLU | CG-CD | -7.19 | 1.41 | 1.51 |
| 1 | A | 151 | TYR | CG-CD2 | 7.18 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 320 | ASN | CB-CG | 7.18 | 1.67 | 1.51 |
| 1 | N | 95 | THR | CB-CG2 | 7.18 | 1.76 | 1.52 |
| 1 | J | 94 | ASP | CB-CG | 7.18 | 1.66 | 1.51 |
| 1 | L | 317 | GLN | CG-CD | 7.18 | 1.67 | 1.51 |
| 1 | H | 462 | PHE | CE1-CZ | -7.17 | 1.23 | 1.37 |
| 1 | B | 168 | HIS | C-O | -7.17 | 1.09 | 1.23 |
| 1 | I | 88 | THR | CB-CG2 | 7.16 | 1.75 | 1.52 |
| 1 | D | 62 | VAL | CB-CG2 | 7.16 | 1.67 | 1.52 |
| 1 | O | 38 | GLY | C-O | 7.16 | 1.35 | 1.23 |
| 1 | C | 462 | PHE | CG-CD1 | -7.16 | 1.28 | 1.38 |
| 1 | G | 447 | TRP | CG-CD1 | 7.16 | 1.46 | 1.36 |
| 1 | B | 298 | SER | CB-OG | -7.16 | 1.32 | 1.42 |
| 1 | E | 396 | SER | C-O | 7.16 | 1.36 | 1.23 |
| 1 | H | 254 | GLN | C-O | 7.15 | 1.36 | 1.23 |
| 1 | L | 116 | GLY | C-O | 7.15 | 1.35 | 1.23 |
| 1 | O | 27 | TYR | CE1-CZ | 7.15 | 1.47 | 1.38 |
| 1 | E | 35 | TYR | CD2-CE2 | -7.15 | 1.28 | 1.39 |
| 1 | H | 89 | SER | CB-OG | 7.15 | 1.51 | 1.42 |
| 1 | N | 201 | VAL | CB-CG1 | -7.15 | 1.37 | 1.52 |
| 1 | O | 149 | MET | CG-SD | 7.15 | 1.99 | 1.81 |
| 1 | H | 67 | GLY | N-CA | -7.14 | 1.35 | 1.46 |
| 1 | O | 26 | GLU | CG-CD | 7.14 | 1.62 | 1.51 |
| 1 | D | 181 | GLN | C-O | 7.14 | 1.36 | 1.23 |
| 1 | E | 280 | SER | C-O | 7.14 | 1.36 | 1.23 |
| 1 | J | 455 | PHE | CD1-CE1 | -7.13 | 1.25 | 1.39 |
| 1 | K | 140 | GLY | N-CA | 7.13 | 1.56 | 1.46 |
| 1 | J | 349 | SER | CA-CB | 7.13 | 1.63 | 1.52 |
| 1 | G | 98 | LEU | CG-CD1 | 7.13 | 1.78 | 1.51 |
| 1 | L | 262 | ASN | C-O | -7.13 | 1.09 | 1.23 |
| 1 | B | 472 | LEU | C-OXT | 7.13 | 1.36 | 1.23 |
| 1 | M | 362 | GLU | CD-OE1 | 7.13 | 1.33 | 1.25 |
| 1 | H | 90 | PHE | CG-CD2 | 7.13 | 1.49 | 1.38 |
| 1 | H | 156 | LEU | C-O | 7.13 | 1.36 | 1.23 |
| 1 | H | 400 | GLU | CD-OE1 | 7.13 | 1.33 | 1.25 |
| 1 | F | 225 | CYS | N-CA | 7.12 | 1.60 | 1.46 |
| 1 | E | 194 | VAL | CB-CG1 | 7.12 | 1.67 | 1.52 |
| 1 | K | 468 | PHE | CD1-CE1 | -7.12 | 1.25 | 1.39 |
| 1 | F | 35 | TYR | CG-CD1 | 7.12 | 1.48 | 1.39 |
| 1 | F | 389 | THR | CB-CG2 | 7.12 | 1.75 | 1.52 |
| 1 | K | 247 | PHE | CG-CD2 | 7.12 | 1.49 | 1.38 |
| 1 | A | 355 | TYR | CG-CD1 | -7.12 | 1.29 | 1.39 |
| 1 | O | 261 | PHE | CG-CD2 | 7.12 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 32 | ASN | CB-CG | 7.11 | 1.67 | 1.51 |
| 1 | D | 174 | PRO | N-CD | 7.11 | 1.57 | 1.47 |
| 1 | H | 114 | GLY | N-CA | 7.11 | 1.56 | 1.46 |
| 1 | O | 379 | CYS | C-O | 7.11 | 1.36 | 1.23 |
| 1 | B | 242 | TYR | CE1-CZ | -7.11 | 1.29 | 1.38 |
| 1 | H | 300 | VAL | C-O | 7.11 | 1.36 | 1.23 |
| 1 | O | 292 | PHE | CE2-CZ | -7.11 | 1.23 | 1.37 |
| 1 | N | 32 | ASN | CG-OD1 | 7.11 | 1.39 | 1.24 |
| 1 | N | 125 | LYS | C-O | 7.11 | 1.36 | 1.23 |
| 1 | B | 142 | ASP | CB-CG | -7.11 | 1.36 | 1.51 |
| 1 | N | 24 | THR | CA-CB | -7.11 | 1.34 | 1.53 |
| 1 | F | 259 | HIS | CA-CB | -7.11 | 1.38 | 1.53 |
| 1 | J | 100 | TRP | CB-CG | -7.11 | 1.37 | 1.50 |
| 1 | N | 269 | GLU | CB-CG | 7.11 | 1.65 | 1.52 |
| 1 | E | 442 | LYS | C-O | 7.10 | 1.36 | 1.23 |
| 1 | H | 467 | LYS | CB-CG | 7.10 | 1.71 | 1.52 |
| 1 | D | 301 | THR | CB-CG2 | 7.10 | 1.75 | 1.52 |
| 1 | F | 239 | SER | CB-OG | 7.10 | 1.51 | 1.42 |
| 1 | G | 162 | LYS | CE-NZ | 7.10 | 1.66 | 1.49 |
| 1 | A | 291 | TYR | CE1-CZ | -7.10 | 1.29 | 1.38 |
| 1 | A | 315 | ARG | CG-CD | 7.10 | 1.69 | 1.51 |
| 1 | B | 124 | ASN | CB-CG | 7.09 | 1.67 | 1.51 |
| 1 | K | 161 | CYS | CB-SG | 7.09 | 1.94 | 1.82 |
| 1 | B | 56 | ASN | C-O | 7.09 | 1.36 | 1.23 |
| 1 | G | 216 | ASN | CG-ND2 | 7.09 | 1.50 | 1.32 |
| 1 | B | 201 | VAL | CA-CB | -7.09 | 1.39 | 1.54 |
| 1 | I | 390 | TYR | CZ-OH | 7.08 | 1.49 | 1.37 |
| 1 | C | 242 | TYR | CE2-CZ | 7.08 | 1.47 | 1.38 |
| 1 | H | 58 | ASN | C-O | 7.08 | 1.36 | 1.23 |
| 1 | K | 452 | LYS | CG-CD | 7.08 | 1.76 | 1.52 |
| 1 | A | 400 | GLU | CD-OE1 | 7.08 | 1.33 | 1.25 |
| 1 | F | 114 | GLY | C-O | 7.08 | 1.34 | 1.23 |
| 1 | I | 231 | TYR | CG-CD2 | -7.08 | 1.29 | 1.39 |
| 1 | L | 340 | THR | CB-CG2 | -7.07 | 1.29 | 1.52 |
| 1 | O | 107 | VAL | C-O | 7.07 | 1.36 | 1.23 |
| 1 | J | 240 | GLU | CD-OE1 | 7.07 | 1.33 | 1.25 |
| 1 | E | 45 | VAL | CB-CG2 | -7.07 | 1.38 | 1.52 |
| 1 | O | 374 | PHE | CG-CD1 | 7.07 | 1.49 | 1.38 |
| 1 | D | 32 | ASN | CG-OD1 | 7.07 | 1.39 | 1.24 |
| 1 | N | 315 | ARG | CG-CD | 7.07 | 1.69 | 1.51 |
| 1 | D | 152 | LYS | CD-CE | 7.06 | 1.69 | 1.51 |
| 1 | J | 215 | ALA | CA-CB | 7.06 | 1.67 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | L | 177 | GLN | C-O | 7.06 | 1.36 | 1.23 |
| 1 | H | 106 | GLU | CD-OE2 | 7.06 | 1.33 | 1.25 |
| 1 | I | 387 | VAL | CA-CB | 7.06 | 1.69 | 1.54 |
| 1 | F | 184 | ASP | CG-OD2 | 7.05 | 1.41 | 1.25 |
| 1 | N | 320 | ASN | C-O | -7.05 | 1.09 | 1.23 |
| 1 | L | 472 | LEU | C-O | 7.05 | 1.36 | 1.23 |
| 1 | M | 200 | MET | C-O | 7.05 | 1.36 | 1.23 |
| 1 | K | 462 | PHE | CG-CD1 | -7.05 | 1.28 | 1.38 |
| 1 | C | 387 | VAL | CB-CG1 | 7.04 | 1.67 | 1.52 |
| 1 | E | 160 | GLY | N-CA | 7.04 | 1.56 | 1.46 |
| 1 | O | 49 | TYR | C-O | 7.04 | 1.36 | 1.23 |
| 1 | D | 189 | GLU | CD-OE1 | 7.04 | 1.33 | 1.25 |
| 1 | B | 241 | PRO | N-CA | 7.04 | 1.59 | 1.47 |
| 1 | C | 173 | SER | CA-CB | 7.04 | 1.63 | 1.52 |
| 1 | D | 369 | GLU | C-O | -7.04 | 1.09 | 1.23 |
| 1 | F | 265 | GLY | N-CA | 7.04 | 1.56 | 1.46 |
| 1 | M | 293 | PRO | C-O | -7.04 | 1.09 | 1.23 |
| 1 | D | 334 | VAL | CB-CG1 | -7.03 | 1.38 | 1.52 |
| 1 | E | 465 | GLY | C-O | -7.03 | 1.12 | 1.23 |
| 1 | D | 240 | GLU | CD-OE1 | 7.03 | 1.33 | 1.25 |
| 1 | B | 117 | ILE | CA-CB | -7.03 | 1.38 | 1.54 |
| 1 | M | 73 | PHE | CG-CD1 | -7.03 | 1.28 | 1.38 |
| 1 | N | 438 | GLU | CD-OE2 | 7.03 | 1.33 | 1.25 |
| 1 | I | 145 | GLU | CD-OE2 | 7.02 | 1.33 | 1.25 |
| 1 | A | 114 | GLY | C-O | 7.02 | 1.34 | 1.23 |
| 1 | E | 173 | SER | C-O | 7.02 | 1.36 | 1.23 |
| 1 | F | 197 | ASP | CG-OD1 | 7.02 | 1.41 | 1.25 |
| 1 | J | 231 | TYR | CD2-CE2 | 7.02 | 1.49 | 1.39 |
| 1 | J | 249 | TYR | C-O | -7.02 | 1.10 | 1.23 |
| 1 | M | 240 | GLU | CG-CD | 7.02 | 1.62 | 1.51 |
| 1 | B | 138 | ASN | CB-CG | 7.01 | 1.67 | 1.51 |
| 1 | G | 226 | THR | CA-CB | -7.01 | 1.35 | 1.53 |
| 1 | N | 202 | ASP | CG-OD2 | 7.01 | 1.41 | 1.25 |
| 1 | O | 169 | TRP | CB-CG | -7.01 | 1.37 | 1.50 |
| 1 | C | 242 | TYR | CG-CD1 | 7.01 | 1.48 | 1.39 |
| 1 | K | 22 | VAL | CB-CG2 | 7.01 | 1.67 | 1.52 |
| 1 | G | 312 | TRP | CE3-CZ3 | -7.00 | 1.26 | 1.38 |
| 1 | J | 456 | SER | CB-OG | 7.00 | 1.51 | 1.42 |
| 1 | O | 159 | ILE | CA-CB | -7.00 | 1.38 | 1.54 |
| 1 | B | 91 | TYR | CE2-CZ | 6.99 | 1.47 | 1.38 |
| 1 | L | 144 | ARG | CZ-NH2 | 6.99 | 1.42 | 1.33 |
| 1 | O | 40 | SER | CA-CB | 6.99 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 34 | TYR | CD1-CE1 | -6.99 | 1.28 | 1.39 |
| 1 | F | 438 | GLU | CB-CG | 6.99 | 1.65 | 1.52 |
| 1 | N | 88 | THR | CA-CB | 6.99 | 1.71 | 1.53 |
| 1 | E | 452 | LYS | CE-NZ | 6.99 | 1.66 | 1.49 |
| 1 | B | 214 | GLN | CB-CG | 6.99 | 1.71 | 1.52 |
| 1 | D | 311 | TYR | CZ-OH | -6.99 | 1.25 | 1.37 |
| 1 | A | 208 | MET | C-O | 6.99 | 1.36 | 1.23 |
| 1 | L | 351 | SER | C-O | 6.99 | 1.36 | 1.23 |
| 1 | B | 177 | GLN | CD-OE1 | 6.98 | 1.39 | 1.24 |
| 1 | C | 83 | PHE | CE2-CZ | 6.98 | 1.50 | 1.37 |
| 1 | F | 276 | TYR | CE2-CZ | 6.98 | 1.47 | 1.38 |
| 1 | K | 106 | GLU | CG-CD | 6.98 | 1.62 | 1.51 |
| 1 | B | 390 | TYR | CE1-CZ | 6.98 | 1.47 | 1.38 |
| 1 | F | 368 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 |
| 1 | N | 205 | PHE | CE2-CZ | 6.98 | 1.50 | 1.37 |
| 1 | A | 307 | PHE | CG-CD1 | -6.98 | 1.28 | 1.38 |
| 1 | C | 104 | GLY | N-CA | -6.98 | 1.35 | 1.46 |
| 1 | D | 213 | LEU | C-O | 6.98 | 1.36 | 1.23 |
| 1 | E | 375 | ILE | C-O | 6.98 | 1.36 | 1.23 |
| 1 | K | 62 | VAL | CB-CG1 | -6.98 | 1.38 | 1.52 |
| 1 | C | 187 | PRO | CG-CD | 6.97 | 1.73 | 1.50 |
| 1 | H | 234 | TYR | CD2-CE2 | -6.97 | 1.28 | 1.39 |
| 1 | F | 117 | ILE | CB-CG2 | 6.97 | 1.74 | 1.52 |
| 1 | K | 115 | VAL | CB-CG2 | -6.97 | 1.38 | 1.52 |
| 1 | L | 151 | TYR | CZ-OH | -6.97 | 1.26 | 1.37 |
| 1 | L | 302 | SER | CA-CB | -6.97 | 1.42 | 1.52 |
| 1 | H | 376 | PHE | CG-CD2 | 6.97 | 1.49 | 1.38 |
| 1 | A | 183 | GLY | C-O | 6.97 | 1.34 | 1.23 |
| 1 | E | 389 | THR | CB-CG2 | 6.97 | 1.75 | 1.52 |
| 1 | I | 117 | ILE | CA-CB | -6.96 | 1.38 | 1.54 |
| 1 | N | 257 | VAL | CA-CB | 6.96 | 1.69 | 1.54 |
| 1 | O | 124 | ASN | CB-CG | 6.96 | 1.67 | 1.51 |
| 1 | F | 353 | THR | CB-CG2 | 6.96 | 1.75 | 1.52 |
| 1 | J | 375 | ILE | C-O | 6.96 | 1.36 | 1.23 |
| 1 | E | 89 | SER | CB-OG | 6.96 | 1.51 | 1.42 |
| 1 | O | 141 | VAL | CB-CG1 | 6.96 | 1.67 | 1.52 |
| 1 | G | 172 | GLY | N-CA | 6.96 | 1.56 | 1.46 |
| 1 | H | 333 | VAL | CB-CG2 | -6.96 | 1.38 | 1.52 |
| 1 | K | 196 | GLN | C-O | -6.96 | 1.10 | 1.23 |
| 1 | L | 177 | GLN | CD-OE1 | 6.95 | 1.39 | 1.24 |
| 1 | I | 263 | ARG | CZ-NH2 | -6.95 | 1.24 | 1.33 |
| 1 | I | 466 | ARG | CB-CG | 6.95 | 1.71 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 61 | LEU | CG-CD1 | 6.94 | 1.77 | 1.51 |
| 1 | B | 271 | VAL | C-O | -6.94 | 1.10 | 1.23 |
| 1 | B | 140 | GLY | CA-C | 6.94 | 1.62 | 1.51 |
| 1 | H | 444 | TYR | CE2-CZ | 6.94 | 1.47 | 1.38 |
| 1 | N | 70 | TYR | CB-CG | -6.94 | 1.41 | 1.51 |
| 1 | N | 369 | GLU | CB-CG | 6.94 | 1.65 | 1.52 |
| 1 | E | 105 | VAL | CB-CG1 | -6.94 | 1.38 | 1.52 |
| 1 | G | 128 | ASP | C-O | 6.94 | 1.36 | 1.23 |
| 1 | N | 88 | THR | CB-CG2 | 6.94 | 1.75 | 1.52 |
| 1 | I | 269 | GLU | CD-OE1 | 6.94 | 1.33 | 1.25 |
| 1 | N | 294 | THR | CB-CG2 | -6.93 | 1.29 | 1.52 |
| 1 | O | 229 | CYS | CB-SG | 6.93 | 1.94 | 1.82 |
| 1 | N | 281 | GLY | CA-C | 6.93 | 1.62 | 1.51 |
| 1 | J | 97 | ARG | NE-CZ | 6.93 | 1.42 | 1.33 |
| 1 | E | 167 | GLU | CD-OE2 | 6.93 | 1.33 | 1.25 |
| 1 | A | 162 | LYS | CD-CE | 6.92 | 1.68 | 1.51 |
| 1 | B | 463 | PRO | CB-CG | 6.92 | 1.84 | 1.50 |
| 1 | J | 380 | LYS | CD-CE | 6.92 | 1.68 | 1.51 |
| 1 | M | 441 | LEU | CG-CD2 | 6.92 | 1.77 | 1.51 |
| 1 | F | 263 | ARG | CZ-NH2 | -6.92 | 1.24 | 1.33 |
| 1 | C | 135 | TYR | CD2-CE2 | -6.91 | 1.28 | 1.39 |
| 1 | F | 148 | SER | CB-OG | 6.91 | 1.51 | 1.42 |
| 1 | H | 331 | VAL | CB-CG1 | -6.91 | 1.38 | 1.52 |
| 1 | O | 86 | PRO | C-O | 6.91 | 1.37 | 1.23 |
| 1 | K | 343 | SER | C-O | 6.91 | 1.36 | 1.23 |
| 1 | M | 82 | LYS | CD-CE | 6.91 | 1.68 | 1.51 |
| 1 | G | 125 | LYS | CD-CE | 6.91 | 1.68 | 1.51 |
| 1 | J | 184 | ASP | C-O | 6.91 | 1.36 | 1.23 |
| 1 | F | 444 | TYR | CZ-OH | 6.91 | 1.49 | 1.37 |
| 1 | K | 105 | VAL | CB-CG1 | -6.90 | 1.38 | 1.52 |
| 1 | I | 189 | GLU | CD-OE1 | 6.90 | 1.33 | 1.25 |
| 1 | O | 240 | GLU | CD-OE1 | 6.90 | 1.33 | 1.25 |
| 1 | B | 400 | GLU | CB-CG | 6.90 | 1.65 | 1.52 |
| 1 | J | 311 | TYR | CD2-CE2 | -6.90 | 1.29 | 1.39 |
| 1 | M | 292 | PHE | CE2-CZ | -6.90 | 1.24 | 1.37 |
| 1 | H | 317 | GLN | CG-CD | 6.90 | 1.67 | 1.51 |
| 1 | M | 97 | ARG | CG-CD | 6.90 | 1.69 | 1.51 |
| 1 | C | 263 | ARG | NE-CZ | -6.89 | 1.24 | 1.33 |
| 1 | A | 145 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | B | 151 | TYR | CZ-OH | -6.89 | 1.26 | 1.37 |
| 1 | I | 106 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | L | 276 | TYR | CD1-CE1 | -6.89 | 1.29 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 368 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | D | 185 | CYS | CB-SG | 6.88 | 1.94 | 1.82 |
| 1 | D | 190 | LEU | C-O | 6.88 | 1.36 | 1.23 |
| 1 | J | 101 | ALA | C-O | 6.88 | 1.36 | 1.23 |
| 1 | L | 73 | PHE | CE2-CZ | -6.88 | 1.24 | 1.37 |
| 1 | N | 93 | PRO | CG-CD | 6.88 | 1.73 | 1.50 |
| 1 | F | 167 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | B | 325 | TRP | CG-CD1 | 6.87 | 1.46 | 1.36 |
| 1 | D | 68 | LEU | CA-C | -6.87 | 1.35 | 1.52 |
| 1 | D | 356 | LYS | CD-CE | 6.87 | 1.68 | 1.51 |
| 1 | O | 200 | MET | CG-SD | 6.87 | 1.99 | 1.81 |
| 1 | M | 215 | ALA | CA-CB | 6.87 | 1.66 | 1.52 |
| 1 | F | 343 | SER | CB-OG | 6.87 | 1.51 | 1.42 |
| 1 | E | 337 | THR | C-O | 6.87 | 1.36 | 1.23 |
| 1 | F | 256 | PHE | CE2-CZ | -6.87 | 1.24 | 1.37 |
| 1 | A | 351 | SER | CB-OG | -6.86 | 1.33 | 1.42 |
| 1 | H | 269 | GLU | CG-CD | 6.86 | 1.62 | 1.51 |
| 1 | L | 240 | GLU | CD-OE2 | -6.86 | 1.18 | 1.25 |
| 1 | M | 438 | GLU | CG-CD | 6.86 | 1.62 | 1.51 |
| 1 | N | 59 | LYS | CD-CE | 6.86 | 1.68 | 1.51 |
| 1 | O | 253 | GLU | CB-CG | 6.86 | 1.65 | 1.52 |
| 1 | B | 400 | GLU | CG-CD | 6.85 | 1.62 | 1.51 |
| 1 | E | 34 | TYR | CZ-OH | 6.85 | 1.49 | 1.37 |
| 1 | H | 144 | ARG | CZ-NH1 | -6.85 | 1.24 | 1.33 |
| 1 | J | 442 | LYS | CE-NZ | 6.85 | 1.66 | 1.49 |
| 1 | O | 322 | GLY | N-CA | 6.85 | 1.56 | 1.46 |
| 1 | H | 179 | ALA | CA-CB | 6.85 | 1.66 | 1.52 |
| 1 | L | 290 | ASN | CG-OD1 | -6.85 | 1.08 | 1.24 |
| 1 | B | 250 | LEU | N-CA | 6.85 | 1.60 | 1.46 |
| 1 | C | 344 | LEU | C-O | 6.85 | 1.36 | 1.23 |
| 1 | F | 31 | THR | CA-C | -6.85 | 1.35 | 1.52 |
| 1 | F | 97 | ARG | CB-CG | 6.84 | 1.71 | 1.52 |
| 1 | H | 100 | TRP | CD2-CE2 | -6.84 | 1.33 | 1.41 |
| 1 | I | 199 | ASP | CG-OD1 | 6.84 | 1.41 | 1.25 |
| 1 | D | 355 | TYR | CZ-OH | 6.84 | 1.49 | 1.37 |
| 1 | J | 234 | TYR | CD2-CE2 | -6.84 | 1.29 | 1.39 |
| 1 | L | 204 | GLY | C-O | -6.84 | 1.12 | 1.23 |
| 1 | L | 141 | VAL | CB-CG1 | -6.84 | 1.38 | 1.52 |
| 1 | L | 205 | PHE | CD1-CE1 | 6.84 | 1.52 | 1.39 |
| 1 | H | 336 | THR | CB-CG2 | -6.84 | 1.29 | 1.52 |
| 1 | H | 370 | TYR | CG-CD1 | -6.84 | 1.30 | 1.39 |
| 1 | O | 208 | MET | CG-SD | 6.84 | 1.99 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 176 | THR | CB-CG2 | 6.83 | 1.74 | 1.52 |
| 1 | H | 237 | MET | C-O | 6.83 | 1.36 | 1.23 |
| 1 | J | 446 | PHE | CD2-CE2 | 6.83 | 1.52 | 1.39 |
| 1 | O | 50 | PHE | CE1-CZ | 6.83 | 1.50 | 1.37 |
| 1 | O | 249 | TYR | CD1-CE1 | -6.83 | 1.29 | 1.39 |
| 1 | O | 370 | TYR | CZ-OH | 6.83 | 1.49 | 1.37 |
| 1 | D | 211 | THR | C-O | -6.83 | 1.10 | 1.23 |
| 1 | E | 181 | GLN | CG-CD | 6.83 | 1.66 | 1.51 |
| 1 | H | 83 | PHE | CE2-CZ | 6.83 | 1.50 | 1.37 |
| 1 | H | 91 | TYR | CG-CD2 | 6.83 | 1.48 | 1.39 |
| 1 | N | 28 | VAL | C-O | 6.83 | 1.36 | 1.23 |
| 1 | A | 400 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | F | 251 | ARG | CZ-NH1 | 6.82 | 1.42 | 1.33 |
| 1 | M | 187 | PRO | CG-CD | 6.82 | 1.73 | 1.50 |
| 1 | A | 231 | TYR | CE2-CZ | 6.82 | 1.47 | 1.38 |
| 1 | G | 75 | ILE | C-O | 6.81 | 1.36 | 1.23 |
| 1 | M | 139 | ALA | C-N | 6.81 | 1.45 | 1.33 |
| 1 | I | 174 | PRO | N-CD | 6.81 | 1.57 | 1.47 |
| 1 | N | 248 | PHE | CD1-CE1 | 6.81 | 1.52 | 1.39 |
| 1 | H | 310 | PRO | N-CA | -6.81 | 1.35 | 1.47 |
| 1 | L | 312 | TRP | CB-CG | -6.81 | 1.38 | 1.50 |
| 1 | A | 34 | TYR | CD2-CE2 | -6.80 | 1.29 | 1.39 |
| 1 | G | 230 | LYS | CB-CG | 6.80 | 1.71 | 1.52 |
| 1 | O | 388 | MET | C-O | 6.80 | 1.36 | 1.23 |
| 1 | A | 380 | LYS | CE-NZ | 6.80 | 1.66 | 1.49 |
| 1 | J | 315 | ARG | C-O | 6.80 | 1.36 | 1.23 |
| 1 | L | 472 | LEU | N-CA | 6.80 | 1.59 | 1.46 |
| 1 | D | 100 | TRP | CE3-CZ3 | 6.80 | 1.50 | 1.38 |
| 1 | L | 152 | LYS | CB-CG | -6.80 | 1.34 | 1.52 |
| 1 | A | 468 | PHE | CG-CD2 | -6.80 | 1.28 | 1.38 |
| 1 | K | 169 | TRP | CB-CG | -6.80 | 1.38 | 1.50 |
| 1 | K | 330 | PHE | CD1-CE1 | -6.80 | 1.25 | 1.39 |
| 1 | N | 49 | TYR | CE2-CZ | 6.80 | 1.47 | 1.38 |
| 1 | F | 347 | ALA | C-O | 6.79 | 1.36 | 1.23 |
| 1 | J | 399 | LEU | N-CA | 6.79 | 1.59 | 1.46 |
| 1 | O | 108 | GLY | N-CA | 6.79 | 1.56 | 1.46 |
| 1 | F | 376 | PHE | CD1-CE1 | -6.79 | 1.25 | 1.39 |
| 1 | C | 295 | PRO | CA-C | -6.79 | 1.39 | 1.52 |
| 1 | A | 307 | PHE | CD1-CE1 | -6.79 | 1.25 | 1.39 |
| 1 | H | 355 | TYR | CE2-CZ | -6.78 | 1.29 | 1.38 |
| 1 | H | 266 | THR | CB-CG2 | 6.78 | 1.74 | 1.52 |
| 1 | J | 109 | ARG | CZ-NH1 | 6.78 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | M | 259 | HIS | C-O | 6.78 | 1.36 | 1.23 |
| 1 | I | 358 | THR | CB-CG2 | 6.77 | 1.74 | 1.52 |
| 1 | C | 241 | PRO | CB-CG | 6.77 | 1.83 | 1.50 |
| 1 | E | 316 | ALA | CA-CB | -6.77 | 1.38 | 1.52 |
| 1 | M | 26 | GLU | CB-CG | -6.77 | 1.39 | 1.52 |
| 1 | M | 453 | GLU | CD-OE2 | 6.77 | 1.33 | 1.25 |
| 1 | M | 27 | TYR | CE2-CZ | -6.77 | 1.29 | 1.38 |
| 1 | N | 306 | ILE | C-O | -6.77 | 1.10 | 1.23 |
| 1 | O | 91 | TYR | CE1-CZ | 6.76 | 1.47 | 1.38 |
| 1 | F | 151 | TYR | CD1-CE1 | -6.76 | 1.29 | 1.39 |
| 1 | G | 337 | THR | CB-CG2 | 6.76 | 1.74 | 1.52 |
| 1 | K | 443 | LYS | C-O | 6.76 | 1.36 | 1.23 |
| 1 | O | 369 | GLU | CB-CG | 6.76 | 1.65 | 1.52 |
| 1 | A | 241 | PRO | N-CA | 6.76 | 1.58 | 1.47 |
| 1 | F | 468 | PHE | CG-CD2 | -6.75 | 1.28 | 1.38 |
| 1 | M | 125 | LYS | CB-CG | -6.75 | 1.34 | 1.52 |
| 1 | M | 372 | LEU | C-O | -6.75 | 1.10 | 1.23 |
| 1 | H | 258 | ARG | CZ-NH2 | -6.75 | 1.24 | 1.33 |
| 1 | K | 312 | TRP | CG-CD1 | -6.75 | 1.27 | 1.36 |
| 1 | I | 205 | PHE | CE2-CZ | 6.75 | 1.50 | 1.37 |
| 1 | A | 135 | TYR | CE1-CZ | 6.74 | 1.47 | 1.38 |
| 1 | B | 276 | TYR | CD2-CE2 | -6.74 | 1.29 | 1.39 |
| 1 | G | 25 | ASP | CB-CG | 6.74 | 1.66 | 1.51 |
| 1 | G | 334 | VAL | CB-CG1 | -6.74 | 1.38 | 1.52 |
| 1 | B | 106 | GLU | CD-OE1 | 6.74 | 1.33 | 1.25 |
| 1 | I | 292 | PHE | CG-CD1 | 6.74 | 1.48 | 1.38 |
| 1 | L | 180 | VAL | CB-CG2 | 6.74 | 1.67 | 1.52 |
| 1 | M | 139 | ALA | C-O | 6.74 | 1.36 | 1.23 |
| 1 | I | 75 | ILE | CB-CG2 | 6.74 | 1.73 | 1.52 |
| 1 | M | 185 | CYS | CB-SG | -6.74 | 1.70 | 1.82 |
| 1 | A | 296 | SER | CA-CB | -6.73 | 1.42 | 1.52 |
| 1 | A | 390 | TYR | CG-CD2 | -6.73 | 1.30 | 1.39 |
| 1 | J | 338 | ARG | CG-CD | 6.73 | 1.68 | 1.51 |
| 1 | L | 34 | TYR | CD1-CE1 | -6.73 | 1.29 | 1.39 |
| 1 | G | 91 | TYR | CE2-CZ | 6.73 | 1.47 | 1.38 |
| 1 | I | 280 | SER | CB-OG | 6.73 | 1.50 | 1.42 |
| 1 | N | 147 | ILE | CA-CB | 6.73 | 1.70 | 1.54 |
| 1 | N | 400 | GLU | CD-OE1 | 6.73 | 1.33 | 1.25 |
| 1 | D | 197 | ASP | C-O | -6.73 | 1.10 | 1.23 |
| 1 | G | 26 | GLU | CD-OE1 | 6.73 | 1.33 | 1.25 |
| 1 | G | 111 | GLN | CB-CG | -6.73 | 1.34 | 1.52 |
| 1 | G | 253 | GLU | CB-CG | 6.73 | 1.65 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 118 | SER | C-O | 6.73 | 1.36 | 1.23 |
| 1 | N | 472 | LEU | C-OXT | 6.73 | 1.36 | 1.23 |
| 1 | K | 107 | VAL | CB-CG1 | -6.72 | 1.38 | 1.52 |
| 1 | M | 201 | VAL | CB-CG1 | -6.72 | 1.38 | 1.52 |
| 1 | B | 167 | GLU | CD-OE2 | 6.72 | 1.33 | 1.25 |
| 1 | D | 109 | ARG | CD-NE | 6.72 | 1.57 | 1.46 |
| 1 | N | 107 | VAL | CB-CG1 | -6.72 | 1.38 | 1.52 |
| 1 | L | 205 | PHE | CD2-CE2 | 6.72 | 1.52 | 1.39 |
| 1 | H | 315 | ARG | CZ-NH2 | 6.72 | 1.41 | 1.33 |
| 1 | J | 446 | PHE | CE1-CZ | 6.72 | 1.50 | 1.37 |
| 1 | D | 227 | SER | CB-OG | 6.71 | 1.50 | 1.42 |
| 1 | H | 169 | TRP | CE3-CZ3 | -6.71 | 1.27 | 1.38 |
| 1 | I | 40 | SER | CA-CB | 6.71 | 1.63 | 1.52 |
| 1 | B | 291 | TYR | CE1-CZ | -6.71 | 1.29 | 1.38 |
| 1 | F | 140 | GLY | CA-C | 6.71 | 1.62 | 1.51 |
| 1 | I | 40 | SER | C-O | 6.71 | 1.36 | 1.23 |
| 1 | H | 268 | GLY | C-O | 6.71 | 1.34 | 1.23 |
| 1 | B | 210 | PHE | CD1-CE1 | -6.71 | 1.25 | 1.39 |
| 1 | L | 156 | LEU | C-O | 6.71 | 1.36 | 1.23 |
| 1 | N | 220 | VAL | CB-CG2 | -6.71 | 1.38 | 1.52 |
| 1 | L | 247 | PHE | CD1-CE1 | -6.71 | 1.25 | 1.39 |
| 1 | J | 131 | ASN | CB-CG | 6.70 | 1.66 | 1.51 |
| 1 | L | 282 | SER | C-O | 6.70 | 1.36 | 1.23 |
| 1 | G | 178 | VAL | C-O | 6.70 | 1.36 | 1.23 |
| 1 | G | 325 | TRP | CG-CD1 | 6.70 | 1.46 | 1.36 |
| 1 | I | 193 | THR | CB-CG2 | 6.70 | 1.74 | 1.52 |
| 1 | J | 25 | ASP | CG-OD2 | 6.70 | 1.40 | 1.25 |
| 1 | A | 440 | PRO | CG-CD | 6.70 | 1.72 | 1.50 |
| 1 | O | 49 | TYR | CG-CD2 | 6.69 | 1.47 | 1.39 |
| 1 | B | 195 | ILE | N-CA | -6.69 | 1.32 | 1.46 |
| 1 | G | 107 | VAL | CA-CB | -6.69 | 1.40 | 1.54 |
| 1 | D | 72 | VAL | CB-CG2 | -6.69 | 1.38 | 1.52 |
| 1 | G | 114 | GLY | C-O | -6.69 | 1.12 | 1.23 |
| 1 | D | 123 | LEU | CG-CD2 | 6.68 | 1.76 | 1.51 |
| 1 | J | 54 | LYS | CE-NZ | 6.68 | 1.65 | 1.49 |
| 1 | J | 85 | PHE | C-O | 6.68 | 1.36 | 1.23 |
| 1 | G | 446 | PHE | CB-CG | -6.68 | 1.40 | 1.51 |
| 1 | E | 199 | ASP | CG-OD2 | 6.67 | 1.40 | 1.25 |
| 1 | E | 97 | ARG | CZ-NH2 | 6.67 | 1.41 | 1.33 |
| 1 | C | 181 | GLN | CD-OE1 | 6.66 | 1.38 | 1.24 |
| 1 | M | 201 | VAL | CB-CG2 | -6.66 | 1.38 | 1.52 |
| 1 | C | 107 | VAL | CB-CG1 | -6.66 | 1.38 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 347 | ALA | C-O | 6.66 | 1.36 | 1.23 |
| 1 | H | 400 | GLU | CG-CD | 6.66 | 1.61 | 1.51 |
| 1 | L | 49 | TYR | CD1-CE1 | -6.66 | 1.29 | 1.39 |
| 1 | E | 234 | TYR | CE2-CZ | -6.66 | 1.29 | 1.38 |
| 1 | C | 349 | SER | CA-CB | 6.65 | 1.62 | 1.52 |
| 1 | A | 365 | ARG | CZ-NH2 | 6.65 | 1.41 | 1.33 |
| 1 | B | 85 | PHE | CE2-CZ | 6.65 | 1.50 | 1.37 |
| 1 | I | 152 | LYS | CB-CG | 6.65 | 1.70 | 1.52 |
| 1 | H | 438 | GLU | CG-CD | 6.65 | 1.61 | 1.51 |
| 1 | K | 240 | GLU | CD-OE1 | 6.65 | 1.32 | 1.25 |
| 1 | B | 171 | LYS | CG-CD | 6.65 | 1.75 | 1.52 |
| 1 | E | 99 | VAL | CB-CG1 | -6.65 | 1.38 | 1.52 |
| 1 | F | 26 | GLU | CG-CD | -6.65 | 1.42 | 1.51 |
| 1 | L | 341 | ASN | C-O | 6.65 | 1.35 | 1.23 |
| 1 | L | 144 | ARG | CD-NE | -6.65 | 1.35 | 1.46 |
| 1 | A | 105 | VAL | CA-CB | -6.64 | 1.40 | 1.54 |
| 1 | D | 174 | PRO | CG-CD | 6.64 | 1.72 | 1.50 |
| 1 | F | 125 | LYS | CD-CE | 6.64 | 1.67 | 1.51 |
| 1 | M | 317 | GLN | N-CA | 6.64 | 1.59 | 1.46 |
| 1 | I | 230 | LYS | CE-NZ | 6.64 | 1.65 | 1.49 |
| 1 | E | 300 | VAL | CB-CG1 | 6.64 | 1.66 | 1.52 |
| 1 | M | 162 | LYS | CE-NZ | 6.64 | 1.65 | 1.49 |
| 1 | N | 299 | MET | C-O | 6.64 | 1.35 | 1.23 |
| 1 | M | 50 | PHE | CG-CD1 | -6.64 | 1.28 | 1.38 |
| 1 | N | 279 | GLY | C-O | -6.64 | 1.13 | 1.23 |
| 1 | E | 67 | GLY | N-CA | 6.63 | 1.56 | 1.46 |
| 1 | O | 33 | ILE | C-O | 6.63 | 1.35 | 1.23 |
| 1 | E | 82 | LYS | CD-CE | 6.63 | 1.67 | 1.51 |
| 1 | K | 70 | TYR | CG-CD1 | -6.63 | 1.30 | 1.39 |
| 1 | N | 296 | SER | C-O | 6.63 | 1.35 | 1.23 |
| 1 | E | 137 | ALA | CA-CB | 6.63 | 1.66 | 1.52 |
| 1 | F | 205 | PHE | CE2-CZ | 6.63 | 1.50 | 1.37 |
| 1 | O | 376 | PHE | CD2-CE2 | -6.63 | 1.25 | 1.39 |
| 1 | E | 459 | LEU | C-O | -6.63 | 1.10 | 1.23 |
| 1 | O | 363 | TYR | CD1-CE1 | 6.63 | 1.49 | 1.39 |
| 1 | I | 150 | ASP | CG-OD2 | 6.62 | 1.40 | 1.25 |
| 1 | B | 23 | SER | CB-OG | 6.62 | 1.50 | 1.42 |
| 1 | F | 379 | CYS | CB-SG | -6.62 | 1.71 | 1.82 |
| 1 | H | 379 | CYS | CB-SG | -6.62 | 1.71 | 1.82 |
| 1 | O | 210 | PHE | CG-CD2 | 6.62 | 1.48 | 1.38 |
| 1 | F | 160 | GLY | C-O | -6.61 | 1.13 | 1.23 |
| 1 | F | 387 | VAL | CB-CG2 | 6.61 | 1.66 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 194 | VAL | CA-CB | -6.61 | 1.40 | 1.54 |
| 1 | B | 104 | GLY | C-O | 6.61 | 1.34 | 1.23 |
| 1 | I | 256 | PHE | CG-CD1 | -6.61 | 1.28 | 1.38 |
| 1 | J | 466 | ARG | C-O | 6.61 | 1.35 | 1.23 |
| 1 | K | 32 | ASN | CB-CG | 6.61 | 1.66 | 1.51 |
| 1 | H | 109 | ARG | CD-NE | 6.61 | 1.57 | 1.46 |
| 1 | L | 139 | ALA | C-O | 6.61 | 1.35 | 1.23 |
| 1 | O | 448 | GLU | CG-CD | 6.61 | 1.61 | 1.51 |
| 1 | B | 327 | ASN | CB-CG | 6.61 | 1.66 | 1.51 |
| 1 | F | 152 | LYS | CE-NZ | 6.61 | 1.65 | 1.49 |
| 1 | G | 202 | ASP | CG-OD1 | 6.61 | 1.40 | 1.25 |
| 1 | B | 324 | CYS | CB-SG | 6.60 | 1.93 | 1.82 |
| 1 | J | 135 | TYR | CD1-CE1 | -6.60 | 1.29 | 1.39 |
| 1 | K | 376 | PHE | CD2-CE2 | -6.60 | 1.26 | 1.39 |
| 1 | M | 98 | LEU | CG-CD1 | 6.60 | 1.76 | 1.51 |
| 1 | O | 238 | VAL | CB-CG1 | 6.60 | 1.66 | 1.52 |
| 1 | B | 374 | PHE | CD1-CE1 | 6.60 | 1.52 | 1.39 |
| 1 | C | 438 | GLU | CD-OE2 | 6.60 | 1.32 | 1.25 |
| 1 | H | 350 | THR | CA-CB | 6.60 | 1.70 | 1.53 |
| 1 | L | 345 | CYS | CB-SG | -6.60 | 1.71 | 1.82 |
| 1 | O | 81 | ASN | CG-ND2 | 6.60 | 1.49 | 1.32 |
| 1 | I | 180 | VAL | CB-CG2 | 6.60 | 1.66 | 1.52 |
| 1 | N | 210 | PHE | CD2-CE2 | -6.59 | 1.26 | 1.39 |
| 1 | A | 176 | THR | CB-CG2 | 6.59 | 1.74 | 1.52 |
| 1 | C | 210 | PHE | CE1-CZ | 6.59 | 1.49 | 1.37 |
| 1 | K | 150 | ASP | C-O | -6.59 | 1.10 | 1.23 |
| 1 | O | 231 | TYR | CD2-CE2 | 6.59 | 1.49 | 1.39 |
| 1 | D | 173 | SER | CA-CB | 6.58 | 1.62 | 1.52 |
| 1 | I | 337 | THR | C-O | 6.58 | 1.35 | 1.23 |
| 1 | E | 210 | PHE | CD2-CE2 | -6.58 | 1.26 | 1.39 |
| 1 | D | 63 | PRO | CB-CG | 6.58 | 1.82 | 1.50 |
| 1 | K | 132 | ALA | CA-CB | -6.58 | 1.38 | 1.52 |
| 1 | N | 38 | GLY | C-O | 6.58 | 1.34 | 1.23 |
| 1 | K | 444 | TYR | CG-CD2 | -6.58 | 1.30 | 1.39 |
| 1 | N | 23 | SER | CB-OG | 6.58 | 1.50 | 1.42 |
| 1 | N | 135 | TYR | CD2-CE2 | -6.58 | 1.29 | 1.39 |
| 1 | C | 201 | VAL | CB-CG2 | 6.57 | 1.66 | 1.52 |
| 1 | C | 72 | VAL | CB-CG1 | -6.57 | 1.39 | 1.52 |
| 1 | I | 135 | TYR | CE1-CZ | -6.56 | 1.30 | 1.38 |
| 1 | N | 253 | GLU | CB-CG | 6.56 | 1.64 | 1.52 |
| 1 | C | 173 | SER | CB-OG | 6.56 | 1.50 | 1.42 |
| 1 | B | 358 | THR | CB-CG2 | 6.56 | 1.74 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 378 | LEU | C-O | -6.56 | 1.10 | 1.23 |
| 1 | K | 343 | SER | CB-OG | 6.56 | 1.50 | 1.42 |
| 1 | N | 65 | VAL | CB-CG1 | -6.56 | 1.39 | 1.52 |
| 1 | N | 319 | HIS | CA-CB | -6.56 | 1.39 | 1.53 |
| 1 | J | 304 | ALA | CA-CB | -6.56 | 1.38 | 1.52 |
| 1 | K | 322 | GLY | N-CA | 6.56 | 1.55 | 1.46 |
| 1 | M | 64 | LYS | CD-CE | 6.56 | 1.67 | 1.51 |
| 1 | N | 54 | LYS | CE-NZ | 6.56 | 1.65 | 1.49 |
| 1 | B | 181 | GLN | CG-CD | 6.56 | 1.66 | 1.51 |
| 1 | B | 355 | TYR | CE2-CZ | 6.56 | 1.47 | 1.38 |
| 1 | A | 447 | TRP | CB-CG | -6.55 | 1.38 | 1.50 |
| 1 | M | 205 | PHE | CE1-CZ | -6.55 | 1.24 | 1.37 |
| 1 | C | 148 | SER | CA-CB | -6.55 | 1.43 | 1.52 |
| 1 | D | 309 | LYS | CB-CG | 6.55 | 1.70 | 1.52 |
| 1 | E | 392 | HIS | C-O | 6.55 | 1.35 | 1.23 |
| 1 | B | 323 | ILE | C-O | 6.55 | 1.35 | 1.23 |
| 1 | D | 139 | ALA | C-N | 6.55 | 1.44 | 1.33 |
| 1 | I | 70 | TYR | CE2-CZ | -6.55 | 1.30 | 1.38 |
| 1 | A | 298 | SER | CB-OG | 6.54 | 1.50 | 1.42 |
| 1 | E | 213 | LEU | CG-CD1 | 6.54 | 1.76 | 1.51 |
| 1 | H | 324 | CYS | CB-SG | 6.54 | 1.93 | 1.82 |
| 1 | A | 59 | LYS | CE-NZ | 6.54 | 1.65 | 1.49 |
| 1 | F | 325 | TRP | CE3-CZ3 | 6.54 | 1.49 | 1.38 |
| 1 | K | 175 | CYS | C-O | 6.54 | 1.35 | 1.23 |
| 1 | O | 370 | TYR | CE1-CZ | 6.54 | 1.47 | 1.38 |
| 1 | B | 177 | GLN | CB-CG | 6.54 | 1.70 | 1.52 |
| 1 | B | 220 | VAL | CB-CG1 | -6.54 | 1.39 | 1.52 |
| 1 | G | 114 | GLY | N-CA | 6.54 | 1.55 | 1.46 |
| 1 | B | 249 | TYR | C-O | 6.54 | 1.35 | 1.23 |
| 1 | G | 332 | THR | CB-OG1 | 6.53 | 1.56 | 1.43 |
| 1 | O | 300 | VAL | CB-CG1 | 6.53 | 1.66 | 1.52 |
| 1 | L | 97 | ARG | CZ-NH1 | 6.53 | 1.41 | 1.33 |
| 1 | M | 282 | SER | CB-OG | 6.53 | 1.50 | 1.42 |
| 1 | H | 242 | TYR | C-O | 6.53 | 1.35 | 1.23 |
| 1 | E | 160 | GLY | C-O | 6.52 | 1.34 | 1.23 |
| 1 | J | 453 | GLU | CB-CG | 6.52 | 1.64 | 1.52 |
| 1 | O | 98 | LEU | CG-CD1 | 6.52 | 1.75 | 1.51 |
| 1 | F | 184 | ASP | CG-OD1 | 6.52 | 1.40 | 1.25 |
| 1 | I | 390 | TYR | CE2-CZ | 6.52 | 1.47 | 1.38 |
| 1 | G | 49 | TYR | C-O | 6.52 | 1.35 | 1.23 |
| 1 | K | 348 | ILE | CA-CB | -6.52 | 1.39 | 1.54 |
| 1 | K | 362 | GLU | CA-CB | -6.52 | 1.39 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | M | 164 | PRO | CA-CB | 6.52 | 1.66 | 1.53 |
| 1 | D | 370 | TYR | CG-CD1 | -6.52 | 1.30 | 1.39 |
| 1 | M | 131 | ASN | C-O | -6.52 | 1.10 | 1.23 |
| 1 | D | 450 | ASN | C-O | 6.52 | 1.35 | 1.23 |
| 1 | C | 462 | PHE | CB-CG | -6.51 | 1.40 | 1.51 |
| 1 | G | 58 | ASN | C-O | 6.51 | 1.35 | 1.23 |
| 1 | I | 35 | TYR | CD1-CE1 | -6.51 | 1.29 | 1.39 |
| 1 | I | 152 | LYS | C-O | 6.51 | 1.35 | 1.23 |
| 1 | L | 34 | TYR | CG-CD1 | -6.51 | 1.30 | 1.39 |
| 1 | B | 28 | VAL | CB-CG1 | 6.51 | 1.66 | 1.52 |
| 1 | K | 385 | ALA | CA-CB | 6.51 | 1.66 | 1.52 |
| 1 | M | 370 | TYR | CG-CD1 | -6.51 | 1.30 | 1.39 |
| 1 | N | 330 | PHE | CE1-CZ | 6.51 | 1.49 | 1.37 |
| 1 | B | 114 | GLY | C-O | 6.50 | 1.34 | 1.23 |
| 1 | B | 301 | THR | CB-CG2 | 6.50 | 1.73 | 1.52 |
| 1 | F | 241 | PRO | CB-CG | 6.50 | 1.82 | 1.50 |
| 1 | D | 276 | TYR | CE2-CZ | 6.50 | 1.47 | 1.38 |
| 1 | F | 70 | TYR | CG-CD1 | -6.50 | 1.30 | 1.39 |
| 1 | F | 70 | TYR | C-O | -6.50 | 1.10 | 1.23 |
| 1 | O | 109 | ARG | C-O | 6.50 | 1.35 | 1.23 |
| 1 | C | 115 | VAL | CA-CB | -6.50 | 1.41 | 1.54 |
| 1 | D | 89 | SER | C-O | 6.50 | 1.35 | 1.23 |
| 1 | H | 323 | ILE | C-O | 6.50 | 1.35 | 1.23 |
| 1 | N | 181 | GLN | CD-OE1 | 6.50 | 1.38 | 1.24 |
| 1 | C | 254 | GLN | CD-OE1 | -6.50 | 1.09 | 1.24 |
| 1 | J | 240 | GLU | CB-CG | 6.50 | 1.64 | 1.52 |
| 1 | N | 210 | PHE | CB-CG | 6.50 | 1.62 | 1.51 |
| 1 | J | 361 | LYS | CD-CE | 6.50 | 1.67 | 1.51 |
| 1 | G | 70 | TYR | CG-CD1 | -6.49 | 1.30 | 1.39 |
| 1 | L | 352 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | E | 309 | LYS | C-O | 6.49 | 1.35 | 1.23 |
| 1 | O | 177 | GLN | CD-OE1 | 6.49 | 1.38 | 1.24 |
| 1 | M | 130 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | B | 294 | THR | CB-CG2 | -6.49 | 1.30 | 1.52 |
| 1 | K | 253 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | O | 162 | LYS | CE-NZ | 6.49 | 1.65 | 1.49 |
| 1 | D | 467 | LYS | CB-CG | 6.48 | 1.70 | 1.52 |
| 1 | J | 146 | CYS | CB-SG | -6.48 | 1.71 | 1.82 |
| 1 | E | 322 | GLY | C-O | 6.48 | 1.34 | 1.23 |
| 1 | A | 35 | TYR | CE1-CZ | -6.48 | 1.30 | 1.38 |
| 1 | A | 62 | VAL | CB-CG2 | 6.48 | 1.66 | 1.52 |
| 1 | C | 150 | ASP | C-O | -6.48 | 1.11 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 144 | ARG | CZ-NH1 | -6.48 | 1.24 | 1.33 |
| 1 | C | 178 | VAL | C-O | 6.47 | 1.35 | 1.23 |
| 1 | G | 370 | TYR | CD2-CE2 | 6.47 | 1.49 | 1.39 |
| 1 | B | 114 | GLY | N-CA | 6.47 | 1.55 | 1.46 |
| 1 | I | 258 | ARG | CZ-NH1 | 6.47 | 1.41 | 1.33 |
| 1 | G | 402 | TRP | CG-CD1 | 6.47 | 1.45 | 1.36 |
| 1 | B | 307 | PHE | CB-CG | -6.47 | 1.40 | 1.51 |
| 1 | G | 325 | TRP | CD2-CE2 | 6.47 | 1.49 | 1.41 |
| 1 | I | 219 | GLU | CD-OE1 | -6.47 | 1.18 | 1.25 |
| 1 | F | 171 | LYS | CG-CD | 6.47 | 1.74 | 1.52 |
| 1 | N | 57 | ASN | CG-ND2 | 6.47 | 1.49 | 1.32 |
| 1 | O | 202 | ASP | N-CA | -6.47 | 1.33 | 1.46 |
| 1 | D | 363 | TYR | CZ-OH | 6.46 | 1.48 | 1.37 |
| 1 | F | 95 | THR | CB-CG2 | -6.46 | 1.31 | 1.52 |
| 1 | I | 189 | GLU | CG-CD | 6.46 | 1.61 | 1.51 |
| 1 | B | 272 | PRO | CG-CD | 6.46 | 1.72 | 1.50 |
| 1 | O | 330 | PHE | CB-CG | 6.46 | 1.62 | 1.51 |
| 1 | I | 53 | LYS | CE-NZ | 6.46 | 1.65 | 1.49 |
| 1 | K | 298 | SER | CB-OG | 6.46 | 1.50 | 1.42 |
| 1 | M | 87 | ASP | C-O | 6.46 | 1.35 | 1.23 |
| 1 | M | 273 | ASP | N-CA | 6.46 | 1.59 | 1.46 |
| 1 | F | 257 | VAL | CB-CG1 | -6.46 | 1.39 | 1.52 |
| 1 | K | 375 | ILE | C-O | 6.45 | 1.35 | 1.23 |
| 1 | O | 271 | VAL | CB-CG1 | 6.45 | 1.66 | 1.52 |
| 1 | F | 178 | VAL | CA-CB | 6.45 | 1.68 | 1.54 |
| 1 | B | 438 | GLU | C-O | 6.45 | 1.35 | 1.23 |
| 1 | D | 181 | GLN | CD-OE1 | 6.45 | 1.38 | 1.24 |
| 1 | E | 280 | SER | CA-CB | 6.45 | 1.62 | 1.52 |
| 1 | J | 132 | ALA | CA-CB | 6.45 | 1.66 | 1.52 |
| 1 | N | 225 | CYS | CB-SG | 6.45 | 1.93 | 1.82 |
| 1 | M | 380 | LYS | C-O | -6.45 | 1.11 | 1.23 |
| 1 | B | 306 | ILE | C-O | -6.45 | 1.11 | 1.23 |
| 1 | A | 172 | GLY | C-O | 6.44 | 1.33 | 1.23 |
| 1 | H | 466 | ARG | NE-CZ | 6.44 | 1.41 | 1.33 |
| 1 | J | 234 | TYR | CD1-CE1 | -6.44 | 1.29 | 1.39 |
| 1 | F | 169 | TRP | CE3-CZ3 | -6.44 | 1.27 | 1.38 |
| 1 | N | 130 | GLU | CD-OE1 | -6.44 | 1.18 | 1.25 |
| 1 | N | 334 | VAL | CB-CG1 | -6.44 | 1.39 | 1.52 |
| 1 | O | 266 | THR | CB-CG2 | 6.44 | 1.73 | 1.52 |
| 1 | A | 256 | PHE | CD1-CE1 | -6.44 | 1.26 | 1.39 |
| 1 | E | 199 | ASP | C-O | -6.43 | 1.11 | 1.23 |
| 1 | F | 400 | GLU | CD-OE1 | 6.43 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 83 | PHE | C-O | 6.43 | 1.35 | 1.23 |
| 1 | B | 303 | ASP | C-O | -6.43 | 1.11 | 1.23 |
| 1 | K | 370 | TYR | CE2-CZ | -6.43 | 1.30 | 1.38 |
| 1 | K | 387 | VAL | CB-CG2 | 6.43 | 1.66 | 1.52 |
| 1 | A | 117 | ILE | CA-CB | -6.43 | 1.40 | 1.54 |
| 1 | E | 341 | ASN | C-O | -6.43 | 1.11 | 1.23 |
| 1 | K | 70 | TYR | CG-CD2 | -6.43 | 1.30 | 1.39 |
| 1 | M | 229 | CYS | CB-SG | -6.43 | 1.71 | 1.82 |
| 1 | O | 138 | ASN | CG-ND2 | 6.43 | 1.49 | 1.32 |
| 1 | C | 26 | GLU | CD-OE1 | 6.42 | 1.32 | 1.25 |
| 1 | O | 49 | TYR | CG-CD1 | 6.42 | 1.47 | 1.39 |
| 1 | C | 314 | GLN | CD-OE1 | 6.42 | 1.38 | 1.24 |
| 1 | I | 362 | GLU | CG-CD | 6.42 | 1.61 | 1.51 |
| 1 | N | 34 | TYR | CE2-CZ | -6.42 | 1.30 | 1.38 |
| 1 | F | 330 | PHE | CD1-CE1 | -6.42 | 1.26 | 1.39 |
| 1 | H | 209 | ASP | CG-OD2 | 6.42 | 1.40 | 1.25 |
| 1 | K | 82 | LYS | CD-CE | 6.42 | 1.67 | 1.51 |
| 1 | K | 338 | ARG | CZ-NH2 | 6.42 | 1.41 | 1.33 |
| 1 | M | 370 | TYR | CG-CD2 | -6.42 | 1.30 | 1.39 |
| 1 | D | 312 | TRP | CA-CB | -6.42 | 1.39 | 1.53 |
| 1 | F | 245 | SER | CB-OG | 6.41 | 1.50 | 1.42 |
| 1 | G | 202 | ASP | N-CA | -6.41 | 1.33 | 1.46 |
| 1 | K | 151 | TYR | CD1-CE1 | -6.41 | 1.29 | 1.39 |
| 1 | L | 472 | LEU | C-OXT | 6.41 | 1.35 | 1.23 |
| 1 | B | 272 | PRO | CB-CG | 6.41 | 1.82 | 1.50 |
| 1 | F | 218 | SER | CB-OG | -6.41 | 1.33 | 1.42 |
| 1 | K | 455 | PHE | CE1-CZ | -6.41 | 1.25 | 1.37 |
| 1 | N | 292 | PHE | C-O | -6.41 | 1.11 | 1.23 |
| 1 | N | 211 | THR | CB-CG2 | -6.41 | 1.31 | 1.52 |
| 1 | F | 107 | VAL | CA-CB | -6.41 | 1.41 | 1.54 |
| 1 | A | 105 | VAL | CB-CG2 | 6.41 | 1.66 | 1.52 |
| 1 | A | 98 | LEU | C-O | 6.40 | 1.35 | 1.23 |
| 1 | E | 32 | ASN | CB-CG | 6.40 | 1.65 | 1.51 |
| 1 | K | 34 | TYR | CE2-CZ | -6.40 | 1.30 | 1.38 |
| 1 | L | 307 | PHE | CB-CG | -6.40 | 1.40 | 1.51 |
| 1 | N | 189 | GLU | CD-OE1 | 6.40 | 1.32 | 1.25 |
| 1 | D | 376 | PHE | CA-CB | -6.40 | 1.39 | 1.53 |
| 1 | E | 152 | LYS | CB-CG | -6.40 | 1.35 | 1.52 |
| 1 | C | 232 | PRO | N-CA | -6.40 | 1.36 | 1.47 |
| 1 | F | 356 | LYS | CD-CE | 6.40 | 1.67 | 1.51 |
| 1 | E | 393 | SER | C-O | 6.40 | 1.35 | 1.23 |
| 1 | G | 241 | PRO | CB-CG | 6.39 | 1.81 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | L | 54 | LYS | CE-NZ | 6.39 | 1.65 | 1.49 |
| 1 | B | 438 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 1 | A | 22 | VAL | CB-CG1 | 6.39 | 1.66 | 1.52 |
| 1 | J | 96 | GLN | CB-CG | 6.39 | 1.69 | 1.52 |
| 1 | O | 116 | GLY | C-O | 6.39 | 1.33 | 1.23 |
| 1 | K | 159 | ILE | CB-CG2 | -6.39 | 1.33 | 1.52 |
| 1 | M | 359 | ASN | CG-ND2 | 6.39 | 1.48 | 1.32 |
| 1 | E | 91 | TYR | CE1-CZ | 6.38 | 1.46 | 1.38 |
| 1 | C | 253 | GLU | CG-CD | -6.38 | 1.42 | 1.51 |
| 1 | G | 216 | ASN | C-O | -6.38 | 1.11 | 1.23 |
| 1 | N | 355 | TYR | CB-CG | 6.38 | 1.61 | 1.51 |
| 1 | O | 63 | PRO | CG-CD | 6.38 | 1.71 | 1.50 |
| 1 | D | 209 | ASP | C-O | 6.37 | 1.35 | 1.23 |
| 1 | M | 374 | PHE | CD2-CE2 | -6.37 | 1.26 | 1.39 |
| 1 | L | 447 | TRP | CE3-CZ3 | -6.37 | 1.27 | 1.38 |
| 1 | M | 438 | GLU | CD-OE1 | 6.37 | 1.32 | 1.25 |
| 1 | G | 227 | SER | CB-OG | 6.37 | 1.50 | 1.42 |
| 1 | H | 231 | TYR | CG-CD1 | 6.37 | 1.47 | 1.39 |
| 1 | H | 402 | TRP | CB-CG | 6.37 | 1.61 | 1.50 |
| 1 | L | 40 | SER | C-O | 6.36 | 1.35 | 1.23 |
| 1 | A | 311 | TYR | CE1-CZ | -6.36 | 1.30 | 1.38 |
| 1 | J | 103 | VAL | C-O | 6.36 | 1.35 | 1.23 |
| 1 | A | 360 | PHE | CG-CD1 | -6.36 | 1.29 | 1.38 |
| 1 | C | 224 | ILE | CB-CG2 | -6.36 | 1.33 | 1.52 |
| 1 | E | 107 | VAL | CB-CG1 | -6.36 | 1.39 | 1.52 |
| 1 | E | 457 | ALA | CA-CB | -6.36 | 1.39 | 1.52 |
| 1 | G | 206 | GLY | CA-C | 6.36 | 1.62 | 1.51 |
| 1 | A | 356 | LYS | C-O | -6.36 | 1.11 | 1.23 |
| 1 | G | 311 | TYR | CG-CD2 | 6.36 | 1.47 | 1.39 |
| 1 | I | 382 | THR | C-O | 6.36 | 1.35 | 1.23 |
| 1 | J | 291 | TYR | CG-CD2 | -6.36 | 1.30 | 1.39 |
| 1 | O | 278 | LYS | CG-CD | 6.36 | 1.74 | 1.52 |
| 1 | D | 132 | ALA | CA-CB | -6.35 | 1.39 | 1.52 |
| 1 | K | 338 | ARG | CG-CD | 6.35 | 1.67 | 1.51 |
| 1 | D | 358 | THR | CB-CG2 | 6.35 | 1.73 | 1.52 |
| 1 | I | 248 | PHE | CG-CD1 | -6.35 | 1.29 | 1.38 |
| 1 | M | 257 | VAL | CB-CG1 | 6.35 | 1.66 | 1.52 |
| 1 | B | 211 | THR | C-O | -6.35 | 1.11 | 1.23 |
| 1 | F | 169 | TRP | CG-CD1 | -6.35 | 1.27 | 1.36 |
| 1 | F | 197 | ASP | CB-CG | 6.35 | 1.65 | 1.51 |
| 1 | J | 269 | GLU | CB-CG | 6.35 | 1.64 | 1.52 |
| 1 | G | 139 | ALA | CA-CB | 6.35 | 1.65 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 307 | PHE | CE1-CZ | 6.35 | 1.49 | 1.37 |
| 1 | H | 201 | VAL | CA-C | -6.34 | 1.36 | 1.52 |
| 1 | N | 53 | LYS | CE-NZ | 6.34 | 1.65 | 1.49 |
| 1 | B | 73 | PHE | CD1-CE1 | 6.34 | 1.51 | 1.39 |
| 1 | K | 27 | TYR | CG-CD2 | 6.34 | 1.47 | 1.39 |
| 1 | L | 376 | PHE | CD2-CE2 | -6.34 | 1.26 | 1.39 |
| 1 | H | 249 | TYR | CG-CD1 | -6.34 | 1.30 | 1.39 |
| 1 | K | 447 | TRP | CE3-CZ3 | 6.34 | 1.49 | 1.38 |
| 1 | D | 376 | PHE | CD2-CE2 | -6.34 | 1.26 | 1.39 |
| 1 | H | 462 | PHE | CG-CD1 | -6.34 | 1.29 | 1.38 |
| 1 | D | 220 | VAL | CB-CG2 | -6.33 | 1.39 | 1.52 |
| 1 | F | 365 | ARG | CZ-NH1 | 6.33 | 1.41 | 1.33 |
| 1 | B | 453 | GLU | CD-OE2 | 6.33 | 1.32 | 1.25 |
| 1 | C | 103 | VAL | CB-CG1 | -6.33 | 1.39 | 1.52 |
| 1 | F | 242 | TYR | CD1-CE1 | 6.33 | 1.48 | 1.39 |
| 1 | J | 243 | GLY | CA-C | 6.33 | 1.61 | 1.51 |
| 1 | C | 54 | LYS | CD-CE | 6.33 | 1.67 | 1.51 |
| 1 | E | 146 | CYS | CB-SG | 6.33 | 1.93 | 1.82 |
| 1 | O | 387 | VAL | CB-CG2 | 6.33 | 1.66 | 1.52 |
| 1 | G | 281 | GLY | C-O | 6.33 | 1.33 | 1.23 |
| 1 | I | 49 | TYR | CG-CD2 | 6.32 | 1.47 | 1.39 |
| 1 | A | 447 | TRP | CD2-CE2 | -6.32 | 1.33 | 1.41 |
| 1 | N | 311 | TYR | C-O | 6.32 | 1.35 | 1.23 |
| 1 | I | 189 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | L | 66 | SER | CA-CB | -6.32 | 1.43 | 1.52 |
| 1 | D | 98 | LEU | C-O | 6.32 | 1.35 | 1.23 |
| 1 | H | 70 | TYR | CD1-CE1 | 6.32 | 1.48 | 1.39 |
| 1 | H | 140 | GLY | N-CA | 6.32 | 1.55 | 1.46 |
| 1 | D | 40 | SER | CA-CB | 6.31 | 1.62 | 1.52 |
| 1 | G | 152 | LYS | CE-NZ | 6.31 | 1.64 | 1.49 |
| 1 | I | 462 | PHE | CE2-CZ | 6.31 | 1.49 | 1.37 |
| 1 | L | 442 | LYS | CE-NZ | 6.31 | 1.64 | 1.49 |
| 1 | N | 273 | ASP | CB-CG | 6.31 | 1.65 | 1.51 |
| 1 | B | 107 | VAL | CB-CG1 | -6.31 | 1.39 | 1.52 |
| 1 | C | 268 | GLY | C-O | 6.31 | 1.33 | 1.23 |
| 1 | D | 311 | TYR | CE1-CZ | -6.31 | 1.30 | 1.38 |
| 1 | D | 346 | ALA | C-O | 6.31 | 1.35 | 1.23 |
| 1 | E | 191 | ILE | CA-CB | -6.31 | 1.40 | 1.54 |
| 1 | I | 162 | LYS | CD-CE | 6.31 | 1.67 | 1.51 |
| 1 | K | 177 | GLN | CG-CD | 6.31 | 1.65 | 1.51 |
| 1 | L | 34 | TYR | CE1-CZ | -6.31 | 1.30 | 1.38 |
| 1 | A | 249 | TYR | CE2-CZ | 6.31 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 256 | PHE | CG-CD1 | -6.31 | 1.29 | 1.38 |
| 1 | N | 361 | LYS | CG-CD | 6.31 | 1.73 | 1.52 |
| 1 | H | 109 | ARG | CZ-NH1 | 6.31 | 1.41 | 1.33 |
| 1 | M | 162 | LYS | CD-CE | 6.31 | 1.67 | 1.51 |
| 1 | B | 390 | TYR | CD1-CE1 | 6.30 | 1.48 | 1.39 |
| 1 | D | 107 | VAL | CB-CG1 | -6.30 | 1.39 | 1.52 |
| 1 | E | 229 | CYS | CB-SG | 6.30 | 1.93 | 1.82 |
| 1 | E | 333 | VAL | C-O | 6.30 | 1.35 | 1.23 |
| 1 | K | 169 | TRP | CE3-CZ3 | -6.30 | 1.27 | 1.38 |
| 1 | G | 337 | THR | C-O | 6.30 | 1.35 | 1.23 |
| 1 | I | 91 | TYR | CE2-CZ | 6.30 | 1.46 | 1.38 |
| 1 | J | 144 | ARG | CB-CG | 6.30 | 1.69 | 1.52 |
| 1 | H | 472 | LEU | C-OXT | 6.29 | 1.35 | 1.23 |
| 1 | M | 300 | VAL | CB-CG2 | -6.29 | 1.39 | 1.52 |
| 1 | D | 174 | PRO | CA-CB | 6.29 | 1.66 | 1.53 |
| 1 | D | 256 | PHE | CG-CD1 | -6.29 | 1.29 | 1.38 |
| 1 | H | 269 | GLU | CD-OE1 | -6.29 | 1.18 | 1.25 |
| 1 | F | 374 | PHE | CE1-CZ | 6.29 | 1.49 | 1.37 |
| 1 | O | 360 | PHE | CB-CG | -6.29 | 1.40 | 1.51 |
| 1 | C | 448 | GLU | C-O | 6.29 | 1.35 | 1.23 |
| 1 | D | 174 | PRO | CB-CG | 6.29 | 1.81 | 1.50 |
| 1 | A | 390 | TYR | CG-CD1 | 6.28 | 1.47 | 1.39 |
| 1 | H | 179 | ALA | CA-C | 6.28 | 1.69 | 1.52 |
| 1 | K | 448 | GLU | CD-OE1 | 6.28 | 1.32 | 1.25 |
| 1 | B | 352 | GLU | CG-CD | 6.28 | 1.61 | 1.51 |
| 1 | A | 85 | PHE | C-O | 6.28 | 1.35 | 1.23 |
| 1 | C | 167 | GLU | CD-OE1 | 6.28 | 1.32 | 1.25 |
| 1 | O | 347 | ALA | C-O | 6.28 | 1.35 | 1.23 |
| 1 | M | 271 | VAL | CA-CB | -6.28 | 1.41 | 1.54 |
| 1 | O | 133 | SER | C-O | 6.28 | 1.35 | 1.23 |
| 1 | E | 165 | ILE | C-O | 6.27 | 1.35 | 1.23 |
| 1 | L | 61 | LEU | CG-CD1 | 6.27 | 1.75 | 1.51 |
| 1 | O | 171 | LYS | CB-CG | 6.27 | 1.69 | 1.52 |
| 1 | A | 285 | ASN | C-O | 6.27 | 1.35 | 1.23 |
| 1 | E | 207 | ALA | CA-CB | 6.27 | 1.65 | 1.52 |
| 1 | I | 49 | TYR | C-O | 6.27 | 1.35 | 1.23 |
| 1 | D | 245 | SER | C-O | 6.26 | 1.35 | 1.23 |
| 1 | L | 153 | GLN | CG-CD | 6.26 | 1.65 | 1.51 |
| 1 | I | 370 | TYR | CA-CB | -6.26 | 1.40 | 1.53 |
| 1 | O | 183 | GLY | C-O | 6.26 | 1.33 | 1.23 |
| 1 | G | 27 | TYR | CB-CG | 6.26 | 1.61 | 1.51 |
| 1 | A | 459 | LEU | C-O | -6.26 | 1.11 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 290 | ASN | C-O | 6.26 | 1.35 | 1.23 |
| 1 | F | 273 | ASP | C-O | 6.26 | 1.35 | 1.23 |
| 1 | N | 236 | LYS | CE-NZ | 6.26 | 1.64 | 1.49 |
| 1 | C | 64 | LYS | CE-NZ | 6.25 | 1.64 | 1.49 |
| 1 | B | 97 | ARG | CG-CD | 6.25 | 1.67 | 1.51 |
| 1 | D | 187 | PRO | CG-CD | 6.25 | 1.71 | 1.50 |
| 1 | G | 470 | LEU | CG-CD1 | 6.25 | 1.75 | 1.51 |
| 1 | H | 375 | ILE | C-O | 6.25 | 1.35 | 1.23 |
| 1 | J | 22 | VAL | CB-CG2 | 6.25 | 1.66 | 1.52 |
| 1 | K | 21 | VAL | CB-CG2 | 6.25 | 1.66 | 1.52 |
| 1 | H | 361 | LYS | CD-CE | 6.25 | 1.66 | 1.51 |
| 1 | J | 253 | GLU | CG-CD | 6.25 | 1.61 | 1.51 |
| 1 | K | 221 | PRO | N-CD | -6.25 | 1.39 | 1.47 |
| 1 | N | 114 | GLY | C-O | 6.25 | 1.33 | 1.23 |
| 1 | O | 32 | ASN | CB-CG | 6.25 | 1.65 | 1.51 |
| 1 | A | 100 | TRP | CG-CD1 | -6.24 | 1.28 | 1.36 |
| 1 | B | 381 | ILE | C-O | -6.24 | 1.11 | 1.23 |
| 1 | G | 374 | PHE | CG-CD2 | 6.24 | 1.48 | 1.38 |
| 1 | G | 452 | LYS | CE-NZ | 6.24 | 1.64 | 1.49 |
| 1 | I | 169 | TRP | CE3-CZ3 | -6.24 | 1.27 | 1.38 |
| 1 | F | 55 | PRO | C-O | 6.24 | 1.35 | 1.23 |
| 1 | A | 237 | MET | CA-C | 6.24 | 1.69 | 1.52 |
| 1 | A | 371 | ASP | N-CA | 6.24 | 1.58 | 1.46 |
| 1 | I | 172 | GLY | N-CA | 6.24 | 1.55 | 1.46 |
| 1 | F | 236 | LYS | CE-NZ | 6.24 | 1.64 | 1.49 |
| 1 | M | 219 | GLU | CD-OE1 | 6.24 | 1.32 | 1.25 |
| 1 | K | 172 | GLY | C-O | 6.24 | 1.33 | 1.23 |
| 1 | K | 203 | THR | CA-CB | -6.24 | 1.37 | 1.53 |
| 1 | I | 352 | GLU | CD-OE1 | 6.23 | 1.32 | 1.25 |
| 1 | I | 61 | LEU | CG-CD1 | 6.23 | 1.75 | 1.51 |
| 1 | K | 180 | VAL | CB-CG1 | 6.23 | 1.66 | 1.52 |
| 1 | L | 103 | VAL | CA-CB | -6.23 | 1.41 | 1.54 |
| 1 | M | 360 | PHE | CG-CD1 | -6.23 | 1.29 | 1.38 |
| 1 | O | 325 | TRP | CD2-CE2 | 6.23 | 1.48 | 1.41 |
| 1 | D | 276 | TYR | CZ-OH | 6.23 | 1.48 | 1.37 |
| 1 | H | 155 | GLN | CB-CG | -6.23 | 1.35 | 1.52 |
| 1 | O | 394 | MET | CG-SD | 6.23 | 1.97 | 1.81 |
| 1 | E | 462 | PHE | CE1-CZ | -6.23 | 1.25 | 1.37 |
| 1 | L | 71 | ARG | CG-CD | -6.23 | 1.36 | 1.51 |
| 1 | F | 178 | VAL | CB-CG2 | 6.23 | 1.66 | 1.52 |
| 1 | H | 454 | LYS | CD-CE | 6.23 | 1.66 | 1.51 |
| 1 | K | 221 | PRO | CB-CG | -6.23 | 1.18 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 259 | HIS | CA-CB | -6.23 | 1.40 | 1.53 |
| 1 | D | 370 | TYR | CA-CB | -6.23 | 1.40 | 1.53 |
| 1 | O | 78 | PRO | CB-CG | -6.23 | 1.18 | 1.50 |
| 1 | O | 311 | TYR | CG-CD1 | 6.23 | 1.47 | 1.39 |
| 1 | F | 176 | THR | C-O | 6.22 | 1.35 | 1.23 |
| 1 | J | 231 | TYR | CB-CG | -6.22 | 1.42 | 1.51 |
| 1 | L | 402 | TRP | CB-CG | -6.22 | 1.39 | 1.50 |
| 1 | M | 178 | VAL | CB-CG2 | 6.22 | 1.66 | 1.52 |
| 1 | A | 100 | TRP | CB-CG | -6.22 | 1.39 | 1.50 |
| 1 | C | 271 | VAL | CA-CB | -6.22 | 1.41 | 1.54 |
| 1 | C | 368 | GLU | CD-OE2 | 6.22 | 1.32 | 1.25 |
| 1 | M | 269 | GLU | C-O | 6.22 | 1.35 | 1.23 |
| 1 | K | 95 | THR | C-O | 6.22 | 1.35 | 1.23 |
| 1 | A | 48 | PRO | C-O | 6.22 | 1.35 | 1.23 |
| 1 | A | 40 | SER | CB-OG | 6.21 | 1.50 | 1.42 |
| 1 | C | 114 | GLY | C-O | -6.21 | 1.13 | 1.23 |
| 1 | D | 304 | ALA | CA-CB | -6.21 | 1.39 | 1.52 |
| 1 | I | 202 | ASP | N-CA | -6.21 | 1.33 | 1.46 |
| 1 | K | 46 | GLY | C-O | 6.21 | 1.33 | 1.23 |
| 1 | N | 361 | LYS | CD-CE | 6.21 | 1.66 | 1.51 |
| 1 | I | 272 | PRO | CA-C | -6.21 | 1.40 | 1.52 |
| 1 | K | 374 | PHE | CG-CD2 | 6.21 | 1.48 | 1.38 |
| 1 | M | 103 | VAL | CB-CG1 | -6.21 | 1.39 | 1.52 |
| 1 | M | 360 | PHE | CE2-CZ | -6.21 | 1.25 | 1.37 |
| 1 | A | 229 | CYS | CB-SG | 6.21 | 1.92 | 1.82 |
| 1 | M | 34 | TYR | CD1-CE1 | -6.21 | 1.30 | 1.39 |
| 1 | C | 400 | GLU | CD-OE1 | 6.21 | 1.32 | 1.25 |
| 1 | C | 446 | PHE | CG-CD1 | 6.21 | 1.48 | 1.38 |
| 1 | G | 23 | SER | CB-OG | 6.21 | 1.50 | 1.42 |
| 1 | H | 242 | TYR | CD1-CE1 | 6.21 | 1.48 | 1.39 |
| 1 | D | 242 | TYR | CD1-CE1 | 6.20 | 1.48 | 1.39 |
| 1 | D | 270 | ASN | C-O | -6.20 | 1.11 | 1.23 |
| 1 | E | 169 | TRP | CE3-CZ3 | -6.20 | 1.27 | 1.38 |
| 1 | E | 176 | THR | CB-CG2 | 6.20 | 1.72 | 1.52 |
| 1 | H | 295 | PRO | CA-C | -6.20 | 1.40 | 1.52 |
| 1 | K | 291 | TYR | CZ-OH | 6.20 | 1.48 | 1.37 |
| 1 | K | 311 | TYR | CB-CG | -6.20 | 1.42 | 1.51 |
| 1 | C | 355 | TYR | CB-CG | 6.20 | 1.60 | 1.51 |
| 1 | G | 233 | ASP | C-O | 6.20 | 1.35 | 1.23 |
| 1 | D | 195 | ILE | C-O | -6.20 | 1.11 | 1.23 |
| 1 | I | 300 | VAL | CB-CG1 | 6.19 | 1.65 | 1.52 |
| 1 | B | 175 | CYS | CB-SG | 6.19 | 1.92 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 390 | TYR | CG-CD2 | -6.19 | 1.31 | 1.39 |
| 1 | C | 396 | SER | CA-CB | 6.19 | 1.62 | 1.52 |
| 1 | F | 125 | LYS | CG-CD | 6.19 | 1.73 | 1.52 |
| 1 | A | 369 | GLU | CA-C | -6.18 | 1.36 | 1.52 |
| 1 | E | 274 | ASP | C-O | 6.18 | 1.35 | 1.23 |
| 1 | E | 325 | TRP | CG-CD1 | 6.18 | 1.45 | 1.36 |
| 1 | H | 443 | LYS | CE-NZ | 6.18 | 1.64 | 1.49 |
| 1 | D | 167 | GLU | CB-CG | -6.18 | 1.40 | 1.52 |
| 1 | L | 263 | ARG | CZ-NH1 | -6.18 | 1.25 | 1.33 |
| 1 | F | 295 | PRO | CG-CD | 6.18 | 1.71 | 1.50 |
| 1 | G | 467 | LYS | CD-CE | 6.18 | 1.66 | 1.51 |
| 1 | O | 231 | TYR | CE2-CZ | 6.18 | 1.46 | 1.38 |
| 1 | F | 283 | THR | CB-CG2 | 6.18 | 1.72 | 1.52 |
| 1 | B | 212 | THR | CB-CG2 | 6.17 | 1.72 | 1.52 |
| 1 | D | 468 | PHE | CD1-CE1 | 6.17 | 1.51 | 1.39 |
| 1 | E | 376 | PHE | CD1-CE1 | -6.17 | 1.26 | 1.39 |
| 1 | K | 312 | TRP | CA-CB | -6.17 | 1.40 | 1.53 |
| 1 | N | 453 | GLU | CD-OE1 | 6.17 | 1.32 | 1.25 |
| 1 | O | 152 | LYS | C-O | 6.17 | 1.35 | 1.23 |
| 1 | M | 107 | VAL | CB-CG2 | -6.17 | 1.39 | 1.52 |
| 1 | B | 142 | ASP | N-CA | 6.17 | 1.58 | 1.46 |
| 1 | I | 125 | LYS | CD-CE | 6.17 | 1.66 | 1.51 |
| 1 | L | 138 | ASN | CG-ND2 | 6.17 | 1.48 | 1.32 |
| 1 | N | 27 | TYR | CA-C | 6.17 | 1.69 | 1.52 |
| 1 | C | 147 | ILE | CB-CG2 | -6.17 | 1.33 | 1.52 |
| 1 | G | 356 | LYS | CE-NZ | 6.17 | 1.64 | 1.49 |
| 1 | D | 400 | GLU | CG-CD | 6.16 | 1.61 | 1.51 |
| 1 | E | 337 | THR | CB-CG2 | -6.16 | 1.32 | 1.52 |
| 1 | D | 301 | THR | C-O | 6.16 | 1.35 | 1.23 |
| 1 | C | 206 | GLY | C-O | 6.16 | 1.33 | 1.23 |
| 1 | K | 284 | ALA | CA-CB | -6.16 | 1.39 | 1.52 |
| 1 | M | 332 | THR | CB-OG1 | 6.16 | 1.55 | 1.43 |
| 1 | E | 83 | PHE | CE2-CZ | 6.16 | 1.49 | 1.37 |
| 1 | G | 315 | ARG | C-O | 6.16 | 1.35 | 1.23 |
| 1 | I | 330 | PHE | CB-CG | 6.16 | 1.61 | 1.51 |
| 1 | B | 138 | ASN | CG-ND2 | 6.15 | 1.48 | 1.32 |
| 1 | G | 278 | LYS | CB-CG | 6.15 | 1.69 | 1.52 |
| 1 | D | 460 | ASP | CG-OD1 | 6.15 | 1.39 | 1.25 |
| 1 | F | 83 | PHE | CD1-CE1 | 6.15 | 1.51 | 1.39 |
| 1 | G | 439 | ASP | N-CA | 6.15 | 1.58 | 1.46 |
| 1 | C | 292 | PHE | CG-CD1 | 6.15 | 1.48 | 1.38 |
| 1 | L | 354 | THR | C-O | 6.15 | 1.35 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 231 | TYR | CD1-CE1 | 6.15 | 1.48 | 1.39 |
| 1 | K | 49 | TYR | CZ-OH | -6.15 | 1.27 | 1.37 |
| 1 | N | 61 | LEU | CG-CD1 | 6.15 | 1.74 | 1.51 |
| 1 | L | 351 | SER | CB-OG | 6.14 | 1.50 | 1.42 |
| 1 | C | 362 | GLU | CD-OE1 | 6.14 | 1.32 | 1.25 |
| 1 | H | 472 | LEU | CG-CD1 | -6.14 | 1.29 | 1.51 |
| 1 | J | 455 | PHE | CD2-CE2 | -6.14 | 1.26 | 1.39 |
| 1 | G | 455 | PHE | CB-CG | -6.14 | 1.41 | 1.51 |
| 1 | O | 50 | PHE | CD1-CE1 | -6.14 | 1.26 | 1.39 |
| 1 | F | 279 | GLY | C-O | -6.13 | 1.13 | 1.23 |
| 1 | A | 24 | THR | CA-CB | -6.13 | 1.37 | 1.53 |
| 1 | J | 147 | ILE | CB-CG2 | -6.13 | 1.33 | 1.52 |
| 1 | K | 231 | TYR | CA-CB | -6.13 | 1.40 | 1.53 |
| 1 | A | 462 | PHE | CG-CD2 | -6.13 | 1.29 | 1.38 |
| 1 | D | 330 | PHE | CD2-CE2 | -6.13 | 1.26 | 1.39 |
| 1 | G | 287 | ALA | C-O | 6.13 | 1.34 | 1.23 |
| 1 | H | 27 | TYR | CD1-CE1 | 6.13 | 1.48 | 1.39 |
| 1 | K | 448 | GLU | CB-CG | 6.13 | 1.63 | 1.52 |
| 1 | B | 291 | TYR | CD2-CE2 | -6.13 | 1.30 | 1.39 |
| 1 | F | 85 | PHE | CG-CD1 | 6.13 | 1.48 | 1.38 |
| 1 | B | 139 | ALA | CA-CB | 6.12 | 1.65 | 1.52 |
| 1 | D | 453 | GLU | CD-OE1 | 6.12 | 1.32 | 1.25 |
| 1 | E | 401 | ASP | C-O | 6.12 | 1.34 | 1.23 |
| 1 | N | 86 | PRO | CA-C | 6.12 | 1.65 | 1.52 |
| 1 | C | 183 | GLY | C-O | 6.12 | 1.33 | 1.23 |
| 1 | E | 291 | TYR | CG-CD1 | -6.12 | 1.31 | 1.39 |
| 1 | A | 447 | TRP | CZ3-CH2 | -6.12 | 1.30 | 1.40 |
| 1 | N | 208 | MET | CB-CG | 6.12 | 1.71 | 1.51 |
| 1 | B | 356 | LYS | CD-CE | 6.12 | 1.66 | 1.51 |
| 1 | I | 267 | VAL | CB-CG2 | 6.11 | 1.65 | 1.52 |
| 1 | M | 177 | GLN | CD-NE2 | 6.11 | 1.48 | 1.32 |
| 1 | E | 402 | TRP | C-O | 6.11 | 1.34 | 1.23 |
| 1 | B | 375 | ILE | C-O | 6.11 | 1.34 | 1.23 |
| 1 | J | 253 | GLU | C-O | -6.11 | 1.11 | 1.23 |
| 1 | O | 176 | THR | CA-CB | 6.11 | 1.69 | 1.53 |
| 1 | M | 112 | PRO | CA-C | 6.11 | 1.65 | 1.52 |
| 1 | A | 331 | VAL | CB-CG2 | -6.11 | 1.40 | 1.52 |
| 1 | A | 468 | PHE | CE2-CZ | -6.11 | 1.25 | 1.37 |
| 1 | M | 141 | VAL | CB-CG2 | -6.11 | 1.40 | 1.52 |
| 1 | N | 343 | SER | C-O | 6.11 | 1.34 | 1.23 |
| 1 | K | 247 | PHE | CE1-CZ | 6.10 | 1.49 | 1.37 |
| 1 | F | 99 | VAL | CB-CG1 | -6.10 | 1.40 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 167 | GLU | CD-OE1 | 6.10 | 1.32 | 1.25 |
| 1 | G | 471 | GLN | CB-CG | -6.10 | 1.36 | 1.52 |
| 1 | K | 457 | ALA | CA-CB | -6.10 | 1.39 | 1.52 |
| 1 | H | 293 | PRO | N-CA | -6.10 | 1.36 | 1.47 |
| 1 | H | 356 | LYS | CE-NZ | 6.10 | 1.64 | 1.49 |
| 1 | J | 269 | GLU | CD-OE2 | 6.10 | 1.32 | 1.25 |
| 1 | O | 395 | ASN | C-O | 6.10 | 1.34 | 1.23 |
| 1 | A | 240 | GLU | CD-OE1 | 6.10 | 1.32 | 1.25 |
| 1 | E | 227 | SER | C-O | 6.10 | 1.34 | 1.23 |
| 1 | K | 300 | VAL | CA-CB | -6.10 | 1.42 | 1.54 |
| 1 | K | 448 | GLU | CD-OE2 | 6.10 | 1.32 | 1.25 |
| 1 | M | 312 | TRP | CB-CG | -6.10 | 1.39 | 1.50 |
| 1 | O | 96 | GLN | CG-CD | 6.10 | 1.65 | 1.51 |
| 1 | D | 317 | GLN | CD-OE1 | 6.10 | 1.37 | 1.24 |
| 1 | M | 169 | TRP | CD2-CE2 | -6.10 | 1.34 | 1.41 |
| 1 | M | 276 | TYR | CD1-CE1 | 6.10 | 1.48 | 1.39 |
| 1 | I | 470 | LEU | CG-CD2 | 6.09 | 1.74 | 1.51 |
| 1 | J | 110 | GLY | C-O | 6.09 | 1.33 | 1.23 |
| 1 | O | 176 | THR | C-O | 6.09 | 1.34 | 1.23 |
| 1 | E | 340 | THR | C-O | 6.09 | 1.34 | 1.23 |
| 1 | O | 247 | PHE | CE1-CZ | 6.09 | 1.49 | 1.37 |
| 1 | D | 472 | LEU | C-OXT | 6.09 | 1.34 | 1.23 |
| 1 | O | 173 | SER | C-O | 6.09 | 1.34 | 1.23 |
| 1 | D | 363 | TYR | CE1-CZ | 6.08 | 1.46 | 1.38 |
| 1 | I | 25 | ASP | CG-OD1 | 6.08 | 1.39 | 1.25 |
| 1 | G | 125 | LYS | CE-NZ | 6.08 | 1.64 | 1.49 |
| 1 | O | 86 | PRO | CG-CD | 6.08 | 1.70 | 1.50 |
| 1 | A | 312 | TRP | CG-CD1 | -6.08 | 1.28 | 1.36 |
| 1 | A | 339 | SER | N-CA | 6.08 | 1.58 | 1.46 |
| 1 | B | 231 | TYR | CG-CD1 | -6.08 | 1.31 | 1.39 |
| 1 | D | 354 | THR | CB-CG2 | -6.08 | 1.32 | 1.52 |
| 1 | B | 72 | VAL | CB-CG2 | -6.07 | 1.40 | 1.52 |
| 1 | C | 348 | ILE | C-O | 6.07 | 1.34 | 1.23 |
| 1 | F | 387 | VAL | CB-CG1 | -6.07 | 1.40 | 1.52 |
| 1 | K | 369 | GLU | CB-CG | 6.07 | 1.63 | 1.52 |
| 1 | F | 240 | GLU | CG-CD | -6.07 | 1.42 | 1.51 |
| 1 | B | 231 | TYR | CZ-OH | 6.07 | 1.48 | 1.37 |
| 1 | C | 177 | GLN | CG-CD | 6.07 | 1.65 | 1.51 |
| 1 | H | 322 | GLY | C-O | 6.07 | 1.33 | 1.23 |
| 1 | A | 149 | MET | CG-SD | -6.07 | 1.65 | 1.81 |
| 1 | F | 465 | GLY | C-O | -6.07 | 1.14 | 1.23 |
| 1 | G | 82 | LYS | CE-NZ | 6.07 | 1.64 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 103 | VAL | CB-CG2 | 6.07 | 1.65 | 1.52 |
| 1 | B | 54 | LYS | CB-CG | 6.07 | 1.69 | 1.52 |
| 1 | C | 373 | GLN | C-O | 6.06 | 1.34 | 1.23 |
| 1 | E | 217 | LYS | CE-NZ | 6.06 | 1.64 | 1.49 |
| 1 | E | 219 | GLU | CB-CG | -6.06 | 1.40 | 1.52 |
| 1 | F | 278 | LYS | CA-CB | 6.06 | 1.67 | 1.53 |
| 1 | G | 90 | PHE | CE1-CZ | 6.06 | 1.48 | 1.37 |
| 1 | K | 356 | LYS | C-O | -6.06 | 1.11 | 1.23 |
| 1 | M | 312 | TRP | CG-CD2 | -6.06 | 1.33 | 1.43 |
| 1 | N | 360 | PHE | CD2-CE2 | 6.06 | 1.51 | 1.39 |
| 1 | G | 309 | LYS | CB-CG | 6.06 | 1.69 | 1.52 |
| 1 | M | 58 | ASN | C-O | 6.06 | 1.34 | 1.23 |
| 1 | N | 96 | GLN | N-CA | -6.06 | 1.34 | 1.46 |
| 1 | O | 84 | GLY | C-O | 6.06 | 1.33 | 1.23 |
| 1 | J | 125 | LYS | CE-NZ | 6.06 | 1.64 | 1.49 |
| 1 | K | 263 | ARG | CZ-NH1 | 6.06 | 1.41 | 1.33 |
| 1 | N | 227 | SER | CB-OG | 6.06 | 1.50 | 1.42 |
| 1 | G | 285 | ASN | C-O | 6.06 | 1.34 | 1.23 |
| 1 | B | 318 | GLY | C-O | -6.05 | 1.14 | 1.23 |
| 1 | E | 135 | TYR | CZ-OH | 6.05 | 1.48 | 1.37 |
| 1 | G | 444 | TYR | CG-CD1 | 6.05 | 1.47 | 1.39 |
| 1 | J | 242 | TYR | CD1-CE1 | 6.05 | 1.48 | 1.39 |
| 1 | C | 62 | VAL | CB-CG2 | 6.05 | 1.65 | 1.52 |
| 1 | E | 472 | LEU | N-CA | 6.05 | 1.58 | 1.46 |
| 1 | N | 118 | SER | CB-OG | 6.05 | 1.50 | 1.42 |
| 1 | A | 200 | MET | CG-SD | 6.05 | 1.96 | 1.81 |
| 1 | I | 252 | ARG | CG-CD | 6.05 | 1.67 | 1.51 |
| 1 | O | 71 | ARG | CZ-NH2 | 6.05 | 1.41 | 1.33 |
| 1 | M | 447 | TRP | CB-CG | -6.05 | 1.39 | 1.50 |
| 1 | O | 369 | GLU | CG-CD | 6.05 | 1.61 | 1.51 |
| 1 | H | 462 | PHE | CB-CG | -6.04 | 1.41 | 1.51 |
| 1 | L | 205 | PHE | CE2-CZ | 6.04 | 1.48 | 1.37 |
| 1 | M | 181 | GLN | CG-CD | 6.04 | 1.65 | 1.51 |
| 1 | N | 447 | TRP | CD2-CE2 | 6.04 | 1.48 | 1.41 |
| 1 | I | 277 | ILE | CA-CB | -6.04 | 1.41 | 1.54 |
| 1 | K | 293 | PRO | CA-C | -6.04 | 1.40 | 1.52 |
| 1 | M | 34 | TYR | CD2-CE2 | -6.04 | 1.30 | 1.39 |
| 1 | J | 96 | GLN | N-CA | 6.04 | 1.58 | 1.46 |
| 1 | M | 361 | LYS | CE-NZ | 6.04 | 1.64 | 1.49 |
| 1 | I | 448 | GLU | CG-CD | 6.04 | 1.61 | 1.51 |
| 1 | D | 365 | ARG | C-O | 6.04 | 1.34 | 1.23 |
| 1 | K | 44 | ALA | CA-CB | -6.04 | 1.39 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 331 | VAL | C-O | 6.04 | 1.34 | 1.23 |
| 1 | O | 248 | PHE | CE1-CZ | 6.04 | 1.48 | 1.37 |
| 1 | K | 463 | PRO | CA-C | -6.04 | 1.40 | 1.52 |
| 1 | O | 198 | GLY | C-O | 6.04 | 1.33 | 1.23 |
| 1 | B | 216 | ASN | CB-CG | -6.03 | 1.37 | 1.51 |
| 1 | E | 242 | TYR | CE1-CZ | -6.03 | 1.30 | 1.38 |
| 1 | G | 180 | VAL | CA-CB | 6.03 | 1.67 | 1.54 |
| 1 | H | 444 | TYR | CG-CD2 | -6.03 | 1.31 | 1.39 |
| 1 | L | 463 | PRO | CB-CG | 6.03 | 1.80 | 1.50 |
| 1 | C | 370 | TYR | CD2-CE2 | 6.03 | 1.48 | 1.39 |
| 1 | G | 182 | PRO | CG-CD | 6.03 | 1.70 | 1.50 |
| 1 | H | 438 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | J | 139 | ALA | CA-CB | 6.03 | 1.65 | 1.52 |
| 1 | B | 316 | ALA | N-CA | 6.03 | 1.58 | 1.46 |
| 1 | H | 253 | GLU | CD-OE1 | 6.03 | 1.32 | 1.25 |
| 1 | M | 333 | VAL | CB-CG2 | -6.03 | 1.40 | 1.52 |
| 1 | B | 294 | THR | N-CA | -6.03 | 1.34 | 1.46 |
| 1 | D | 37 | ALA | CA-CB | 6.03 | 1.65 | 1.52 |
| 1 | G | 51 | PRO | N-CD | 6.03 | 1.56 | 1.47 |
| 1 | J | 34 | TYR | CD2-CE2 | -6.03 | 1.30 | 1.39 |
| 1 | L | 462 | PHE | CG-CD2 | -6.03 | 1.29 | 1.38 |
| 1 | O | 400 | GLU | CB-CG | 6.03 | 1.63 | 1.52 |
| 1 | L | 309 | LYS | CE-NZ | 6.02 | 1.64 | 1.49 |
| 1 | F | 184 | ASP | CB-CG | 6.02 | 1.64 | 1.51 |
| 1 | F | 271 | VAL | CB-CG2 | 6.02 | 1.65 | 1.52 |
| 1 | I | 214 | GLN | CD-OE1 | 6.02 | 1.37 | 1.24 |
| 1 | I | 467 | LYS | CB-CG | 6.02 | 1.68 | 1.52 |
| 1 | L | 70 | TYR | CD2-CE2 | -6.02 | 1.30 | 1.39 |
| 1 | D | 326 | GLY | C-O | -6.02 | 1.14 | 1.23 |
| 1 | N | 316 | ALA | N-CA | 6.02 | 1.58 | 1.46 |
| 1 | H | 355 | TYR | CD2-CE2 | 6.01 | 1.48 | 1.39 |
| 1 | J | 234 | TYR | CE1-CZ | -6.01 | 1.30 | 1.38 |
| 1 | B | 315 | ARG | CG-CD | 6.01 | 1.67 | 1.51 |
| 1 | D | 173 | SER | C-O | 6.01 | 1.34 | 1.23 |
| 1 | N | 223 | ASP | C-O | 6.01 | 1.34 | 1.23 |
| 1 | M | 78 | PRO | N-CA | -6.01 | 1.37 | 1.47 |
| 1 | N | 273 | ASP | C-O | 6.01 | 1.34 | 1.23 |
| 1 | O | 74 | ARG | CG-CD | -6.01 | 1.36 | 1.51 |
| 1 | G | 177 | GLN | CD-OE1 | 6.01 | 1.37 | 1.24 |
| 1 | B | 41 | ARG | CZ-NH1 | 6.01 | 1.40 | 1.33 |
| 1 | F | 95 | THR | CA-CB | -6.01 | 1.37 | 1.53 |
| 1 | I | 176 | THR | N-CA | 6.01 | 1.58 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 242 | TYR | CG-CD2 | 6.01 | 1.47 | 1.39 |
| 1 | D | 356 | LYS | N-CA | -6.01 | 1.34 | 1.46 |
| 1 | F | 169 | TRP | CB-CG | -6.01 | 1.39 | 1.50 |
| 1 | I | 179 | ALA | N-CA | 6.01 | 1.58 | 1.46 |
| 1 | J | 452 | LYS | CD-CE | 6.01 | 1.66 | 1.51 |
| 1 | B | 272 | PRO | CA-C | -6.00 | 1.40 | 1.52 |
| 1 | L | 349 | SER | C-O | 6.00 | 1.34 | 1.23 |
| 1 | F | 35 | TYR | CG-CD2 | 6.00 | 1.47 | 1.39 |
| 1 | F | 352 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | K | 30 | ARG | C-O | -6.00 | 1.11 | 1.23 |
| 1 | C | 99 | VAL | CA-CB | 6.00 | 1.67 | 1.54 |
| 1 | A | 471 | GLN | CA-CB | -6.00 | 1.40 | 1.53 |
| 1 | C | 189 | GLU | CD-OE1 | 6.00 | 1.32 | 1.25 |
| 1 | L | 175 | CYS | C-O | 6.00 | 1.34 | 1.23 |
| 1 | E | 471 | GLN | C-O | 6.00 | 1.34 | 1.23 |
| 1 | I | 110 | GLY | CA-C | 5.99 | 1.61 | 1.51 |
| 1 | K | 341 | ASN | CA-C | -5.99 | 1.37 | 1.52 |
| 1 | C | 160 | GLY | C-O | 5.99 | 1.33 | 1.23 |
| 1 | J | 330 | PHE | CD2-CE2 | 5.99 | 1.51 | 1.39 |
| 1 | J | 471 | GLN | C-O | 5.99 | 1.34 | 1.23 |
| 1 | B | 177 | GLN | CG-CD | 5.99 | 1.64 | 1.51 |
| 1 | F | 330 | PHE | CD2-CE2 | -5.99 | 1.27 | 1.39 |
| 1 | B | 22 | VAL | C-O | 5.99 | 1.34 | 1.23 |
| 1 | D | 272 | PRO | C-O | -5.99 | 1.11 | 1.23 |
| 1 | H | 287 | ALA | CA-CB | 5.99 | 1.65 | 1.52 |
| 1 | H | 235 | ILE | CA-CB | -5.98 | 1.41 | 1.54 |
| 1 | C | 444 | TYR | CG-CD2 | 5.98 | 1.47 | 1.39 |
| 1 | H | 139 | ALA | C-N | 5.98 | 1.43 | 1.33 |
| 1 | D | 140 | GLY | N-CA | 5.98 | 1.55 | 1.46 |
| 1 | F | 351 | SER | CB-OG | 5.98 | 1.50 | 1.42 |
| 1 | H | 106 | GLU | CB-CG | 5.98 | 1.63 | 1.52 |
| 1 | M | 455 | PHE | CE2-CZ | 5.98 | 1.48 | 1.37 |
| 1 | N | 194 | VAL | CB-CG1 | 5.98 | 1.65 | 1.52 |
| 1 | M | 361 | LYS | CD-CE | 5.98 | 1.66 | 1.51 |
| 1 | C | 347 | ALA | CA-CB | 5.97 | 1.65 | 1.52 |
| 1 | I | 196 | GLN | CB-CG | -5.97 | 1.36 | 1.52 |
| 1 | A | 139 | ALA | CA-CB | 5.97 | 1.65 | 1.52 |
| 1 | D | 162 | LYS | CE-NZ | 5.97 | 1.64 | 1.49 |
| 1 | J | 288 | SER | CB-OG | 5.97 | 1.50 | 1.42 |
| 1 | O | 355 | TYR | CG-CD1 | -5.97 | 1.31 | 1.39 |
| 1 | N | 353 | THR | CB-CG2 | 5.97 | 1.72 | 1.52 |
| 1 | A | 398 | ILE | CA-CB | -5.97 | 1.41 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 472 | LEU | CA-CB | 5.97 | 1.67 | 1.53 |
| 1 | G | 97 | ARG | CB-CG | 5.97 | 1.68 | 1.52 |
| 1 | O | 176 | THR | N-CA | 5.97 | 1.58 | 1.46 |
| 1 | L | 239 | SER | CB-OG | 5.97 | 1.50 | 1.42 |
| 1 | D | 60 | ILE | CG1-CD1 | 5.97 | 1.91 | 1.50 |
| 1 | E | 130 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | G | 222 | LEU | C-O | 5.97 | 1.34 | 1.23 |
| 1 | L | 346 | ALA | CA-CB | 5.97 | 1.65 | 1.52 |
| 1 | A | 35 | TYR | CG-CD2 | -5.96 | 1.31 | 1.39 |
| 1 | E | 276 | TYR | CA-CB | -5.96 | 1.40 | 1.53 |
| 1 | L | 241 | PRO | N-CA | 5.96 | 1.57 | 1.47 |
| 1 | O | 390 | TYR | CE1-CZ | 5.96 | 1.46 | 1.38 |
| 1 | J | 163 | PRO | C-O | 5.96 | 1.35 | 1.23 |
| 1 | J | 269 | GLU | CG-CD | 5.96 | 1.60 | 1.51 |
| 1 | B | 210 | PHE | CD2-CE2 | -5.96 | 1.27 | 1.39 |
| 1 | C | 32 | ASN | CB-CG | 5.96 | 1.64 | 1.51 |
| 1 | I | 307 | PHE | CD2-CE2 | -5.96 | 1.27 | 1.39 |
| 1 | F | 50 | PHE | CD2-CE2 | -5.96 | 1.27 | 1.39 |
| 1 | F | 65 | VAL | CB-CG1 | -5.95 | 1.40 | 1.52 |
| 1 | L | 256 | PHE | CD2-CE2 | 5.95 | 1.51 | 1.39 |
| 1 | O | 307 | PHE | C-O | 5.95 | 1.34 | 1.23 |
| 1 | L | 334 | VAL | CB-CG2 | -5.95 | 1.40 | 1.52 |
| 1 | J | 324 | CYS | CB-SG | 5.95 | 1.92 | 1.82 |
| 1 | H | 356 | LYS | CG-CD | 5.95 | 1.72 | 1.52 |
| 1 | D | 317 | GLN | CG-CD | 5.95 | 1.64 | 1.51 |
| 1 | H | 293 | PRO | CB-CG | -5.95 | 1.20 | 1.50 |
| 1 | G | 130 | GLU | CD-OE2 | 5.95 | 1.32 | 1.25 |
| 1 | K | 301 | THR | CB-CG2 | 5.95 | 1.72 | 1.52 |
| 1 | J | 198 | GLY | C-O | 5.94 | 1.33 | 1.23 |
| 1 | M | 220 | VAL | C-N | -5.94 | 1.23 | 1.34 |
| 1 | C | 376 | PHE | CG-CD1 | 5.94 | 1.47 | 1.38 |
| 1 | F | 268 | GLY | CA-C | 5.94 | 1.61 | 1.51 |
| 1 | I | 258 | ARG | CZ-NH2 | -5.94 | 1.25 | 1.33 |
| 1 | K | 448 | GLU | C-O | 5.94 | 1.34 | 1.23 |
| 1 | K | 171 | LYS | CG-CD | 5.94 | 1.72 | 1.52 |
| 1 | B | 395 | ASN | CB-CG | 5.94 | 1.64 | 1.51 |
| 1 | C | 453 | GLU | CB-CG | 5.94 | 1.63 | 1.52 |
| 1 | K | 89 | SER | CB-OG | 5.94 | 1.50 | 1.42 |
| 1 | D | 168 | HIS | C-O | 5.93 | 1.34 | 1.23 |
| 1 | H | 137 | ALA | C-O | 5.93 | 1.34 | 1.23 |
| 1 | G | 396 | SER | CB-OG | 5.93 | 1.50 | 1.42 |
| 1 | H | 438 | GLU | CB-CG | 5.93 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 46 | GLY | N-CA | 5.93 | 1.54 | 1.46 |
| 1 | E | 156 | LEU | C-O | 5.93 | 1.34 | 1.23 |
| 1 | K | 295 | PRO | N-CA | -5.93 | 1.37 | 1.47 |
| 1 | A | 20 | ALA | C-O | 5.93 | 1.34 | 1.23 |
| 1 | B | 463 | PRO | N-CA | 5.93 | 1.57 | 1.47 |
| 1 | E | 390 | TYR | CG-CD1 | 5.93 | 1.46 | 1.39 |
| 1 | E | 76 | HIS | C-O | 5.93 | 1.34 | 1.23 |
| 1 | H | 370 | TYR | CD1-CE1 | 5.93 | 1.48 | 1.39 |
| 1 | J | 355 | TYR | CD2-CE2 | 5.93 | 1.48 | 1.39 |
| 1 | L | 199 | ASP | CB-CG | 5.92 | 1.64 | 1.51 |
| 1 | N | 272 | PRO | C-O | -5.92 | 1.11 | 1.23 |
| 1 | O | 231 | TYR | CD1-CE1 | 5.92 | 1.48 | 1.39 |
| 1 | I | 241 | PRO | CB-CG | 5.92 | 1.79 | 1.50 |
| 1 | J | 281 | GLY | C-O | 5.92 | 1.33 | 1.23 |
| 1 | A | 267 | VAL | CB-CG2 | 5.92 | 1.65 | 1.52 |
| 1 | G | 144 | ARG | CZ-NH2 | 5.92 | 1.40 | 1.33 |
| 1 | H | 310 | PRO | C-O | -5.92 | 1.11 | 1.23 |
| 1 | H | 454 | LYS | CE-NZ | 5.92 | 1.63 | 1.49 |
| 1 | J | 257 | VAL | CA-CB | -5.92 | 1.42 | 1.54 |
| 1 | K | 30 | ARG | N-CA | -5.92 | 1.34 | 1.46 |
| 1 | N | 145 | GLU | CD-OE1 | 5.92 | 1.32 | 1.25 |
| 1 | B | 127 | ASP | N-CA | 5.91 | 1.58 | 1.46 |
| 1 | E | 138 | ASN | CG-ND2 | 5.91 | 1.47 | 1.32 |
| 1 | K | 353 | THR | C-O | 5.91 | 1.34 | 1.23 |
| 1 | N | 178 | VAL | N-CA | 5.91 | 1.58 | 1.46 |
| 1 | O | 269 | GLU | CD-OE1 | 5.91 | 1.32 | 1.25 |
| 1 | G | 73 | PHE | CE1-CZ | 5.91 | 1.48 | 1.37 |
| 1 | O | 128 | ASP | C-O | 5.91 | 1.34 | 1.23 |
| 1 | A | 243 | GLY | C-O | 5.91 | 1.33 | 1.23 |
| 1 | B | 207 | ALA | CA-CB | -5.91 | 1.40 | 1.52 |
| 1 | C | 312 | TRP | CE3-CZ3 | -5.91 | 1.28 | 1.38 |
| 1 | G | 376 | PHE | CE2-CZ | 5.91 | 1.48 | 1.37 |
| 1 | H | 171 | LYS | C-O | 5.91 | 1.34 | 1.23 |
| 1 | O | 180 | VAL | C-O | 5.91 | 1.34 | 1.23 |
| 1 | H | 57 | ASN | C-O | 5.91 | 1.34 | 1.23 |
| 1 | N | 35 | TYR | C-O | 5.91 | 1.34 | 1.23 |
| 1 | L | 70 | TYR | CG-CD2 | -5.91 | 1.31 | 1.39 |
| 1 | F | 362 | GLU | CD-OE1 | 5.91 | 1.32 | 1.25 |
| 1 | I | 320 | ASN | CG-OD1 | 5.91 | 1.36 | 1.24 |
| 1 | D | 296 | SER | CA-CB | -5.90 | 1.44 | 1.52 |
| 1 | E | 222 | LEU | CG-CD2 | 5.90 | 1.73 | 1.51 |
| 1 | N | 134 | ALA | C-O | 5.90 | 1.34 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 45 | VAL | CB-CG2 | -5.90 | 1.40 | 1.52 |
| 1 | D | 55 | PRO | CA-C | 5.90 | 1.64 | 1.52 |
| 1 | D | 300 | VAL | C-O | 5.90 | 1.34 | 1.23 |
| 1 | I | 390 | TYR | CD1-CE1 | -5.90 | 1.30 | 1.39 |
| 1 | H | 235 | ILE | C-O | 5.90 | 1.34 | 1.23 |
| 1 | L | 26 | GLU | CG-CD | 5.90 | 1.60 | 1.51 |
| 1 | I | 330 | PHE | CE2-CZ | 5.90 | 1.48 | 1.37 |
| 1 | N | 93 | PRO | CA-CB | 5.90 | 1.65 | 1.53 |
| 1 | O | 217 | LYS | CD-CE | 5.90 | 1.66 | 1.51 |
| 1 | O | 472 | LEU | N-CA | 5.90 | 1.58 | 1.46 |
| 1 | B | 453 | GLU | C-O | 5.90 | 1.34 | 1.23 |
| 1 | J | 159 | ILE | CB-CG2 | -5.90 | 1.34 | 1.52 |
| 1 | F | 365 | ARG | NE-CZ | 5.89 | 1.40 | 1.33 |
| 1 | G | 164 | PRO | C-O | 5.89 | 1.35 | 1.23 |
| 1 | G | 202 | ASP | CG-OD2 | 5.89 | 1.39 | 1.25 |
| 1 | J | 446 | PHE | CE2-CZ | 5.89 | 1.48 | 1.37 |
| 1 | L | 70 | TYR | CE2-CZ | -5.89 | 1.30 | 1.38 |
| 1 | N | 365 | ARG | CZ-NH1 | 5.89 | 1.40 | 1.33 |
| 1 | B | 288 | SER | C-O | -5.89 | 1.12 | 1.23 |
| 1 | C | 179 | ALA | CA-CB | 5.89 | 1.64 | 1.52 |
| 1 | E | 106 | GLU | CG-CD | 5.89 | 1.60 | 1.51 |
| 1 | D | 291 | TYR | CB-CG | -5.89 | 1.42 | 1.51 |
| 1 | H | 233 | ASP | CB-CG | 5.89 | 1.64 | 1.51 |
| 1 | M | 64 | LYS | C-O | 5.89 | 1.34 | 1.23 |
| 1 | O | 66 | SER | CB-OG | 5.89 | 1.50 | 1.42 |
| 1 | G | 391 | ILE | CB-CG2 | 5.88 | 1.71 | 1.52 |
| 1 | M | 240 | GLU | CD-OE1 | 5.88 | 1.32 | 1.25 |
| 1 | A | 280 | SER | CB-OG | 5.88 | 1.49 | 1.42 |
| 1 | O | 443 | LYS | CG-CD | 5.88 | 1.72 | 1.52 |
| 1 | F | 78 | PRO | CA-CB | 5.88 | 1.65 | 1.53 |
| 1 | J | 56 | ASN | CG-OD1 | 5.88 | 1.36 | 1.24 |
| 1 | A | 30 | ARG | CA-C | -5.88 | 1.37 | 1.52 |
| 1 | B | 343 | SER | CB-OG | 5.88 | 1.49 | 1.42 |
| 1 | C | 278 | LYS | CB-CG | 5.88 | 1.68 | 1.52 |
| 1 | D | 276 | TYR | CD1-CE1 | -5.88 | 1.30 | 1.39 |
| 1 | M | 91 | TYR | CE2-CZ | 5.88 | 1.46 | 1.38 |
| 1 | E | 362 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | G | 299 | MET | N-CA | 5.88 | 1.58 | 1.46 |
| 1 | I | 169 | TRP | CG-CD1 | -5.88 | 1.28 | 1.36 |
| 1 | O | 210 | PHE | CD1-CE1 | -5.88 | 1.27 | 1.39 |
| 1 | A | 342 | MET | SD-CE | 5.87 | 2.10 | 1.77 |
| 1 | B | 342 | MET | C-O | 5.87 | 1.34 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 218 | SER | CB-OG | -5.87 | 1.34 | 1.42 |
| 1 | E | 296 | SER | C-O | -5.87 | 1.12 | 1.23 |
| 1 | H | 106 | GLU | CG-CD | 5.87 | 1.60 | 1.51 |
| 1 | K | 74 | ARG | CB-CG | -5.87 | 1.36 | 1.52 |
| 1 | E | 224 | ILE | CB-CG2 | -5.87 | 1.34 | 1.52 |
| 1 | J | 376 | PHE | C-O | 5.87 | 1.34 | 1.23 |
| 1 | C | 262 | ASN | CB-CG | -5.87 | 1.37 | 1.51 |
| 1 | N | 355 | TYR | C-O | 5.87 | 1.34 | 1.23 |
| 1 | A | 90 | PHE | CD1-CE1 | 5.87 | 1.50 | 1.39 |
| 1 | D | 311 | TYR | C-O | 5.87 | 1.34 | 1.23 |
| 1 | K | 370 | TYR | CB-CG | -5.87 | 1.42 | 1.51 |
| 1 | G | 181 | GLN | CD-NE2 | 5.86 | 1.47 | 1.32 |
| 1 | K | 227 | SER | CA-CB | 5.86 | 1.61 | 1.52 |
| 1 | K | 261 | PHE | CB-CG | 5.86 | 1.61 | 1.51 |
| 1 | L | 363 | TYR | CB-CG | -5.86 | 1.42 | 1.51 |
| 1 | N | 49 | TYR | CG-CD1 | 5.86 | 1.46 | 1.39 |
| 1 | K | 276 | TYR | CD1-CE1 | 5.86 | 1.48 | 1.39 |
| 1 | D | 200 | MET | C-O | 5.86 | 1.34 | 1.23 |
| 1 | O | 329 | LEU | C-O | 5.86 | 1.34 | 1.23 |
| 1 | B | 247 | PHE | CE2-CZ | -5.86 | 1.26 | 1.37 |
| 1 | D | 170 | GLY | C-O | 5.86 | 1.33 | 1.23 |
| 1 | J | 293 | PRO | CA-C | -5.86 | 1.41 | 1.52 |
| 1 | D | 106 | GLU | C-O | 5.86 | 1.34 | 1.23 |
| 1 | F | 61 | LEU | CG-CD1 | 5.86 | 1.73 | 1.51 |
| 1 | N | 249 | TYR | CB-CG | -5.86 | 1.42 | 1.51 |
| 1 | H | 61 | LEU | CG-CD1 | 5.86 | 1.73 | 1.51 |
| 1 | N | 263 | ARG | C-O | 5.86 | 1.34 | 1.23 |
| 1 | B | 271 | VAL | CB-CG2 | 5.85 | 1.65 | 1.52 |
| 1 | C | 55 | PRO | CA-C | 5.85 | 1.64 | 1.52 |
| 1 | K | 438 | GLU | CB-CG | 5.85 | 1.63 | 1.52 |
| 1 | B | 446 | PHE | CG-CD1 | 5.85 | 1.47 | 1.38 |
| 1 | L | 307 | PHE | CG-CD2 | -5.85 | 1.29 | 1.38 |
| 1 | O | 152 | LYS | CE-NZ | 5.85 | 1.63 | 1.49 |
| 1 | O | 282 | SER | CB-OG | 5.85 | 1.49 | 1.42 |
| 1 | D | 29 | ALA | CA-CB | 5.84 | 1.64 | 1.52 |
| 1 | I | 85 | PHE | CE2-CZ | 5.84 | 1.48 | 1.37 |
| 1 | E | 130 | GLU | CD-OE1 | 5.84 | 1.32 | 1.25 |
| 1 | B | 455 | PHE | CE2-CZ | -5.84 | 1.26 | 1.37 |
| 1 | G | 72 | VAL | CB-CG2 | -5.84 | 1.40 | 1.52 |
| 1 | J | 352 | GLU | CB-CG | -5.84 | 1.41 | 1.52 |
| 1 | L | 120 | HIS | N-CA | 5.84 | 1.58 | 1.46 |
| 1 | O | 194 | VAL | C-O | 5.84 | 1.34 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 452 | LYS | CD-CE | 5.84 | 1.65 | 1.51 |
| 1 | I | 88 | THR | C-O | 5.84 | 1.34 | 1.23 |
| 1 | L | 336 | THR | CB-CG2 | -5.84 | 1.33 | 1.52 |
| 1 | A | 191 | ILE | CA-CB | -5.83 | 1.41 | 1.54 |
| 1 | H | 142 | ASP | C-O | 5.83 | 1.34 | 1.23 |
| 1 | M | 44 | ALA | CA-CB | 5.83 | 1.64 | 1.52 |
| 1 | D | 462 | PHE | CE1-CZ | 5.83 | 1.48 | 1.37 |
| 1 | B | 21 | VAL | CA-CB | -5.83 | 1.42 | 1.54 |
| 1 | C | 251 | ARG | CZ-NH1 | 5.83 | 1.40 | 1.33 |
| 1 | H | 28 | VAL | C-O | 5.83 | 1.34 | 1.23 |
| 1 | I | 314 | GLN | CD-OE1 | 5.83 | 1.36 | 1.24 |
| 1 | I | 452 | LYS | C-O | 5.83 | 1.34 | 1.23 |
| 1 | O | 50 | PHE | CD2-CE2 | -5.83 | 1.27 | 1.39 |
| 1 | D | 199 | ASP | C-O | -5.83 | 1.12 | 1.23 |
| 1 | G | 38 | GLY | C-O | 5.83 | 1.32 | 1.23 |
| 1 | I | 320 | ASN | C-O | -5.83 | 1.12 | 1.23 |
| 1 | A | 290 | ASN | C-O | 5.83 | 1.34 | 1.23 |
| 1 | D | 199 | ASP | CB-CG | -5.83 | 1.39 | 1.51 |
| 1 | F | 73 | PHE | CB-CG | -5.83 | 1.41 | 1.51 |
| 1 | H | 221 | PRO | CG-CD | 5.83 | 1.69 | 1.50 |
| 1 | A | 467 | LYS | CG-CD | 5.82 | 1.72 | 1.52 |
| 1 | C | 148 | SER | CB-OG | 5.82 | 1.49 | 1.42 |
| 1 | K | 103 | VAL | CB-CG1 | 5.82 | 1.65 | 1.52 |
| 1 | H | 101 | ALA | C-O | 5.82 | 1.34 | 1.23 |
| 1 | L | 93 | PRO | CB-CG | -5.82 | 1.20 | 1.50 |
| 1 | N | 383 | LEU | CG-CD1 | 5.82 | 1.73 | 1.51 |
| 1 | O | 206 | GLY | C-O | 5.82 | 1.32 | 1.23 |
| 1 | I | 334 | VAL | C-O | 5.82 | 1.34 | 1.23 |
| 1 | K | 24 | THR | CA-CB | -5.82 | 1.38 | 1.53 |
| 1 | B | 394 | MET | CB-CG | -5.82 | 1.32 | 1.51 |
| 1 | L | 165 | ILE | CG1-CD1 | 5.82 | 1.90 | 1.50 |
| 1 | A | 370 | TYR | CE1-CZ | -5.82 | 1.30 | 1.38 |
| 1 | E | 132 | ALA | CA-CB | -5.82 | 1.40 | 1.52 |
| 1 | F | 249 | TYR | CD2-CE2 | 5.82 | 1.48 | 1.39 |
| 1 | G | 453 | GLU | CB-CG | 5.82 | 1.63 | 1.52 |
| 1 | L | 95 | THR | CB-OG1 | 5.82 | 1.54 | 1.43 |
| 1 | L | 315 | ARG | CZ-NH2 | 5.82 | 1.40 | 1.33 |
| 1 | G | 306 | ILE | CB-CG2 | -5.81 | 1.34 | 1.52 |
| 1 | B | 169 | TRP | CG-CD1 | -5.81 | 1.28 | 1.36 |
| 1 | C | 295 | PRO | C-O | -5.81 | 1.11 | 1.23 |
| 1 | A | 242 | TYR | CE2-CZ | -5.81 | 1.30 | 1.38 |
| 1 | G | 56 | ASN | C-O | 5.81 | 1.34 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | M | 400 | GLU | CG-CD | 5.81 | 1.60 | 1.51 |
| 1 | J | 466 | ARG | CG-CD | 5.81 | 1.66 | 1.51 |
| 1 | C | 471 | GLN | CD-OE1 | 5.80 | 1.36 | 1.24 |
| 1 | F | 41 | ARG | CD-NE | 5.80 | 1.56 | 1.46 |
| 1 | E | 390 | TYR | CZ-OH | 5.80 | 1.47 | 1.37 |
| 1 | B | 248 | PHE | CB-CG | -5.80 | 1.41 | 1.51 |
| 1 | E | 141 | VAL | CA-CB | -5.80 | 1.42 | 1.54 |
| 1 | E | 83 | PHE | CB-CG | 5.80 | 1.61 | 1.51 |
| 1 | G | 91 | TYR | CE1-CZ | 5.80 | 1.46 | 1.38 |
| 1 | J | 370 | TYR | CG-CD2 | -5.80 | 1.31 | 1.39 |
| 1 | O | 111 | GLN | CG-CD | 5.80 | 1.64 | 1.51 |
| 1 | G | 55 | PRO | CA-C | 5.80 | 1.64 | 1.52 |
| 1 | G | 312 | TRP | CE2-CZ2 | -5.80 | 1.29 | 1.39 |
| 1 | I | 45 | VAL | CB-CG1 | -5.80 | 1.40 | 1.52 |
| 1 | J | 167 | GLU | CD-OE1 | 5.80 | 1.32 | 1.25 |
| 1 | D | 151 | TYR | C-O | 5.79 | 1.34 | 1.23 |
| 1 | C | 471 | GLN | CD-NE2 | 5.79 | 1.47 | 1.32 |
| 1 | E | 234 | TYR | CG-CD1 | -5.79 | 1.31 | 1.39 |
| 1 | I | 97 | ARG | CG-CD | 5.79 | 1.66 | 1.51 |
| 1 | J | 68 | LEU | CA-C | -5.79 | 1.37 | 1.52 |
| 1 | B | 32 | ASN | CB-CG | 5.79 | 1.64 | 1.51 |
| 1 | K | 445 | THR | CB-CG2 | 5.79 | 1.71 | 1.52 |
| 1 | J | 454 | LYS | CD-CE | 5.79 | 1.65 | 1.51 |
| 1 | N | 113 | LEU | C-O | 5.79 | 1.34 | 1.23 |
| 1 | F | 55 | PRO | CA-C | 5.79 | 1.64 | 1.52 |
| 1 | C | 130 | GLU | CG-CD | -5.79 | 1.43 | 1.51 |
| 1 | C | 141 | VAL | CB-CG1 | 5.79 | 1.65 | 1.52 |
| 1 | D | 248 | PHE | CG-CD1 | -5.79 | 1.30 | 1.38 |
| 1 | G | 62 | VAL | C-O | 5.79 | 1.34 | 1.23 |
| 1 | H | 296 | SER | CB-OG | -5.79 | 1.34 | 1.42 |
| 1 | M | 352 | GLU | CG-CD | 5.79 | 1.60 | 1.51 |
| 1 | J | 299 | MET | N-CA | 5.78 | 1.57 | 1.46 |
| 1 | B | 152 | LYS | CE-NZ | 5.78 | 1.63 | 1.49 |
| 1 | O | 195 | ILE | C-O | -5.78 | 1.12 | 1.23 |
| 1 | B | 51 | PRO | CG-CD | -5.78 | 1.31 | 1.50 |
| 1 | E | 257 | VAL | CB-CG2 | 5.78 | 1.65 | 1.52 |
| 1 | J | 219 | GLU | C-O | -5.78 | 1.12 | 1.23 |
| 1 | L | 98 | LEU | CG-CD1 | 5.78 | 1.73 | 1.51 |
| 1 | J | 86 | PRO | C-O | 5.78 | 1.34 | 1.23 |
| 1 | K | 379 | CYS | CB-SG | -5.78 | 1.72 | 1.81 |
| 1 | M | 42 | LEU | CG-CD2 | 5.78 | 1.73 | 1.51 |
| 1 | M | 471 | GLN | CB-CG | -5.78 | 1.36 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 80 | PRO | CB-CG | 5.77 | 1.78 | 1.50 |
| 1 | B | 60 | ILE | C-O | -5.77 | 1.12 | 1.23 |
| 1 | B | 246 | LEU | CG-CD1 | -5.77 | 1.30 | 1.51 |
| 1 | M | 316 | ALA | N-CA | 5.77 | 1.57 | 1.46 |
| 1 | O | 327 | ASN | CB-CG | 5.77 | 1.64 | 1.51 |
| 1 | O | 438 | GLU | CG-CD | 5.77 | 1.60 | 1.51 |
| 1 | D | 368 | GLU | CG-CD | -5.77 | 1.43 | 1.51 |
| 1 | H | 176 | THR | CB-CG2 | 5.77 | 1.71 | 1.52 |
| 1 | I | 285 | ASN | C-O | 5.77 | 1.34 | 1.23 |
| 1 | N | 85 | PHE | CE1-CZ | 5.77 | 1.48 | 1.37 |
| 1 | G | 108 | GLY | C-O | 5.77 | 1.32 | 1.23 |
| 1 | D | 267 | VAL | C-O | -5.77 | 1.12 | 1.23 |
| 1 | H | 312 | TRP | CD2-CE2 | 5.77 | 1.48 | 1.41 |
| 1 | L | 124 | ASN | CB-CG | 5.77 | 1.64 | 1.51 |
| 1 | O | 312 | TRP | C-O | 5.77 | 1.34 | 1.23 |
| 1 | C | 91 | TYR | CE2-CZ | 5.76 | 1.46 | 1.38 |
| 1 | H | 66 | SER | CB-OG | 5.76 | 1.49 | 1.42 |
| 1 | J | 86 | PRO | CA-C | 5.76 | 1.64 | 1.52 |
| 1 | N | 442 | LYS | C-O | 5.76 | 1.34 | 1.23 |
| 1 | D | 202 | ASP | N-CA | -5.76 | 1.34 | 1.46 |
| 1 | G | 248 | PHE | CD2-CE2 | -5.76 | 1.27 | 1.39 |
| 1 | C | 454 | LYS | C-O | 5.76 | 1.34 | 1.23 |
| 1 | D | 463 | PRO | N-CA | -5.76 | 1.37 | 1.47 |
| 1 | G | 348 | ILE | CB-CG2 | 5.76 | 1.70 | 1.52 |
| 1 | K | 21 | VAL | CA-CB | -5.76 | 1.42 | 1.54 |
| 1 | B | 350 | THR | CA-CB | 5.76 | 1.68 | 1.53 |
| 1 | E | 92 | ASN | CG-OD1 | 5.76 | 1.36 | 1.24 |
| 1 | G | 306 | ILE | CA-CB | -5.76 | 1.41 | 1.54 |
| 1 | O | 391 | ILE | C-O | 5.76 | 1.34 | 1.23 |
| 1 | C | 158 | LEU | C-O | 5.76 | 1.34 | 1.23 |
| 1 | M | 442 | LYS | CD-CE | 5.76 | 1.65 | 1.51 |
| 1 | N | 368 | GLU | C-O | 5.75 | 1.34 | 1.23 |
| 1 | G | 315 | ARG | CG-CD | 5.75 | 1.66 | 1.51 |
| 1 | H | 390 | TYR | N-CA | 5.75 | 1.57 | 1.46 |
| 1 | I | 363 | TYR | CB-CG | -5.75 | 1.43 | 1.51 |
| 1 | D | 244 | ASP | CG-OD1 | 5.75 | 1.38 | 1.25 |
| 1 | G | 116 | GLY | C-O | 5.75 | 1.32 | 1.23 |
| 1 | L | 221 | PRO | CG-CD | -5.75 | 1.31 | 1.50 |
| 1 | M | 320 | ASN | C-O | -5.75 | 1.12 | 1.23 |
| 1 | H | 472 | LEU | N-CA | 5.75 | 1.57 | 1.46 |
| 1 | E | 90 | PHE | CE2-CZ | 5.75 | 1.48 | 1.37 |
| 1 | E | 448 | GLU | CB-CG | 5.75 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | L | 63 | PRO | C-O | 5.75 | 1.34 | 1.23 |
| 1 | N | 91 | TYR | C-O | 5.75 | 1.34 | 1.23 |
| 1 | O | 32 | ASN | C-O | 5.75 | 1.34 | 1.23 |
| 1 | D | 139 | ALA | C-O | 5.74 | 1.34 | 1.23 |
| 1 | C | 81 | ASN | CG-OD1 | 5.74 | 1.36 | 1.24 |
| 1 | F | 215 | ALA | CA-CB | -5.74 | 1.40 | 1.52 |
| 1 | G | 208 | MET | C-O | 5.74 | 1.34 | 1.23 |
| 1 | G | 265 | GLY | N-CA | 5.74 | 1.54 | 1.46 |
| 1 | J | 75 | ILE | C-O | 5.74 | 1.34 | 1.23 |
| 1 | A | 236 | LYS | CE-NZ | 5.74 | 1.63 | 1.49 |
| 1 | C | 225 | CYS | C-O | 5.74 | 1.34 | 1.23 |
| 1 | G | 176 | THR | CB-CG2 | 5.74 | 1.71 | 1.52 |
| 1 | N | 280 | SER | CB-OG | 5.74 | 1.49 | 1.42 |
| 1 | O | 278 | LYS | CD-CE | 5.74 | 1.65 | 1.51 |
| 1 | A | 287 | ALA | CA-CB | 5.74 | 1.64 | 1.52 |
| 1 | B | 54 | LYS | CD-CE | 5.74 | 1.65 | 1.51 |
| 1 | E | 374 | PHE | CE1-CZ | 5.74 | 1.48 | 1.37 |
| 1 | H | 296 | SER | CA-CB | -5.74 | 1.44 | 1.52 |
| 1 | L | 159 | ILE | CG1-CD1 | 5.74 | 1.90 | 1.50 |
| 1 | M | 78 | PRO | CG-CD | -5.74 | 1.31 | 1.50 |
| 1 | M | 148 | SER | CB-OG | 5.74 | 1.49 | 1.42 |
| 1 | N | 114 | GLY | N-CA | 5.74 | 1.54 | 1.46 |
| 1 | J | 174 | PRO | C-O | 5.73 | 1.34 | 1.23 |
| 1 | L | 188 | LEU | CG-CD2 | -5.73 | 1.30 | 1.51 |
| 1 | E | 338 | ARG | CZ-NH1 | 5.73 | 1.40 | 1.33 |
| 1 | G | 55 | PRO | C-O | 5.73 | 1.34 | 1.23 |
| 1 | M | 71 | ARG | C-O | -5.73 | 1.12 | 1.23 |
| 1 | M | 453 | GLU | CD-OE1 | 5.73 | 1.31 | 1.25 |
| 1 | G | 225 | CYS | C-O | 5.73 | 1.34 | 1.23 |
| 1 | J | 139 | ALA | CA-C | 5.73 | 1.67 | 1.52 |
| 1 | M | 370 | TYR | CZ-OH | 5.73 | 1.47 | 1.37 |
| 1 | B | 323 | ILE | CB-CG2 | 5.73 | 1.70 | 1.52 |
| 1 | C | 135 | TYR | CG-CD1 | 5.73 | 1.46 | 1.39 |
| 1 | D | 104 | GLY | N-CA | -5.73 | 1.37 | 1.46 |
| 1 | D | 144 | ARG | CB-CG | 5.73 | 1.68 | 1.52 |
| 1 | J | 57 | ASN | CA-C | 5.73 | 1.67 | 1.52 |
| 1 | G | 455 | PHE | C-O | 5.72 | 1.34 | 1.23 |
| 1 | E | 318 | GLY | CA-C | -5.72 | 1.42 | 1.51 |
| 1 | K | 170 | GLY | C-O | 5.72 | 1.32 | 1.23 |
| 1 | C | 236 | LYS | CG-CD | 5.72 | 1.72 | 1.52 |
| 1 | M | 390 | TYR | CB-CG | 5.72 | 1.60 | 1.51 |
| 1 | E | 255 | MET | C-O | -5.72 | 1.12 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 123 | LEU | C-O | -5.72 | 1.12 | 1.23 |
| 1 | J | 389 | THR | CB-CG2 | 5.72 | 1.71 | 1.52 |
| 1 | K | 138 | ASN | C-O | 5.72 | 1.34 | 1.23 |
| 1 | A | 341 | ASN | C-O | 5.71 | 1.34 | 1.23 |
| 1 | F | 43 | LEU | C-O | 5.71 | 1.34 | 1.23 |
| 1 | G | 68 | LEU | CG-CD2 | -5.71 | 1.30 | 1.51 |
| 1 | J | 137 | ALA | CA-CB | 5.71 | 1.64 | 1.52 |
| 1 | J | 35 | TYR | C-O | 5.71 | 1.34 | 1.23 |
| 1 | H | 175 | CYS | N-CA | 5.71 | 1.57 | 1.46 |
| 1 | L | 135 | TYR | CD2-CE2 | -5.71 | 1.30 | 1.39 |
| 1 | O | 140 | GLY | C-O | 5.71 | 1.32 | 1.23 |
| 1 | O | 294 | THR | CB-CG2 | -5.71 | 1.33 | 1.52 |
| 1 | B | 472 | LEU | CA-CB | 5.71 | 1.66 | 1.53 |
| 1 | F | 393 | SER | CB-OG | -5.71 | 1.34 | 1.42 |
| 1 | G | 467 | LYS | CG-CD | 5.71 | 1.71 | 1.52 |
| 1 | K | 245 | SER | CA-CB | 5.71 | 1.61 | 1.52 |
| 1 | N | 94 | ASP | C-O | 5.71 | 1.34 | 1.23 |
| 1 | D | 130 | GLU | C-O | 5.71 | 1.34 | 1.23 |
| 1 | O | 444 | TYR | CD1-CE1 | 5.71 | 1.48 | 1.39 |
| 1 | E | 291 | TYR | CZ-OH | 5.70 | 1.47 | 1.37 |
| 1 | H | 40 | SER | CB-OG | 5.70 | 1.49 | 1.42 |
| 1 | I | 151 | TYR | CG-CD1 | 5.70 | 1.46 | 1.39 |
| 1 | K | 299 | MET | N-CA | 5.70 | 1.57 | 1.46 |
| 1 | D | 174 | PRO | N-CA | 5.70 | 1.56 | 1.47 |
| 1 | I | 248 | PHE | CB-CG | -5.70 | 1.41 | 1.51 |
| 1 | J | 75 | ILE | CA-CB | -5.70 | 1.41 | 1.54 |
| 1 | J | 207 | ALA | CA-CB | -5.70 | 1.40 | 1.52 |
| 1 | M | 273 | ASP | CG-OD2 | 5.70 | 1.38 | 1.25 |
| 1 | O | 97 | ARG | CB-CG | 5.70 | 1.68 | 1.52 |
| 1 | D | 292 | PHE | CE1-CZ | 5.70 | 1.48 | 1.37 |
| 1 | F | 231 | TYR | CZ-OH | 5.70 | 1.47 | 1.37 |
| 1 | H | 218 | SER | CB-OG | 5.70 | 1.49 | 1.42 |
| 1 | H | 390 | TYR | CD2-CE2 | 5.70 | 1.47 | 1.39 |
| 1 | B | 402 | TRP | CB-CG | 5.70 | 1.60 | 1.50 |
| 1 | C | 75 | ILE | CA-CB | -5.70 | 1.41 | 1.54 |
| 1 | O | 443 | LYS | CB-CG | 5.70 | 1.68 | 1.52 |
| 1 | J | 285 | ASN | C-O | 5.69 | 1.34 | 1.23 |
| 1 | N | 31 | THR | CB-CG2 | 5.69 | 1.71 | 1.52 |
| 1 | I | 34 | TYR | CD1-CE1 | 5.69 | 1.47 | 1.39 |
| 1 | I | 70 | TYR | CD1-CE1 | 5.69 | 1.47 | 1.39 |
| 1 | L | 322 | GLY | C-O | 5.69 | 1.32 | 1.23 |
| 1 | D | 95 | THR | CB-OG1 | 5.69 | 1.54 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 468 | PHE | CD2-CE2 | 5.69 | 1.50 | 1.39 |
| 1 | K | 269 | GLU | CB-CG | 5.69 | 1.62 | 1.52 |
| 1 | M | 438 | GLU | CB-CG | 5.69 | 1.62 | 1.52 |
| 1 | N | 266 | THR | CB-CG2 | 5.69 | 1.71 | 1.52 |
| 1 | L | 283 | THR | C-O | -5.69 | 1.12 | 1.23 |
| 1 | N | 256 | PHE | CE2-CZ | -5.69 | 1.26 | 1.37 |
| 1 | B | 138 | ASN | C-O | 5.68 | 1.34 | 1.23 |
| 1 | C | 234 | TYR | CE1-CZ | -5.68 | 1.31 | 1.38 |
| 1 | E | 230 | LYS | CB-CG | 5.68 | 1.67 | 1.52 |
| 1 | F | 268 | GLY | C-O | 5.68 | 1.32 | 1.23 |
| 1 | F | 471 | GLN | C-O | 5.68 | 1.34 | 1.23 |
| 1 | I | 468 | PHE | CE1-CZ | 5.68 | 1.48 | 1.37 |
| 1 | L | 311 | TYR | CZ-OH | -5.68 | 1.28 | 1.37 |
| 1 | N | 162 | LYS | C-O | 5.68 | 1.34 | 1.23 |
| 1 | O | 212 | THR | CA-CB | -5.68 | 1.38 | 1.53 |
| 1 | H | 81 | ASN | C-O | -5.68 | 1.12 | 1.23 |
| 1 | I | 25 | ASP | CG-OD2 | 5.68 | 1.38 | 1.25 |
| 1 | K | 370 | TYR | CE1-CZ | -5.68 | 1.31 | 1.38 |
| 1 | F | 102 | CYS | CB-SG | -5.68 | 1.72 | 1.81 |
| 1 | M | 51 | PRO | N-CD | 5.68 | 1.55 | 1.47 |
| 1 | N | 155 | GLN | CG-CD | 5.68 | 1.64 | 1.51 |
| 1 | A | 400 | GLU | CG-CD | 5.68 | 1.60 | 1.51 |
| 1 | H | 103 | VAL | C-O | 5.68 | 1.34 | 1.23 |
| 1 | H | 171 | LYS | CB-CG | 5.68 | 1.67 | 1.52 |
| 1 | L | 42 | LEU | CG-CD2 | 5.68 | 1.72 | 1.51 |
| 1 | O | 362 | GLU | CD-OE1 | 5.68 | 1.31 | 1.25 |
| 1 | G | 247 | PHE | CE1-CZ | 5.68 | 1.48 | 1.37 |
| 1 | J | 50 | PHE | CE2-CZ | -5.68 | 1.26 | 1.37 |
| 1 | J | 98 | LEU | CG-CD1 | 5.68 | 1.72 | 1.51 |
| 1 | A | 82 | LYS | CD-CE | 5.67 | 1.65 | 1.51 |
| 1 | A | 392 | HIS | C-O | 5.67 | 1.34 | 1.23 |
| 1 | C | 64 | LYS | CB-CG | 5.67 | 1.67 | 1.52 |
| 1 | D | 203 | THR | C-O | 5.67 | 1.34 | 1.23 |
| 1 | J | 298 | SER | CB-OG | 5.67 | 1.49 | 1.42 |
| 1 | N | 250 | LEU | C-O | 5.67 | 1.34 | 1.23 |
| 1 | D | 70 | TYR | CE1-CZ | 5.67 | 1.46 | 1.38 |
| 1 | D | 472 | LEU | N-CA | 5.67 | 1.57 | 1.46 |
| 1 | H | 362 | GLU | CD-OE1 | 5.67 | 1.31 | 1.25 |
| 1 | J | 130 | GLU | CD-OE1 | -5.67 | 1.19 | 1.25 |
| 1 | H | 183 | GLY | C-O | 5.67 | 1.32 | 1.23 |
| 1 | G | 48 | PRO | CA-C | -5.67 | 1.41 | 1.52 |
| 1 | O | 241 | PRO | CB-CG | 5.67 | 1.78 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 145 | GLU | C-O | 5.66 | 1.34 | 1.23 |
| 1 | K | 202 | ASP | CG-OD1 | 5.66 | 1.38 | 1.25 |
| 1 | N | 361 | LYS | CE-NZ | 5.66 | 1.63 | 1.49 |
| 1 | K | 251 | ARG | CZ-NH1 | -5.66 | 1.25 | 1.33 |
| 1 | L | 462 | PHE | CG-CD1 | -5.66 | 1.30 | 1.38 |
| 1 | G | 364 | LEU | C-O | 5.66 | 1.34 | 1.23 |
| 1 | J | 136 | ALA | C-O | 5.66 | 1.34 | 1.23 |
| 1 | L | 332 | THR | CB-CG2 | -5.66 | 1.33 | 1.52 |
| 1 | M | 82 | LYS | C-O | -5.66 | 1.12 | 1.23 |
| 1 | A | 312 | TRP | CZ3-CH2 | 5.66 | 1.49 | 1.40 |
| 1 | E | 369 | GLU | CB-CG | 5.66 | 1.62 | 1.52 |
| 1 | E | 390 | TYR | CE1-CZ | 5.66 | 1.46 | 1.38 |
| 1 | L | 137 | ALA | CA-CB | 5.66 | 1.64 | 1.52 |
| 1 | M | 159 | ILE | CB-CG2 | -5.66 | 1.35 | 1.52 |
| 1 | N | 50 | PHE | CE1-CZ | 5.66 | 1.48 | 1.37 |
| 1 | A | 111 | GLN | CG-CD | 5.66 | 1.64 | 1.51 |
| 1 | H | 321 | ASN | CB-CG | 5.66 | 1.64 | 1.51 |
| 1 | D | 462 | PHE | CB-CG | -5.65 | 1.41 | 1.51 |
| 1 | L | 40 | SER | CA-C | 5.65 | 1.67 | 1.52 |
| 1 | I | 162 | LYS | CG-CD | 5.65 | 1.71 | 1.52 |
| 1 | N | 391 | ILE | C-O | 5.65 | 1.34 | 1.23 |
| 1 | E | 184 | ASP | CB-CG | 5.65 | 1.63 | 1.51 |
| 1 | O | 249 | TYR | CG-CD2 | -5.65 | 1.31 | 1.39 |
| 1 | H | 363 | TYR | CB-CG | 5.65 | 1.60 | 1.51 |
| 1 | O | 403 | ASN | CG-ND2 | 5.65 | 1.47 | 1.32 |
| 1 | D | 362 | GLU | C-O | 5.65 | 1.34 | 1.23 |
| 1 | J | 471 | GLN | CB-CG | -5.65 | 1.37 | 1.52 |
| 1 | O | 276 | TYR | CG-CD2 | 5.65 | 1.46 | 1.39 |
| 1 | E | 396 | SER | CA-C | 5.64 | 1.67 | 1.52 |
| 1 | G | 387 | VAL | CB-CG1 | 5.64 | 1.64 | 1.52 |
| 1 | A | 462 | PHE | CB-CG | -5.64 | 1.41 | 1.51 |
| 1 | F | 158 | LEU | C-O | 5.64 | 1.34 | 1.23 |
| 1 | L | 111 | GLN | CD-OE1 | 5.64 | 1.36 | 1.24 |
| 1 | N | 455 | PHE | CD2-CE2 | 5.64 | 1.50 | 1.39 |
| 1 | F | 149 | MET | CB-CG | 5.64 | 1.69 | 1.51 |
| 1 | N | 380 | LYS | CD-CE | 5.64 | 1.65 | 1.51 |
| 1 | H | 349 | SER | CB-OG | 5.64 | 1.49 | 1.42 |
| 1 | I | 150 | ASP | N-CA | 5.64 | 1.57 | 1.46 |
| 1 | A | 261 | PHE | CE2-CZ | 5.64 | 1.48 | 1.37 |
| 1 | H | 56 | ASN | CB-CG | 5.64 | 1.64 | 1.51 |
| 1 | H | 205 | PHE | CG-CD1 | 5.64 | 1.47 | 1.38 |
| 1 | J | 31 | THR | C-O | -5.64 | 1.12 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | L | 91 | TYR | CD1-CE1 | -5.64 | 1.30 | 1.39 |
| 1 | L | 444 | TYR | CG-CD1 | 5.64 | 1.46 | 1.39 |
| 1 | A | 118 | SER | CA-CB | -5.63 | 1.44 | 1.52 |
| 1 | C | 329 | LEU | CG-CD1 | -5.63 | 1.31 | 1.51 |
| 1 | F | 130 | GLU | C-O | 5.63 | 1.34 | 1.23 |
| 1 | G | 363 | TYR | CG-CD2 | 5.63 | 1.46 | 1.39 |
| 1 | M | 75 | ILE | CB-CG2 | -5.63 | 1.35 | 1.52 |
| 1 | I | 368 | GLU | CD-OE1 | 5.63 | 1.31 | 1.25 |
| 1 | K | 91 | TYR | CZ-OH | 5.63 | 1.47 | 1.37 |
| 1 | M | 63 | PRO | CB-CG | 5.63 | 1.78 | 1.50 |
| 1 | J | 376 | PHE | CG-CD1 | 5.63 | 1.47 | 1.38 |
| 1 | C | 299 | MET | CA-CB | -5.63 | 1.41 | 1.53 |
| 1 | D | 286 | LEU | CA-CB | -5.63 | 1.40 | 1.53 |
| 1 | I | 106 | GLU | CD-OE1 | 5.63 | 1.31 | 1.25 |
| 1 | D | 273 | ASP | CB-CG | 5.63 | 1.63 | 1.51 |
| 1 | J | 468 | PHE | CE2-CZ | -5.63 | 1.26 | 1.37 |
| 1 | M | 248 | PHE | CA-CB | -5.63 | 1.41 | 1.53 |
| 1 | N | 468 | PHE | C-O | 5.63 | 1.34 | 1.23 |
| 1 | A | 297 | GLY | C-O | 5.62 | 1.32 | 1.23 |
| 1 | B | 225 | CYS | N-CA | 5.62 | 1.57 | 1.46 |
| 1 | N | 247 | PHE | N-CA | -5.62 | 1.35 | 1.46 |
| 1 | N | 438 | GLU | CG-CD | 5.62 | 1.60 | 1.51 |
| 1 | A | 295 | PRO | N-CD | -5.62 | 1.40 | 1.47 |
| 1 | B | 86 | PRO | CG-CD | 5.62 | 1.69 | 1.50 |
| 1 | B | 187 | PRO | CA-C | -5.62 | 1.41 | 1.52 |
| 1 | C | 123 | LEU | CG-CD2 | 5.62 | 1.72 | 1.51 |
| 1 | E | 102 | CYS | CB-SG | -5.62 | 1.72 | 1.81 |
| 1 | E | 138 | ASN | C-O | 5.62 | 1.34 | 1.23 |
| 1 | G | 210 | PHE | CG-CD2 | 5.62 | 1.47 | 1.38 |
| 1 | N | 234 | TYR | CE2-CZ | -5.62 | 1.31 | 1.38 |
| 1 | H | 367 | GLY | N-CA | 5.62 | 1.54 | 1.46 |
| 1 | E | 70 | TYR | CG-CD1 | -5.62 | 1.31 | 1.39 |
| 1 | F | 453 | GLU | CD-OE1 | 5.62 | 1.31 | 1.25 |
| 1 | K | 149 | MET | CG-SD | -5.62 | 1.66 | 1.81 |
| 1 | K | 335 | ASP | CB-CG | -5.62 | 1.40 | 1.51 |
| 1 | O | 448 | GLU | CD-OE2 | 5.62 | 1.31 | 1.25 |
| 1 | L | 390 | TYR | CB-CG | -5.62 | 1.43 | 1.51 |
| 1 | M | 327 | ASN | CB-CG | 5.62 | 1.64 | 1.51 |
| 1 | A | 164 | PRO | C-O | -5.62 | 1.12 | 1.23 |
| 1 | F | 139 | ALA | C-O | 5.62 | 1.34 | 1.23 |
| 1 | L | 463 | PRO | N-CA | 5.62 | 1.56 | 1.47 |
| 1 | N | 89 | SER | N-CA | 5.62 | 1.57 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 97 | ARG | NE-CZ | 5.61 | 1.40 | 1.33 |
| 1 | E | 455 | PHE | CD2-CE2 | 5.61 | 1.50 | 1.39 |
| 1 | M | 272 | PRO | N-CA | -5.61 | 1.37 | 1.47 |
| 1 | M | 390 | TYR | CE1-CZ | -5.61 | 1.31 | 1.38 |
| 1 | N | 34 | TYR | CG-CD1 | -5.61 | 1.31 | 1.39 |
| 1 | D | 446 | PHE | CA-CB | -5.61 | 1.41 | 1.53 |
| 1 | G | 352 | GLU | C-O | 5.61 | 1.34 | 1.23 |
| 1 | J | 352 | GLU | CG-CD | 5.61 | 1.60 | 1.51 |
| 1 | K | 73 | PHE | CD1-CE1 | 5.61 | 1.50 | 1.39 |
| 1 | M | 312 | TRP | CG-CD1 | -5.61 | 1.28 | 1.36 |
| 1 | M | 336 | THR | C-O | 5.61 | 1.34 | 1.23 |
| 1 | D | 280 | SER | CA-C | -5.61 | 1.38 | 1.52 |
| 1 | F | 237 | MET | C-O | 5.61 | 1.34 | 1.23 |
| 1 | G | 194 | VAL | C-O | 5.61 | 1.34 | 1.23 |
| 1 | K | 401 | ASP | C-O | 5.61 | 1.34 | 1.23 |
| 1 | A | 378 | LEU | C-O | -5.61 | 1.12 | 1.23 |
| 1 | G | 28 | VAL | CB-CG1 | 5.61 | 1.64 | 1.52 |
| 1 | J | 169 | TRP | CE3-CZ3 | 5.61 | 1.48 | 1.38 |
| 1 | O | 268 | GLY | C-O | 5.61 | 1.32 | 1.23 |
| 1 | A | 75 | ILE | C-O | 5.60 | 1.33 | 1.23 |
| 1 | A | 124 | ASN | C-O | -5.60 | 1.12 | 1.23 |
| 1 | C | 208 | MET | C-O | 5.60 | 1.33 | 1.23 |
| 1 | F | 317 | GLN | CG-CD | 5.60 | 1.64 | 1.51 |
| 1 | G | 219 | GLU | CG-CD | 5.60 | 1.60 | 1.51 |
| 1 | L | 372 | LEU | CB-CG | 5.60 | 1.68 | 1.52 |
| 1 | C | 51 | PRO | CA-C | 5.60 | 1.64 | 1.52 |
| 1 | D | 376 | PHE | CD1-CE1 | -5.60 | 1.28 | 1.39 |
| 1 | O | 64 | LYS | CB-CG | 5.60 | 1.67 | 1.52 |
| 1 | D | 308 | ASN | CG-ND2 | 5.60 | 1.46 | 1.32 |
| 1 | A | 160 | GLY | CA-C | 5.60 | 1.60 | 1.51 |
| 1 | C | 363 | TYR | CE1-CZ | 5.60 | 1.45 | 1.38 |
| 1 | D | 67 | GLY | N-CA | -5.60 | 1.37 | 1.46 |
| 1 | M | 236 | LYS | CD-CE | 5.60 | 1.65 | 1.51 |
| 1 | I | 70 | TYR | CG-CD2 | -5.60 | 1.31 | 1.39 |
| 1 | J | 229 | CYS | CB-SG | -5.60 | 1.72 | 1.81 |
| 1 | L | 455 | PHE | CD1-CE1 | 5.60 | 1.50 | 1.39 |
| 1 | N | 446 | PHE | CD2-CE2 | 5.60 | 1.50 | 1.39 |
| 1 | O | 252 | ARG | N-CA | -5.60 | 1.35 | 1.46 |
| 1 | H | 46 | GLY | N-CA | 5.59 | 1.54 | 1.46 |
| 1 | M | 87 | ASP | N-CA | 5.59 | 1.57 | 1.46 |
| 1 | O | 162 | LYS | CD-CE | 5.59 | 1.65 | 1.51 |
| 1 | B | 105 | VAL | CB-CG2 | -5.59 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 216 | ASN | C-O | -5.59 | 1.12 | 1.23 |
| 1 | E | 310 | PRO | CG-CD | -5.59 | 1.32 | 1.50 |
| 1 | F | 294 | THR | C-O | -5.59 | 1.12 | 1.23 |
| 1 | I | 178 | VAL | CA-C | 5.59 | 1.67 | 1.52 |
| 1 | A | 386 | ASP | CB-CG | 5.59 | 1.63 | 1.51 |
| 1 | G | 249 | TYR | CG-CD2 | -5.59 | 1.31 | 1.39 |
| 1 | G | 359 | ASN | CA-C | 5.59 | 1.67 | 1.52 |
| 1 | N | 105 | VAL | CB-CG1 | -5.59 | 1.41 | 1.52 |
| 1 | O | 26 | GLU | CD-OE1 | 5.59 | 1.31 | 1.25 |
| 1 | H | 294 | THR | C-O | 5.59 | 1.33 | 1.23 |
| 1 | K | 341 | ASN | CG-ND2 | 5.59 | 1.46 | 1.32 |
| 1 | E | 252 | ARG | NE-CZ | -5.59 | 1.25 | 1.33 |
| 1 | F | 181 | GLN | CD-OE1 | 5.59 | 1.36 | 1.24 |
| 1 | J | 98 | LEU | C-O | 5.59 | 1.33 | 1.23 |
| 1 | M | 230 | LYS | CD-CE | 5.59 | 1.65 | 1.51 |
| 1 | N | 449 | VAL | N-CA | 5.59 | 1.57 | 1.46 |
| 1 | L | 468 | PHE | CE1-CZ | 5.58 | 1.48 | 1.37 |
| 1 | M | 438 | GLU | C-O | 5.58 | 1.33 | 1.23 |
| 1 | D | 23 | SER | CA-CB | 5.58 | 1.61 | 1.52 |
| 1 | B | 40 | SER | C-O | 5.58 | 1.33 | 1.23 |
| 1 | K | 282 | SER | C-O | 5.58 | 1.33 | 1.23 |
| 1 | M | 248 | PHE | CD2-CE2 | -5.58 | 1.28 | 1.39 |
| 1 | J | 151 | TYR | CE2-CZ | 5.58 | 1.45 | 1.38 |
| 1 | K | 110 | GLY | N-CA | 5.58 | 1.54 | 1.46 |
| 1 | K | 326 | GLY | C-O | -5.58 | 1.14 | 1.23 |
| 1 | N | 178 | VAL | CB-CG1 | 5.58 | 1.64 | 1.52 |
| 1 | C | 146 | CYS | N-CA | -5.58 | 1.35 | 1.46 |
| 1 | J | 91 | TYR | CE1-CZ | -5.58 | 1.31 | 1.38 |
| 1 | N | 95 | THR | N-CA | 5.58 | 1.57 | 1.46 |
| 1 | D | 447 | TRP | CB-CG | -5.57 | 1.40 | 1.50 |
| 1 | F | 32 | ASN | C-O | 5.57 | 1.33 | 1.23 |
| 1 | F | 247 | PHE | CE1-CZ | 5.57 | 1.48 | 1.37 |
| 1 | F | 363 | TYR | CZ-OH | 5.57 | 1.47 | 1.37 |
| 1 | O | 261 | PHE | CE1-CZ | 5.57 | 1.48 | 1.37 |
| 1 | O | 314 | GLN | C-O | 5.57 | 1.33 | 1.23 |
| 1 | F | 307 | PHE | CE1-CZ | 5.57 | 1.48 | 1.37 |
| 1 | I | 192 | ASN | CG-ND2 | 5.57 | 1.46 | 1.32 |
| 1 | N | 30 | ARG | CB-CG | 5.57 | 1.67 | 1.52 |
| 1 | E | 309 | LYS | CE-NZ | 5.57 | 1.62 | 1.49 |
| 1 | J | 124 | ASN | C-O | -5.57 | 1.12 | 1.23 |
| 1 | J | 330 | PHE | C-O | 5.57 | 1.33 | 1.23 |
| 1 | C | 331 | VAL | CB-CG2 | -5.57 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 311 | TYR | CD1-CE1 | 5.57 | 1.47 | 1.39 |
| 1 | D | 471 | GLN | CD-OE1 | 5.57 | 1.36 | 1.24 |
| 1 | H | 219 | GLU | N-CA | 5.57 | 1.57 | 1.46 |
| 1 | B | 51 | PRO | CA-CB | -5.56 | 1.42 | 1.53 |
| 1 | H | 311 | TYR | CG-CD1 | -5.56 | 1.31 | 1.39 |
| 1 | H | 363 | TYR | C-O | 5.56 | 1.33 | 1.23 |
| 1 | I | 21 | VAL | CA-CB | -5.56 | 1.43 | 1.54 |
| 1 | I | 229 | CYS | CB-SG | 5.56 | 1.91 | 1.82 |
| 1 | M | 89 | SER | CB-OG | 5.56 | 1.49 | 1.42 |
| 1 | J | 85 | PHE | CG-CD1 | 5.56 | 1.47 | 1.38 |
| 1 | J | 169 | TRP | CZ3-CH2 | 5.56 | 1.49 | 1.40 |
| 1 | M | 41 | ARG | CG-CD | -5.56 | 1.38 | 1.51 |
| 1 | C | 31 | THR | CB-CG2 | 5.56 | 1.70 | 1.52 |
| 1 | D | 70 | TYR | CG-CD1 | 5.56 | 1.46 | 1.39 |
| 1 | I | 242 | TYR | CG-CD2 | 5.56 | 1.46 | 1.39 |
| 1 | A | 348 | ILE | N-CA | -5.56 | 1.35 | 1.46 |
| 1 | N | 278 | LYS | CE-NZ | 5.56 | 1.62 | 1.49 |
| 1 | F | 40 | SER | CA-CB | 5.56 | 1.61 | 1.52 |
| 1 | M | 171 | LYS | CG-CD | 5.56 | 1.71 | 1.52 |
| 1 | N | 271 | VAL | CB-CG1 | 5.55 | 1.64 | 1.52 |
| 1 | I | 66 | SER | C-O | 5.55 | 1.33 | 1.23 |
| 1 | B | 50 | PHE | CD1-CE1 | -5.55 | 1.28 | 1.39 |
| 1 | D | 376 | PHE | N-CA | -5.55 | 1.35 | 1.46 |
| 1 | F | 110 | GLY | C-O | 5.55 | 1.32 | 1.23 |
| 1 | L | 228 | ILE | CG1-CD1 | 5.55 | 1.88 | 1.50 |
| 1 | O | 125 | LYS | CG-CD | 5.55 | 1.71 | 1.52 |
| 1 | A | 356 | LYS | CG-CD | 5.55 | 1.71 | 1.52 |
| 1 | B | 268 | GLY | C-O | 5.55 | 1.32 | 1.23 |
| 1 | C | 396 | SER | C-O | 5.55 | 1.33 | 1.23 |
| 1 | K | 180 | VAL | CB-CG2 | 5.55 | 1.64 | 1.52 |
| 1 | M | 349 | SER | CA-CB | 5.55 | 1.61 | 1.52 |
| 1 | O | 403 | ASN | CG-OD1 | 5.55 | 1.36 | 1.24 |
| 1 | H | 343 | SER | C-O | 5.55 | 1.33 | 1.23 |
| 1 | H | 374 | PHE | CG-CD2 | 5.55 | 1.47 | 1.38 |
| 1 | M | 258 | ARG | C-O | 5.55 | 1.33 | 1.23 |
| 1 | B | 31 | THR | CB-CG2 | 5.54 | 1.70 | 1.52 |
| 1 | M | 269 | GLU | CB-CG | 5.54 | 1.62 | 1.52 |
| 1 | C | 367 | GLY | N-CA | 5.54 | 1.54 | 1.46 |
| 1 | F | 203 | THR | CA-CB | -5.54 | 1.39 | 1.53 |
| 1 | B | 271 | VAL | C-N | -5.54 | 1.23 | 1.34 |
| 1 | B | 311 | TYR | CG-CD2 | 5.54 | 1.46 | 1.39 |
| 1 | D | 362 | GLU | CA-CB | -5.54 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 86 | PRO | CA-C | 5.54 | 1.64 | 1.52 |
| 1 | M | 279 | GLY | CA-C | 5.54 | 1.60 | 1.51 |
| 1 | M | 375 | ILE | CB-CG2 | -5.54 | 1.35 | 1.52 |
| 1 | N | 452 | LYS | CG-CD | 5.54 | 1.71 | 1.52 |
| 1 | O | 83 | PHE | CE1-CZ | 5.54 | 1.47 | 1.37 |
| 1 | O | 325 | TRP | CG-CD1 | 5.54 | 1.44 | 1.36 |
| 1 | E | 181 | GLN | C-O | 5.53 | 1.33 | 1.23 |
| 1 | F | 443 | LYS | CE-NZ | 5.53 | 1.62 | 1.49 |
| 1 | J | 91 | TYR | C-O | 5.53 | 1.33 | 1.23 |
| 1 | I | 116 | GLY | CA-C | 5.53 | 1.60 | 1.51 |
| 1 | F | 400 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | L | 24 | THR | C-O | 5.53 | 1.33 | 1.23 |
| 1 | F | 157 | CYS | C-O | -5.53 | 1.12 | 1.23 |
| 1 | A | 180 | VAL | CB-CG2 | 5.52 | 1.64 | 1.52 |
| 1 | C | 98 | LEU | CG-CD1 | 5.52 | 1.72 | 1.51 |
| 1 | C | 234 | TYR | CD2-CE2 | -5.52 | 1.31 | 1.39 |
| 1 | O | 439 | ASP | N-CA | 5.52 | 1.57 | 1.46 |
| 1 | D | 146 | CYS | C-O | 5.52 | 1.33 | 1.23 |
| 1 | A | 205 | PHE | N-CA | -5.52 | 1.35 | 1.46 |
| 1 | B | 330 | PHE | CE1-CZ | -5.52 | 1.26 | 1.37 |
| 1 | J | 310 | PRO | CG-CD | -5.52 | 1.32 | 1.50 |
| 1 | K | 53 | LYS | CB-CG | 5.52 | 1.67 | 1.52 |
| 1 | M | 129 | THR | CA-CB | -5.52 | 1.39 | 1.53 |
| 1 | D | 145 | GLU | CB-CG | 5.52 | 1.62 | 1.52 |
| 1 | I | 403 | ASN | C-O | 5.52 | 1.33 | 1.23 |
| 1 | D | 35 | TYR | CG-CD2 | -5.52 | 1.31 | 1.39 |
| 1 | J | 220 | VAL | CA-CB | -5.52 | 1.43 | 1.54 |
| 1 | A | 459 | LEU | CA-CB | -5.51 | 1.41 | 1.53 |
| 1 | D | 365 | ARG | CG-CD | 5.51 | 1.65 | 1.51 |
| 1 | G | 198 | GLY | N-CA | 5.51 | 1.54 | 1.46 |
| 1 | G | 307 | PHE | CB-CG | -5.51 | 1.42 | 1.51 |
| 1 | I | 380 | LYS | CD-CE | 5.51 | 1.65 | 1.51 |
| 1 | K | 374 | PHE | CE2-CZ | 5.51 | 1.47 | 1.37 |
| 1 | K | 396 | SER | CB-OG | 5.51 | 1.49 | 1.42 |
| 1 | M | 49 | TYR | CD2-CE2 | 5.51 | 1.47 | 1.39 |
| 1 | M | 353 | THR | CB-CG2 | 5.51 | 1.70 | 1.52 |
| 1 | N | 63 | PRO | C-O | 5.51 | 1.34 | 1.23 |
| 1 | D | 361 | LYS | CE-NZ | 5.51 | 1.62 | 1.49 |
| 1 | F | 262 | ASN | C-O | 5.51 | 1.33 | 1.23 |
| 1 | L | 129 | THR | N-CA | -5.51 | 1.35 | 1.46 |
| 1 | D | 114 | GLY | N-CA | 5.51 | 1.54 | 1.46 |
| 1 | M | 363 | TYR | CD1-CE1 | -5.51 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 126 | LEU | C-O | 5.51 | 1.33 | 1.23 |
| 1 | C | 198 | GLY | N-CA | 5.51 | 1.54 | 1.46 |
| 1 | D | 356 | LYS | CG-CD | 5.51 | 1.71 | 1.52 |
| 1 | L | 100 | TRP | CA-C | -5.51 | 1.38 | 1.52 |
| 1 | D | 202 | ASP | CB-CG | 5.51 | 1.63 | 1.51 |
| 1 | E | 188 | LEU | C-O | -5.51 | 1.12 | 1.23 |
| 1 | K | 354 | THR | CA-CB | -5.51 | 1.39 | 1.53 |
| 1 | M | 453 | GLU | CG-CD | 5.51 | 1.60 | 1.51 |
| 1 | C | 314 | GLN | CD-NE2 | 5.50 | 1.46 | 1.32 |
| 1 | M | 70 | TYR | CD2-CE2 | -5.50 | 1.31 | 1.39 |
| 1 | A | 438 | GLU | CD-OE1 | 5.50 | 1.31 | 1.25 |
| 1 | D | 189 | GLU | C-O | 5.50 | 1.33 | 1.23 |
| 1 | F | 233 | ASP | CG-OD1 | 5.50 | 1.38 | 1.25 |
| 1 | G | 167 | GLU | N-CA | -5.50 | 1.35 | 1.46 |
| 1 | I | 215 | ALA | CA-CB | 5.50 | 1.64 | 1.52 |
| 1 | J | 189 | GLU | CB-CG | 5.50 | 1.62 | 1.52 |
| 1 | L | 372 | LEU | CG-CD2 | 5.50 | 1.72 | 1.51 |
| 1 | C | 365 | ARG | CZ-NH2 | -5.50 | 1.25 | 1.33 |
| 1 | I | 469 | LEU | C-O | -5.50 | 1.12 | 1.23 |
| 1 | O | 85 | PHE | CG-CD1 | 5.50 | 1.47 | 1.38 |
| 1 | O | 264 | ALA | CA-CB | 5.50 | 1.64 | 1.52 |
| 1 | O | 360 | PHE | CE1-CZ | -5.50 | 1.26 | 1.37 |
| 1 | B | 306 | ILE | N-CA | -5.50 | 1.35 | 1.46 |
| 1 | C | 216 | ASN | CG-OD1 | 5.50 | 1.36 | 1.24 |
| 1 | K | 235 | ILE | CA-CB | -5.50 | 1.42 | 1.54 |
| 1 | C | 242 | TYR | CE1-CZ | 5.50 | 1.45 | 1.38 |
| 1 | G | 206 | GLY | C-O | 5.50 | 1.32 | 1.23 |
| 1 | N | 59 | LYS | C-O | 5.50 | 1.33 | 1.23 |
| 1 | F | 146 | CYS | CB-SG | 5.50 | 1.91 | 1.82 |
| 1 | C | 34 | TYR | CG-CD1 | -5.49 | 1.32 | 1.39 |
| 1 | E | 55 | PRO | CA-C | 5.49 | 1.63 | 1.52 |
| 1 | E | 217 | LYS | C-O | 5.49 | 1.33 | 1.23 |
| 1 | L | 348 | ILE | CA-CB | -5.49 | 1.42 | 1.54 |
| 1 | O | 338 | ARG | CB-CG | 5.49 | 1.67 | 1.52 |
| 1 | D | 266 | THR | CB-CG2 | 5.49 | 1.70 | 1.52 |
| 1 | E | 307 | PHE | CE1-CZ | 5.49 | 1.47 | 1.37 |
| 1 | F | 129 | THR | CA-CB | -5.49 | 1.39 | 1.53 |
| 1 | J | 253 | GLU | CB-CG | 5.49 | 1.62 | 1.52 |
| 1 | N | 86 | PRO | CG-CD | 5.49 | 1.68 | 1.50 |
| 1 | C | 93 | PRO | CG-CD | 5.49 | 1.68 | 1.50 |
| 1 | D | 307 | PHE | CE2-CZ | -5.49 | 1.26 | 1.37 |
| 1 | K | 442 | LYS | CD-CE | 5.49 | 1.65 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 129 | THR | CB-CG2 | -5.49 | 1.34 | 1.52 |
| 1 | I | 352 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | J | 94 | ASP | CG-OD1 | 5.49 | 1.38 | 1.25 |
| 1 | M | 64 | LYS | CG-CD | 5.49 | 1.71 | 1.52 |
| 1 | C | 317 | GLN | CD-OE1 | 5.49 | 1.36 | 1.24 |
| 1 | K | 220 | VAL | CB-CG1 | -5.49 | 1.41 | 1.52 |
| 1 | K | 402 | TRP | CE3-CZ3 | 5.49 | 1.47 | 1.38 |
| 1 | L | 49 | TYR | CG-CD1 | -5.49 | 1.32 | 1.39 |
| 1 | N | 51 | PRO | C-O | 5.49 | 1.34 | 1.23 |
| 1 | N | 135 | TYR | CE2-CZ | 5.48 | 1.45 | 1.38 |
| 1 | N | 249 | TYR | CD1-CE1 | 5.48 | 1.47 | 1.39 |
| 1 | D | 180 | VAL | CB-CG2 | 5.48 | 1.64 | 1.52 |
| 1 | F | 26 | GLU | CB-CG | -5.48 | 1.41 | 1.52 |
| 1 | H | 63 | PRO | CB-CG | 5.48 | 1.77 | 1.50 |
| 1 | H | 87 | ASP | C-O | 5.48 | 1.33 | 1.23 |
| 1 | N | 95 | THR | CB-OG1 | 5.48 | 1.54 | 1.43 |
| 1 | N | 270 | ASN | CB-CG | 5.48 | 1.63 | 1.51 |
| 1 | C | 73 | PHE | CD1-CE1 | 5.48 | 1.50 | 1.39 |
| 1 | H | 240 | GLU | CD-OE1 | 5.48 | 1.31 | 1.25 |
| 1 | I | 334 | VAL | CA-CB | -5.48 | 1.43 | 1.54 |
| 1 | O | 448 | GLU | CB-CG | 5.48 | 1.62 | 1.52 |
| 1 | J | 462 | PHE | CG-CD1 | -5.48 | 1.30 | 1.38 |
| 1 | F | 218 | SER | C-O | 5.48 | 1.33 | 1.23 |
| 1 | A | 93 | PRO | N-CD | 5.47 | 1.55 | 1.47 |
| 1 | F | 225 | CYS | CB-SG | 5.47 | 1.91 | 1.82 |
| 1 | L | 71 | ARG | C-O | 5.47 | 1.33 | 1.23 |
| 1 | L | 438 | GLU | C-O | 5.47 | 1.33 | 1.23 |
| 1 | J | 151 | TYR | CB-CG | -5.47 | 1.43 | 1.51 |
| 1 | K | 58 | ASN | CG-OD1 | 5.47 | 1.35 | 1.24 |
| 1 | M | 83 | PHE | CE1-CZ | -5.47 | 1.26 | 1.37 |
| 1 | N | 446 | PHE | CA-CB | -5.47 | 1.42 | 1.53 |
| 1 | B | 146 | CYS | CB-SG | -5.47 | 1.72 | 1.81 |
| 1 | D | 27 | TYR | CD2-CE2 | 5.47 | 1.47 | 1.39 |
| 1 | G | 56 | ASN | CG-OD1 | 5.47 | 1.35 | 1.24 |
| 1 | I | 34 | TYR | C-O | 5.47 | 1.33 | 1.23 |
| 1 | J | 187 | PRO | CG-CD | 5.47 | 1.68 | 1.50 |
| 1 | K | 56 | ASN | CB-CG | 5.47 | 1.63 | 1.51 |
| 1 | N | 70 | TYR | C-O | -5.47 | 1.12 | 1.23 |
| 1 | N | 240 | GLU | CD-OE1 | 5.47 | 1.31 | 1.25 |
| 1 | A | 33 | ILE | C-O | 5.47 | 1.33 | 1.23 |
| 1 | B | 165 | ILE | CB-CG2 | 5.47 | 1.69 | 1.52 |
| 1 | C | 144 | ARG | CZ-NH2 | -5.47 | 1.25 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 89 | SER | C-O | 5.46 | 1.33 | 1.23 |
| 1 | D | 160 | GLY | CA-C | 5.46 | 1.60 | 1.51 |
| 1 | O | 346 | ALA | CA-C | -5.46 | 1.38 | 1.52 |
| 1 | D | 314 | GLN | CB-CG | 5.46 | 1.67 | 1.52 |
| 1 | G | 267 | VAL | CB-CG2 | 5.46 | 1.64 | 1.52 |
| 1 | K | 187 | PRO | CG-CD | 5.46 | 1.68 | 1.50 |
| 1 | O | 381 | ILE | C-O | 5.46 | 1.33 | 1.23 |
| 1 | D | 363 | TYR | CE2-CZ | 5.46 | 1.45 | 1.38 |
| 1 | I | 363 | TYR | C-O | 5.46 | 1.33 | 1.23 |
| 1 | L | 52 | ILE | CB-CG2 | 5.46 | 1.69 | 1.52 |
| 1 | L | 315 | ARG | CB-CG | 5.46 | 1.67 | 1.52 |
| 1 | F | 304 | ALA | C-O | -5.46 | 1.12 | 1.23 |
| 1 | H | 402 | TRP | C-O | 5.46 | 1.33 | 1.23 |
| 1 | D | 28 | VAL | CB-CG2 | -5.45 | 1.41 | 1.52 |
| 1 | F | 230 | LYS | C-O | 5.45 | 1.33 | 1.23 |
| 1 | A | 104 | GLY | N-CA | 5.45 | 1.54 | 1.46 |
| 1 | C | 355 | TYR | CZ-OH | 5.45 | 1.47 | 1.37 |
| 1 | I | 217 | LYS | C-O | 5.45 | 1.33 | 1.23 |
| 1 | J | 400 | GLU | CG-CD | 5.45 | 1.60 | 1.51 |
| 1 | N | 106 | GLU | CB-CG | 5.45 | 1.62 | 1.52 |
| 1 | E | 121 | PRO | CA-C | -5.45 | 1.42 | 1.52 |
| 1 | J | 211 | THR | CA-CB | -5.45 | 1.39 | 1.53 |
| 1 | O | 156 | LEU | C-O | 5.45 | 1.33 | 1.23 |
| 1 | A | 27 | TYR | CZ-OH | -5.45 | 1.28 | 1.37 |
| 1 | I | 163 | PRO | CB-CG | 5.45 | 1.77 | 1.50 |
| 1 | F | 104 | GLY | C-O | 5.45 | 1.32 | 1.23 |
| 1 | I | 364 | LEU | CG-CD2 | 5.45 | 1.72 | 1.51 |
| 1 | L | 32 | ASN | C-O | 5.45 | 1.33 | 1.23 |
| 1 | E | 272 | PRO | N-CA | -5.44 | 1.38 | 1.47 |
| 1 | B | 311 | TYR | CD2-CE2 | 5.44 | 1.47 | 1.39 |
| 1 | N | 284 | ALA | CA-CB | -5.44 | 1.41 | 1.52 |
| 1 | N | 312 | TRP | CZ3-CH2 | 5.44 | 1.48 | 1.40 |
| 1 | M | 70 | TYR | CG-CD1 | -5.44 | 1.32 | 1.39 |
| 1 | N | 472 | LEU | CA-CB | 5.44 | 1.66 | 1.53 |
| 1 | N | 335 | ASP | CG-OD2 | 5.44 | 1.37 | 1.25 |
| 1 | F | 241 | PRO | N-CA | 5.44 | 1.56 | 1.47 |
| 1 | G | 291 | TYR | CD1-CE1 | -5.44 | 1.31 | 1.39 |
| 1 | E | 192 | ASN | CB-CG | 5.44 | 1.63 | 1.51 |
| 1 | H | 350 | THR | CB-CG2 | 5.44 | 1.70 | 1.52 |
| 1 | L | 69 | GLN | C-O | -5.44 | 1.13 | 1.23 |
| 1 | O | 375 | ILE | CB-CG2 | -5.43 | 1.36 | 1.52 |
| 1 | G | 400 | GLU | CB-CG | 5.43 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 326 | GLY | C-O | -5.43 | 1.15 | 1.23 |
| 1 | N | 347 | ALA | C-O | 5.43 | 1.33 | 1.23 |
| 1 | C | 146 | CYS | CB-SG | 5.43 | 1.91 | 1.82 |
| 1 | E | 257 | VAL | CA-CB | -5.43 | 1.43 | 1.54 |
| 1 | F | 91 | TYR | CE1-CZ | -5.43 | 1.31 | 1.38 |
| 1 | F | 311 | TYR | CD1-CE1 | 5.43 | 1.47 | 1.39 |
| 1 | A | 45 | VAL | C-O | 5.43 | 1.33 | 1.23 |
| 1 | E | 270 | ASN | N-CA | -5.43 | 1.35 | 1.46 |
| 1 | F | 82 | LYS | CD-CE | 5.43 | 1.64 | 1.51 |
| 1 | H | 145 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | I | 144 | ARG | CG-CD | -5.43 | 1.38 | 1.51 |
| 1 | C | 38 | GLY | N-CA | 5.42 | 1.54 | 1.46 |
| 1 | N | 155 | GLN | CA-CB | -5.42 | 1.42 | 1.53 |
| 1 | N | 469 | LEU | CG-CD2 | 5.42 | 1.72 | 1.51 |
| 1 | I | 346 | ALA | C-O | 5.42 | 1.33 | 1.23 |
| 1 | A | 363 | TYR | CD1-CE1 | 5.42 | 1.47 | 1.39 |
| 1 | E | 69 | GLN | CA-C | 5.42 | 1.67 | 1.52 |
| 1 | G | 54 | LYS | CE-NZ | 5.42 | 1.62 | 1.49 |
| 1 | E | 128 | ASP | CB-CG | 5.42 | 1.63 | 1.51 |
| 1 | G | 347 | ALA | CA-CB | 5.42 | 1.63 | 1.52 |
| 1 | I | 155 | GLN | CB-CG | -5.42 | 1.38 | 1.52 |
| 1 | M | 346 | ALA | CA-CB | 5.42 | 1.63 | 1.52 |
| 1 | A | 390 | TYR | CZ-OH | 5.42 | 1.47 | 1.37 |
| 1 | D | 64 | LYS | CE-NZ | -5.42 | 1.35 | 1.49 |
| 1 | I | 242 | TYR | N-CA | -5.42 | 1.35 | 1.46 |
| 1 | L | 21 | VAL | CB-CG2 | 5.42 | 1.64 | 1.52 |
| 1 | O | 22 | VAL | CB-CG2 | 5.42 | 1.64 | 1.52 |
| 1 | O | 70 | TYR | CD1-CE1 | 5.42 | 1.47 | 1.39 |
| 1 | O | 460 | ASP | CG-OD1 | 5.42 | 1.37 | 1.25 |
| 1 | B | 271 | VAL | N-CA | -5.42 | 1.35 | 1.46 |
| 1 | E | 324 | CYS | CB-SG | 5.42 | 1.91 | 1.82 |
| 1 | F | 454 | LYS | C-O | 5.42 | 1.33 | 1.23 |
| 1 | G | 355 | TYR | CG-CD1 | -5.42 | 1.32 | 1.39 |
| 1 | K | 365 | ARG | CA-CB | 5.42 | 1.65 | 1.53 |
| 1 | A | 348 | ILE | CA-CB | -5.41 | 1.42 | 1.54 |
| 1 | E | 40 | SER | CA-CB | 5.41 | 1.61 | 1.52 |
| 1 | I | 41 | ARG | CD-NE | 5.41 | 1.55 | 1.46 |
| 1 | J | 370 | TYR | CE2-CZ | -5.41 | 1.31 | 1.38 |
| 1 | I | 155 | GLN | CG-CD | 5.41 | 1.63 | 1.51 |
| 1 | K | 226 | THR | C-O | 5.41 | 1.33 | 1.23 |
| 1 | B | 375 | ILE | CB-CG2 | -5.41 | 1.36 | 1.52 |
| 1 | F | 267 | VAL | N-CA | 5.41 | 1.57 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 270 | ASN | CG-ND2 | 5.41 | 1.46 | 1.32 |
| 1 | O | 365 | ARG | CA-CB | -5.41 | 1.42 | 1.53 |
| 1 | B | 106 | GLU | CG-CD | 5.41 | 1.60 | 1.51 |
| 1 | G | 250 | LEU | C-O | 5.41 | 1.33 | 1.23 |
| 1 | D | 267 | VAL | CB-CG1 | 5.41 | 1.64 | 1.52 |
| 1 | K | 151 | TYR | CE1-CZ | -5.41 | 1.31 | 1.38 |
| 1 | G | 336 | THR | CB-CG2 | -5.40 | 1.34 | 1.52 |
| 1 | A | 210 | PHE | CG-CD1 | -5.40 | 1.30 | 1.38 |
| 1 | B | 361 | LYS | C-O | 5.40 | 1.33 | 1.23 |
| 1 | C | 472 | LEU | N-CA | 5.40 | 1.57 | 1.46 |
| 1 | E | 139 | ALA | CA-CB | 5.40 | 1.63 | 1.52 |
| 1 | E | 331 | VAL | CB-CG2 | 5.40 | 1.64 | 1.52 |
| 1 | M | 64 | LYS | N-CA | -5.40 | 1.35 | 1.46 |
| 1 | N | 236 | LYS | CG-CD | 5.40 | 1.70 | 1.52 |
| 1 | O | 390 | TYR | CG-CD2 | 5.40 | 1.46 | 1.39 |
| 1 | G | 316 | ALA | N-CA | 5.40 | 1.57 | 1.46 |
| 1 | L | 178 | VAL | CB-CG1 | 5.40 | 1.64 | 1.52 |
| 1 | C | 63 | PRO | C-O | 5.40 | 1.34 | 1.23 |
| 1 | I | 150 | ASP | C-O | 5.40 | 1.33 | 1.23 |
| 1 | C | 167 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | I | 90 | PHE | C-O | 5.40 | 1.33 | 1.23 |
| 1 | J | 298 | SER | N-CA | -5.40 | 1.35 | 1.46 |
| 1 | O | 447 | TRP | CG-CD1 | 5.40 | 1.44 | 1.36 |
| 1 | A | 244 | ASP | C-O | 5.40 | 1.33 | 1.23 |
| 1 | A | 447 | TRP | CG-CD1 | -5.39 | 1.29 | 1.36 |
| 1 | D | 444 | TYR | C-O | 5.39 | 1.33 | 1.23 |
| 1 | J | 360 | PHE | CD2-CE2 | 5.39 | 1.50 | 1.39 |
| 1 | K | 50 | PHE | CE1-CZ | -5.39 | 1.27 | 1.37 |
| 1 | K | 204 | GLY | N-CA | -5.39 | 1.38 | 1.46 |
| 1 | O | 112 | PRO | CA-C | 5.39 | 1.63 | 1.52 |
| 1 | F | 453 | GLU | CG-CD | 5.39 | 1.60 | 1.51 |
| 1 | H | 256 | PHE | CG-CD2 | -5.39 | 1.30 | 1.38 |
| 1 | M | 291 | TYR | CD2-CE2 | -5.39 | 1.31 | 1.39 |
| 1 | F | 293 | PRO | CA-CB | -5.39 | 1.42 | 1.53 |
| 1 | G | 330 | PHE | CE1-CZ | 5.39 | 1.47 | 1.37 |
| 1 | O | 356 | LYS | CB-CG | 5.39 | 1.67 | 1.52 |
| 1 | D | 135 | TYR | CG-CD1 | -5.39 | 1.32 | 1.39 |
| 1 | D | 158 | LEU | C-O | 5.39 | 1.33 | 1.23 |
| 1 | G | 214 | GLN | CD-OE1 | 5.39 | 1.35 | 1.24 |
| 1 | M | 216 | ASN | C-O | -5.39 | 1.13 | 1.23 |
| 1 | O | 290 | ASN | CG-ND2 | 5.39 | 1.46 | 1.32 |
| 1 | E | 448 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 108 | GLY | CA-C | 5.38 | 1.60 | 1.51 |
| 1 | N | 140 | GLY | N-CA | 5.38 | 1.54 | 1.46 |
| 1 | N | 276 | TYR | C-O | 5.38 | 1.33 | 1.23 |
| 1 | B | 55 | PRO | C-O | 5.38 | 1.34 | 1.23 |
| 1 | B | 380 | LYS | CB-CG | -5.38 | 1.38 | 1.52 |
| 1 | F | 307 | PHE | CD1-CE1 | 5.38 | 1.50 | 1.39 |
| 1 | L | 460 | ASP | CA-CB | 5.38 | 1.65 | 1.53 |
| 1 | M | 205 | PHE | CG-CD1 | 5.38 | 1.46 | 1.38 |
| 1 | N | 106 | GLU | CD-OE1 | 5.38 | 1.31 | 1.25 |
| 1 | A | 118 | SER | CB-OG | -5.38 | 1.35 | 1.42 |
| 1 | B | 248 | PHE | CE2-CZ | 5.38 | 1.47 | 1.37 |
| 1 | F | 161 | CYS | CB-SG | 5.38 | 1.91 | 1.82 |
| 1 | G | 472 | LEU | N-CA | 5.38 | 1.57 | 1.46 |
| 1 | K | 181 | GLN | CG-CD | 5.38 | 1.63 | 1.51 |
| 1 | D | 68 | LEU | C-O | -5.38 | 1.13 | 1.23 |
| 1 | F | 294 | THR | C-N | -5.38 | 1.24 | 1.34 |
| 1 | K | 272 | PRO | CB-CG | 5.38 | 1.76 | 1.50 |
| 1 | N | 89 | SER | CA-C | 5.38 | 1.67 | 1.52 |
| 1 | D | 240 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | E | 39 | THR | N-CA | 5.38 | 1.57 | 1.46 |
| 1 | J | 85 | PHE | CD2-CE2 | 5.38 | 1.50 | 1.39 |
| 1 | B | 276 | TYR | CD1-CE1 | -5.37 | 1.31 | 1.39 |
| 1 | I | 256 | PHE | CG-CD2 | 5.37 | 1.46 | 1.38 |
| 1 | J | 159 | ILE | CA-CB | -5.37 | 1.42 | 1.54 |
| 1 | L | 248 | PHE | CE1-CZ | -5.37 | 1.27 | 1.37 |
| 1 | M | 201 | VAL | CA-CB | -5.37 | 1.43 | 1.54 |
| 1 | L | 376 | PHE | CD1-CE1 | -5.37 | 1.28 | 1.39 |
| 1 | O | 53 | LYS | CD-CE | 5.37 | 1.64 | 1.51 |
| 1 | B | 368 | GLU | CB-CG | -5.37 | 1.42 | 1.52 |
| 1 | D | 210 | PHE | CG-CD1 | 5.37 | 1.46 | 1.38 |
| 1 | B | 105 | VAL | CB-CG1 | -5.37 | 1.41 | 1.52 |
| 1 | G | 96 | GLN | C-O | 5.37 | 1.33 | 1.23 |
| 1 | A | 166 | GLY | N-CA | 5.37 | 1.54 | 1.46 |
| 1 | F | 147 | ILE | CA-CB | 5.37 | 1.67 | 1.54 |
| 1 | F | 169 | TRP | CZ3-CH2 | -5.37 | 1.31 | 1.40 |
| 1 | K | 467 | LYS | CG-CD | 5.37 | 1.70 | 1.52 |
| 1 | L | 230 | LYS | CG-CD | -5.37 | 1.34 | 1.52 |
| 1 | O | 161 | CYS | C-O | 5.37 | 1.33 | 1.23 |
| 1 | L | 26 | GLU | C-O | -5.36 | 1.13 | 1.23 |
| 1 | M | 457 | ALA | C-O | -5.36 | 1.13 | 1.23 |
| 1 | O | 177 | GLN | C-O | 5.36 | 1.33 | 1.23 |
| 1 | J | 55 | PRO | N-CA | 5.36 | 1.56 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | M | 22 | VAL | CB-CG2 | -5.36 | 1.41 | 1.52 |
| 1 | H | 283 | THR | CB-CG2 | 5.36 | 1.70 | 1.52 |
| 1 | I | 231 | TYR | CB-CG | -5.36 | 1.43 | 1.51 |
| 1 | K | 278 | LYS | CD-CE | 5.36 | 1.64 | 1.51 |
| 1 | B | 169 | TRP | CB-CG | -5.36 | 1.40 | 1.50 |
| 1 | O | 95 | THR | CB-CG2 | 5.36 | 1.70 | 1.52 |
| 1 | J | 56 | ASN | CB-CG | 5.36 | 1.63 | 1.51 |
| 1 | J | 446 | PHE | CD1-CE1 | 5.36 | 1.50 | 1.39 |
| 1 | L | 135 | TYR | CG-CD2 | 5.36 | 1.46 | 1.39 |
| 1 | A | 284 | ALA | CA-CB | 5.36 | 1.63 | 1.52 |
| 1 | A | 390 | TYR | CE1-CZ | 5.36 | 1.45 | 1.38 |
| 1 | D | 312 | TRP | NE1-CE2 | -5.36 | 1.30 | 1.37 |
| 1 | H | 267 | VAL | CB-CG2 | 5.35 | 1.64 | 1.52 |
| 1 | E | 282 | SER | CA-CB | 5.35 | 1.60 | 1.52 |
| 1 | F | 207 | ALA | N-CA | -5.35 | 1.35 | 1.46 |
| 1 | F | 374 | PHE | CE2-CZ | 5.35 | 1.47 | 1.37 |
| 1 | F | 376 | PHE | CE1-CZ | 5.35 | 1.47 | 1.37 |
| 1 | H | 455 | PHE | CB-CG | -5.35 | 1.42 | 1.51 |
| 1 | O | 96 | GLN | CD-OE1 | 5.35 | 1.35 | 1.24 |
| 1 | L | 199 | ASP | CG-OD2 | 5.35 | 1.37 | 1.25 |
| 1 | D | 109 | ARG | NE-CZ | 5.35 | 1.40 | 1.33 |
| 1 | E | 112 | PRO | N-CD | -5.35 | 1.40 | 1.47 |
| 1 | J | 387 | VAL | CB-CG2 | -5.35 | 1.41 | 1.52 |
| 1 | I | 187 | PRO | N-CA | 5.35 | 1.56 | 1.47 |
| 1 | M | 49 | TYR | CE2-CZ | -5.35 | 1.31 | 1.38 |
| 1 | N | 72 | VAL | CB-CG1 | 5.35 | 1.64 | 1.52 |
| 1 | D | 179 | ALA | CA-CB | 5.34 | 1.63 | 1.52 |
| 1 | G | 159 | ILE | CB-CG2 | -5.34 | 1.36 | 1.52 |
| 1 | H | 442 | LYS | CE-NZ | 5.34 | 1.62 | 1.49 |
| 1 | O | 21 | VAL | CB-CG2 | 5.34 | 1.64 | 1.52 |
| 1 | D | 300 | VAL | CA-CB | -5.34 | 1.43 | 1.54 |
| 1 | H | 90 | PHE | CB-CG | 5.34 | 1.60 | 1.51 |
| 1 | H | 90 | PHE | CE1-CZ | 5.34 | 1.47 | 1.37 |
| 1 | K | 178 | VAL | C-O | 5.34 | 1.33 | 1.23 |
| 1 | L | 317 | GLN | CB-CG | 5.34 | 1.67 | 1.52 |
| 1 | N | 132 | ALA | CA-CB | 5.34 | 1.63 | 1.52 |
| 1 | A | 20 | ALA | N-CA | 5.34 | 1.57 | 1.46 |
| 1 | C | 77 | LEU | CG-CD1 | 5.34 | 1.71 | 1.51 |
| 1 | K | 163 | PRO | CG-CD | -5.34 | 1.33 | 1.50 |
| 1 | O | 317 | GLN | CD-OE1 | 5.34 | 1.35 | 1.24 |
| 1 | B | 383 | LEU | CG-CD1 | 5.34 | 1.71 | 1.51 |
| 1 | D | 135 | TYR | CD2-CE2 | 5.34 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 393 | SER | C-O | 5.34 | 1.33 | 1.23 |
| 1 | B | 123 | LEU | C-O | -5.34 | 1.13 | 1.23 |
| 1 | D | 287 | ALA | CA-CB | 5.34 | 1.63 | 1.52 |
| 1 | F | 50 | PHE | CA-CB | -5.34 | 1.42 | 1.53 |
| 1 | J | 181 | GLN | C-O | 5.34 | 1.33 | 1.23 |
| 1 | J | 330 | PHE | CG-CD2 | 5.34 | 1.46 | 1.38 |
| 1 | L | 302 | SER | N-CA | -5.34 | 1.35 | 1.46 |
| 1 | N | 49 | TYR | CD2-CE2 | 5.34 | 1.47 | 1.39 |
| 1 | D | 144 | ARG | CZ-NH1 | -5.34 | 1.26 | 1.33 |
| 1 | D | 293 | PRO | CA-CB | -5.34 | 1.42 | 1.53 |
| 1 | G | 231 | TYR | CE1-CZ | -5.34 | 1.31 | 1.38 |
| 1 | B | 24 | THR | C-O | 5.33 | 1.33 | 1.23 |
| 1 | C | 60 | ILE | CG1-CD1 | 5.33 | 1.87 | 1.50 |
| 1 | E | 145 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 1 | H | 341 | ASN | N-CA | 5.33 | 1.57 | 1.46 |
| 1 | K | 368 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 1 | O | 85 | PHE | CG-CD2 | 5.33 | 1.46 | 1.38 |
| 1 | B | 171 | LYS | CD-CE | 5.33 | 1.64 | 1.51 |
| 1 | C | 369 | GLU | CD-OE1 | 5.33 | 1.31 | 1.25 |
| 1 | I | 100 | TRP | CB-CG | -5.33 | 1.40 | 1.50 |
| 1 | F | 66 | SER | C-O | 5.33 | 1.33 | 1.23 |
| 1 | J | 147 | ILE | CA-CB | -5.33 | 1.42 | 1.54 |
| 1 | C | 152 | LYS | CE-NZ | 5.33 | 1.62 | 1.49 |
| 1 | C | 215 | ALA | C-O | 5.33 | 1.33 | 1.23 |
| 1 | C | 469 | LEU | CG-CD2 | 5.33 | 1.71 | 1.51 |
| 1 | D | 263 | ARG | CZ-NH1 | 5.33 | 1.40 | 1.33 |
| 1 | B | 278 | LYS | CE-NZ | 5.33 | 1.62 | 1.49 |
| 1 | D | 60 | ILE | CA-CB | -5.33 | 1.42 | 1.54 |
| 1 | M | 91 | TYR | CG-CD2 | 5.33 | 1.46 | 1.39 |
| 1 | A | 387 | VAL | C-O | 5.32 | 1.33 | 1.23 |
| 1 | D | 108 | GLY | C-O | 5.32 | 1.32 | 1.23 |
| 1 | E | 252 | ARG | CZ-NH2 | -5.32 | 1.26 | 1.33 |
| 1 | G | 127 | ASP | C-O | 5.32 | 1.33 | 1.23 |
| 1 | G | 162 | LYS | CD-CE | 5.32 | 1.64 | 1.51 |
| 1 | I | 374 | PHE | CG-CD2 | 5.32 | 1.46 | 1.38 |
| 1 | K | 276 | TYR | CE2-CZ | 5.32 | 1.45 | 1.38 |
| 1 | N | 55 | PRO | CA-C | 5.32 | 1.63 | 1.52 |
| 1 | K | 205 | PHE | CE2-CZ | 5.32 | 1.47 | 1.37 |
| 1 | F | 230 | LYS | CB-CG | 5.32 | 1.67 | 1.52 |
| 1 | G | 22 | VAL | C-O | 5.32 | 1.33 | 1.23 |
| 1 | J | 215 | ALA | N-CA | 5.32 | 1.56 | 1.46 |
| 1 | J | 468 | PHE | CD1-CE1 | -5.32 | 1.28 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 360 | PHE | CB-CG | -5.32 | 1.42 | 1.51 |
| 1 | O | 270 | ASN | CB-CG | 5.32 | 1.63 | 1.51 |
| 1 | C | 248 | PHE | CD1-CE1 | 5.32 | 1.49 | 1.39 |
| 1 | F | 199 | ASP | CB-CG | -5.32 | 1.40 | 1.51 |
| 1 | I | 469 | LEU | CG-CD2 | 5.32 | 1.71 | 1.51 |
| 1 | L | 251 | ARG | C-O | 5.32 | 1.33 | 1.23 |
| 1 | H | 27 | TYR | CG-CD2 | 5.32 | 1.46 | 1.39 |
| 1 | J | 338 | ARG | CZ-NH2 | 5.32 | 1.40 | 1.33 |
| 1 | B | 348 | ILE | CA-CB | -5.31 | 1.42 | 1.54 |
| 1 | C | 361 | LYS | CE-NZ | 5.31 | 1.62 | 1.49 |
| 1 | E | 144 | ARG | CZ-NH1 | 5.31 | 1.40 | 1.33 |
| 1 | N | 83 | PHE | C-O | 5.31 | 1.33 | 1.23 |
| 1 | B | 159 | ILE | CB-CG2 | -5.31 | 1.36 | 1.52 |
| 1 | E | 86 | PRO | N-CA | 5.31 | 1.56 | 1.47 |
| 1 | F | 206 | GLY | N-CA | 5.31 | 1.54 | 1.46 |
| 1 | H | 312 | TRP | CE3-CZ3 | -5.31 | 1.29 | 1.38 |
| 1 | I | 261 | PHE | CG-CD2 | -5.31 | 1.30 | 1.38 |
| 1 | J | 241 | PRO | C-O | 5.31 | 1.33 | 1.23 |
| 1 | O | 112 | PRO | N-CD | -5.31 | 1.40 | 1.47 |
| 1 | K | 76 | HIS | C-O | -5.31 | 1.13 | 1.23 |
| 1 | A | 70 | TYR | CD1-CE1 | 5.31 | 1.47 | 1.39 |
| 1 | F | 355 | TYR | CD1-CE1 | -5.31 | 1.31 | 1.39 |
| 1 | H | 468 | PHE | CG-CD2 | -5.31 | 1.30 | 1.38 |
| 1 | K | 455 | PHE | CA-CB | -5.31 | 1.42 | 1.53 |
| 1 | L | 311 | TYR | CG-CD1 | 5.31 | 1.46 | 1.39 |
| 1 | E | 398 | ILE | C-O | 5.30 | 1.33 | 1.23 |
| 1 | E | 452 | LYS | CD-CE | 5.30 | 1.64 | 1.51 |
| 1 | F | 46 | GLY | C-O | 5.30 | 1.32 | 1.23 |
| 1 | K | 173 | SER | C-O | 5.30 | 1.33 | 1.23 |
| 1 | B | 155 | GLN | CB-CG | -5.30 | 1.38 | 1.52 |
| 1 | D | 187 | PRO | N-CA | 5.30 | 1.56 | 1.47 |
| 1 | E | 201 | VAL | CB-CG2 | -5.30 | 1.41 | 1.52 |
| 1 | G | 376 | PHE | CG-CD1 | 5.30 | 1.46 | 1.38 |
| 1 | K | 221 | PRO | CG-CD | -5.30 | 1.33 | 1.50 |
| 1 | C | 177 | GLN | CB-CG | 5.30 | 1.66 | 1.52 |
| 1 | D | 390 | TYR | CE1-CZ | 5.30 | 1.45 | 1.38 |
| 1 | C | 309 | LYS | CD-CE | 5.30 | 1.64 | 1.51 |
| 1 | H | 148 | SER | C-O | 5.30 | 1.33 | 1.23 |
| 1 | N | 465 | GLY | N-CA | 5.30 | 1.53 | 1.46 |
| 1 | C | 466 | ARG | CZ-NH1 | -5.29 | 1.26 | 1.33 |
| 1 | L | 271 | VAL | C-O | -5.29 | 1.13 | 1.23 |
| 1 | M | 442 | LYS | CE-NZ | 5.29 | 1.62 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 363 | TYR | CE2-CZ | 5.29 | 1.45 | 1.38 |
| 1 | H | 365 | ARG | C-O | 5.29 | 1.33 | 1.23 |
| 1 | L | 45 | VAL | C-O | 5.29 | 1.33 | 1.23 |
| 1 | O | 60 | ILE | CB-CG2 | -5.29 | 1.36 | 1.52 |
| 1 | H | 214 | GLN | CD-OE1 | 5.29 | 1.35 | 1.24 |
| 1 | N | 99 | VAL | CB-CG2 | -5.29 | 1.41 | 1.52 |
| 1 | A | 138 | ASN | CB-CG | 5.29 | 1.63 | 1.51 |
| 1 | H | 313 | LEU | C-O | 5.29 | 1.33 | 1.23 |
| 1 | M | 462 | PHE | CD1-CE1 | -5.29 | 1.28 | 1.39 |
| 1 | J | 181 | GLN | CD-OE1 | 5.29 | 1.35 | 1.24 |
| 1 | B | 181 | GLN | CD-NE2 | 5.29 | 1.46 | 1.32 |
| 1 | E | 298 | SER | N-CA | -5.29 | 1.35 | 1.46 |
| 1 | G | 374 | PHE | CD2-CE2 | -5.29 | 1.28 | 1.39 |
| 1 | I | 23 | SER | CB-OG | -5.29 | 1.35 | 1.42 |
| 1 | L | 174 | PRO | CG-CD | 5.29 | 1.68 | 1.50 |
| 1 | C | 261 | PHE | CG-CD2 | -5.29 | 1.30 | 1.38 |
| 1 | D | 469 | LEU | CA-C | 5.29 | 1.66 | 1.52 |
| 1 | E | 150 | ASP | CG-OD2 | 5.29 | 1.37 | 1.25 |
| 1 | H | 224 | ILE | C-O | 5.29 | 1.33 | 1.23 |
| 1 | I | 247 | PHE | CE2-CZ | -5.29 | 1.27 | 1.37 |
| 1 | I | 329 | LEU | CG-CD2 | 5.29 | 1.71 | 1.51 |
| 1 | I | 359 | ASN | CG-OD1 | 5.29 | 1.35 | 1.24 |
| 1 | D | 249 | TYR | CZ-OH | 5.28 | 1.46 | 1.37 |
| 1 | E | 243 | GLY | CA-C | 5.28 | 1.60 | 1.51 |
| 1 | H | 23 | SER | CB-OG | 5.28 | 1.49 | 1.42 |
| 1 | L | 455 | PHE | CD2-CE2 | 5.28 | 1.49 | 1.39 |
| 1 | M | 147 | ILE | CG1-CD1 | 5.28 | 1.86 | 1.50 |
| 1 | N | 261 | PHE | N-CA | -5.28 | 1.35 | 1.46 |
| 1 | I | 153 | GLN | N-CA | 5.28 | 1.56 | 1.46 |
| 1 | B | 28 | VAL | CB-CG2 | -5.28 | 1.41 | 1.52 |
| 1 | B | 125 | LYS | CB-CG | -5.28 | 1.38 | 1.52 |
| 1 | C | 309 | LYS | CB-CG | 5.28 | 1.66 | 1.52 |
| 1 | G | 49 | TYR | CE2-CZ | 5.28 | 1.45 | 1.38 |
| 1 | O | 181 | GLN | CG-CD | 5.28 | 1.63 | 1.51 |
| 1 | B | 253 | GLU | CB-CG | -5.28 | 1.42 | 1.52 |
| 1 | C | 455 | PHE | CB-CG | -5.28 | 1.42 | 1.51 |
| 1 | E | 43 | LEU | C-O | -5.28 | 1.13 | 1.23 |
| 1 | K | 328 | GLN | C-O | 5.28 | 1.33 | 1.23 |
| 1 | N | 464 | LEU | CG-CD1 | 5.28 | 1.71 | 1.51 |
| 1 | O | 123 | LEU | CG-CD1 | 5.28 | 1.71 | 1.51 |
| 1 | I | 260 | LEU | CG-CD2 | -5.28 | 1.32 | 1.51 |
| 1 | H | 248 | PHE | CG-CD2 | -5.28 | 1.30 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 308 | ASN | CB-CG | 5.28 | 1.63 | 1.51 |
| 1 | F | 171 | LYS | CB-CG | 5.27 | 1.66 | 1.52 |
| 1 | H | 157 | CYS | C-O | 5.27 | 1.33 | 1.23 |
| 1 | O | 225 | CYS | CB-SG | 5.27 | 1.91 | 1.82 |
| 1 | A | 374 | PHE | CE2-CZ | 5.27 | 1.47 | 1.37 |
| 1 | B | 197 | ASP | CB-CG | 5.27 | 1.62 | 1.51 |
| 1 | C | 370 | TYR | CB-CG | -5.27 | 1.43 | 1.51 |
| 1 | D | 292 | PHE | C-O | -5.27 | 1.13 | 1.23 |
| 1 | G | 355 | TYR | CE1-CZ | -5.27 | 1.31 | 1.38 |
| 1 | L | 50 | PHE | CD1-CE1 | -5.27 | 1.28 | 1.39 |
| 1 | G | 34 | TYR | CG-CD1 | 5.27 | 1.46 | 1.39 |
| 1 | L | 135 | TYR | CZ-OH | 5.27 | 1.46 | 1.37 |
| 1 | M | 205 | PHE | CE2-CZ | 5.27 | 1.47 | 1.37 |
| 1 | D | 70 | TYR | CE2-CZ | -5.27 | 1.31 | 1.38 |
| 1 | L | 130 | GLU | CG-CD | 5.27 | 1.59 | 1.51 |
| 1 | I | 358 | THR | CB-OG1 | 5.27 | 1.53 | 1.43 |
| 1 | M | 253 | GLU | C-O | -5.27 | 1.13 | 1.23 |
| 1 | C | 343 | SER | CB-OG | 5.27 | 1.49 | 1.42 |
| 1 | L | 269 | GLU | CB-CG | 5.27 | 1.62 | 1.52 |
| 1 | E | 270 | ASN | CA-C | -5.26 | 1.39 | 1.52 |
| 1 | G | 470 | LEU | C-O | 5.26 | 1.33 | 1.23 |
| 1 | H | 208 | MET | N-CA | -5.26 | 1.35 | 1.46 |
| 1 | N | 256 | PHE | CD2-CE2 | -5.26 | 1.28 | 1.39 |
| 1 | G | 182 | PRO | N-CA | 5.26 | 1.56 | 1.47 |
| 1 | K | 255 | MET | N-CA | 5.26 | 1.56 | 1.46 |
| 1 | M | 333 | VAL | C-O | 5.26 | 1.33 | 1.23 |
| 1 | B | 370 | TYR | CZ-OH | 5.26 | 1.46 | 1.37 |
| 1 | F | 20 | ALA | CA-CB | 5.26 | 1.63 | 1.52 |
| 1 | L | 50 | PHE | CD2-CE2 | -5.26 | 1.28 | 1.39 |
| 1 | L | 330 | PHE | CG-CD2 | 5.26 | 1.46 | 1.38 |
| 1 | N | 139 | ALA | C-N | 5.26 | 1.42 | 1.33 |
| 1 | N | 338 | ARG | CZ-NH1 | 5.26 | 1.39 | 1.33 |
| 1 | N | 439 | ASP | CB-CG | 5.26 | 1.62 | 1.51 |
| 1 | N | 470 | LEU | C-O | -5.26 | 1.13 | 1.23 |
| 1 | C | 298 | SER | CA-CB | -5.26 | 1.45 | 1.52 |
| 1 | H | 227 | SER | CA-CB | 5.26 | 1.60 | 1.52 |
| 1 | J | 307 | PHE | CG-CD1 | -5.26 | 1.30 | 1.38 |
| 1 | J | 380 | LYS | CG-CD | 5.26 | 1.70 | 1.52 |
| 1 | K | 361 | LYS | CG-CD | 5.26 | 1.70 | 1.52 |
| 1 | M | 344 | LEU | C-O | 5.26 | 1.33 | 1.23 |
| 1 | N | 128 | ASP | CG-OD2 | 5.26 | 1.37 | 1.25 |
| 1 | F | 346 | ALA | CA-CB | 5.26 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 393 | SER | C-O | 5.26 | 1.33 | 1.23 |
| 1 | K | 463 | PRO | CA-CB | -5.26 | 1.43 | 1.53 |
| 1 | G | 135 | TYR | C-O | -5.26 | 1.13 | 1.23 |
| 1 | H | 144 | ARG | NE-CZ | -5.26 | 1.26 | 1.33 |
| 1 | L | 439 | ASP | C-O | 5.26 | 1.33 | 1.23 |
| 1 | K | 222 | LEU | CG-CD1 | -5.25 | 1.32 | 1.51 |
| 1 | A | 91 | TYR | C-O | 5.25 | 1.33 | 1.23 |
| 1 | B | 27 | TYR | CZ-OH | 5.25 | 1.46 | 1.37 |
| 1 | G | 178 | VAL | CA-C | 5.25 | 1.66 | 1.52 |
| 1 | J | 362 | GLU | C-O | 5.25 | 1.33 | 1.23 |
| 1 | K | 263 | ARG | CZ-NH2 | 5.25 | 1.39 | 1.33 |
| 1 | D | 80 | PRO | N-CD | 5.25 | 1.55 | 1.47 |
| 1 | E | 368 | GLU | CA-CB | -5.25 | 1.42 | 1.53 |
| 1 | H | 140 | GLY | CA-C | 5.25 | 1.60 | 1.51 |
| 1 | J | 343 | SER | CB-OG | 5.25 | 1.49 | 1.42 |
| 1 | K | 217 | LYS | N-CA | -5.25 | 1.35 | 1.46 |
| 1 | A | 65 | VAL | CB-CG1 | 5.25 | 1.63 | 1.52 |
| 1 | C | 82 | LYS | CD-CE | 5.25 | 1.64 | 1.51 |
| 1 | E | 470 | LEU | CG-CD1 | 5.25 | 1.71 | 1.51 |
| 1 | F | 455 | PHE | CE1-CZ | 5.25 | 1.47 | 1.37 |
| 1 | H | 385 | ALA | CA-CB | 5.25 | 1.63 | 1.52 |
| 1 | I | 64 | LYS | C-O | 5.25 | 1.33 | 1.23 |
| 1 | L | 138 | ASN | CB-CG | 5.25 | 1.63 | 1.51 |
| 1 | A | 298 | SER | CA-CB | -5.25 | 1.45 | 1.52 |
| 1 | D | 464 | LEU | CG-CD2 | -5.25 | 1.32 | 1.51 |
| 1 | G | 110 | GLY | C-O | -5.25 | 1.15 | 1.23 |
| 1 | J | 102 | CYS | CB-SG | 5.25 | 1.91 | 1.82 |
| 1 | J | 169 | TRP | CD2-CE2 | 5.25 | 1.47 | 1.41 |
| 1 | N | 356 | LYS | C-O | -5.25 | 1.13 | 1.23 |
| 1 | B | 219 | GLU | CB-CG | -5.25 | 1.42 | 1.52 |
| 1 | B | 230 | LYS | CB-CG | 5.25 | 1.66 | 1.52 |
| 1 | G | 22 | VAL | CB-CG2 | 5.24 | 1.63 | 1.52 |
| 1 | I | 289 | SER | CB-OG | 5.24 | 1.49 | 1.42 |
| 1 | K | 217 | LYS | CD-CE | 5.24 | 1.64 | 1.51 |
| 1 | L | 298 | SER | CA-CB | -5.24 | 1.45 | 1.52 |
| 1 | O | 453 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | F | 265 | GLY | C-O | 5.24 | 1.32 | 1.23 |
| 1 | G | 34 | TYR | CB-CG | 5.24 | 1.59 | 1.51 |
| 1 | O | 462 | PHE | CB-CG | -5.24 | 1.42 | 1.51 |
| 1 | A | 127 | ASP | CG-OD2 | 5.24 | 1.37 | 1.25 |
| 1 | G | 381 | ILE | C-O | 5.24 | 1.33 | 1.23 |
| 1 | M | 73 | PHE | CD1-CE1 | -5.24 | 1.28 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | M | 362 | GLU | C-O | 5.24 | 1.33 | 1.23 |
| 1 | H | 99 | VAL | CB-CG1 | -5.24 | 1.41 | 1.52 |
| 1 | B | 443 | LYS | CD-CE | 5.24 | 1.64 | 1.51 |
| 1 | C | 97 | ARG | CZ-NH1 | 5.24 | 1.39 | 1.33 |
| 1 | F | 177 | GLN | C-O | 5.24 | 1.33 | 1.23 |
| 1 | H | 35 | TYR | CE1-CZ | -5.24 | 1.31 | 1.38 |
| 1 | M | 376 | PHE | CG-CD1 | 5.24 | 1.46 | 1.38 |
| 1 | N | 181 | GLN | N-CA | -5.24 | 1.35 | 1.46 |
| 1 | N | 471 | GLN | CD-OE1 | 5.24 | 1.35 | 1.24 |
| 1 | B | 144 | ARG | CD-NE | -5.23 | 1.37 | 1.46 |
| 1 | F | 22 | VAL | CB-CG2 | -5.23 | 1.41 | 1.52 |
| 1 | F | 73 | PHE | CD1-CE1 | 5.23 | 1.49 | 1.39 |
| 1 | G | 345 | CYS | C-O | -5.23 | 1.13 | 1.23 |
| 1 | I | 53 | LYS | C-O | 5.23 | 1.33 | 1.23 |
| 1 | I | 448 | GLU | CD-OE1 | 5.23 | 1.31 | 1.25 |
| 1 | M | 75 | ILE | C-O | 5.23 | 1.33 | 1.23 |
| 1 | N | 27 | TYR | CB-CG | -5.23 | 1.43 | 1.51 |
| 1 | A | 282 | SER | CB-OG | 5.23 | 1.49 | 1.42 |
| 1 | D | 367 | GLY | CA-C | 5.23 | 1.60 | 1.51 |
| 1 | G | 190 | LEU | CG-CD1 | 5.23 | 1.71 | 1.51 |
| 1 | K | 75 | ILE | CB-CG2 | -5.23 | 1.36 | 1.52 |
| 1 | L | 322 | GLY | N-CA | -5.23 | 1.38 | 1.46 |
| 1 | D | 30 | ARG | N-CA | -5.23 | 1.35 | 1.46 |
| 1 | F | 188 | LEU | C-O | -5.23 | 1.13 | 1.23 |
| 1 | G | 245 | SER | CB-OG | 5.23 | 1.49 | 1.42 |
| 1 | K | 459 | LEU | CG-CD2 | -5.23 | 1.32 | 1.51 |
| 1 | A | 356 | LYS | CA-C | -5.23 | 1.39 | 1.52 |
| 1 | H | 396 | SER | CB-OG | 5.23 | 1.49 | 1.42 |
| 1 | D | 35 | TYR | CG-CD1 | -5.22 | 1.32 | 1.39 |
| 1 | G | 336 | THR | CB-OG1 | 5.22 | 1.53 | 1.43 |
| 1 | K | 249 | TYR | CE2-CZ | -5.22 | 1.31 | 1.38 |
| 1 | K | 255 | MET | CG-SD | -5.22 | 1.67 | 1.81 |
| 1 | M | 271 | VAL | CB-CG1 | 5.22 | 1.63 | 1.52 |
| 1 | F | 291 | TYR | CZ-OH | 5.22 | 1.46 | 1.37 |
| 1 | K | 444 | TYR | CG-CD1 | -5.22 | 1.32 | 1.39 |
| 1 | N | 278 | LYS | CB-CG | 5.22 | 1.66 | 1.52 |
| 1 | B | 140 | GLY | N-CA | 5.22 | 1.53 | 1.46 |
| 1 | F | 281 | GLY | N-CA | 5.22 | 1.53 | 1.46 |
| 1 | M | 312 | TRP | NE1-CE2 | -5.22 | 1.30 | 1.37 |
| 1 | N | 264 | ALA | CA-CB | -5.22 | 1.41 | 1.52 |
| 1 | D | 203 | THR | CA-CB | -5.22 | 1.39 | 1.53 |
| 1 | K | 21 | VAL | N-CA | -5.22 | 1.35 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 22 | VAL | CB-CG2 | 5.21 | 1.63 | 1.52 |
| 1 | C | 234 | TYR | CE2-CZ | 5.21 | 1.45 | 1.38 |
| 1 | I | 73 | PHE | CG-CD1 | 5.21 | 1.46 | 1.38 |
| 1 | O | 258 | ARG | CG-CD | 5.21 | 1.65 | 1.51 |
| 1 | E | 103 | VAL | C-O | 5.21 | 1.33 | 1.23 |
| 1 | F | 376 | PHE | CG-CD2 | 5.21 | 1.46 | 1.38 |
| 1 | H | 312 | TRP | CA-CB | -5.21 | 1.42 | 1.53 |
| 1 | L | 460 | ASP | CB-CG | 5.21 | 1.62 | 1.51 |
| 1 | C | 124 | ASN | C-O | -5.21 | 1.13 | 1.23 |
| 1 | N | 335 | ASP | CB-CG | 5.21 | 1.62 | 1.51 |
| 1 | A | 377 | GLN | CB-CG | 5.21 | 1.66 | 1.52 |
| 1 | F | 148 | SER | C-O | 5.21 | 1.33 | 1.23 |
| 1 | G | 394 | MET | CG-SD | 5.21 | 1.94 | 1.81 |
| 1 | J | 234 | TYR | CG-CD1 | -5.21 | 1.32 | 1.39 |
| 1 | J | 360 | PHE | CG-CD2 | -5.21 | 1.30 | 1.38 |
| 1 | L | 201 | VAL | CA-CB | -5.21 | 1.43 | 1.54 |
| 1 | F | 85 | PHE | CE2-CZ | 5.21 | 1.47 | 1.37 |
| 1 | F | 272 | PRO | CA-C | -5.21 | 1.42 | 1.52 |
| 1 | H | 247 | PHE | CG-CD2 | 5.21 | 1.46 | 1.38 |
| 1 | J | 363 | TYR | CG-CD1 | 5.21 | 1.46 | 1.39 |
| 1 | F | 400 | GLU | CG-CD | 5.21 | 1.59 | 1.51 |
| 1 | F | 396 | SER | CB-OG | 5.20 | 1.49 | 1.42 |
| 1 | G | 176 | THR | N-CA | 5.20 | 1.56 | 1.46 |
| 1 | I | 105 | VAL | CB-CG2 | 5.20 | 1.63 | 1.52 |
| 1 | I | 351 | SER | CB-OG | -5.20 | 1.35 | 1.42 |
| 1 | K | 30 | ARG | CB-CG | 5.20 | 1.66 | 1.52 |
| 1 | K | 315 | ARG | CG-CD | 5.20 | 1.65 | 1.51 |
| 1 | J | 141 | VAL | CB-CG1 | 5.20 | 1.63 | 1.52 |
| 1 | F | 23 | SER | N-CA | 5.20 | 1.56 | 1.46 |
| 1 | I | 370 | TYR | CG-CD1 | -5.20 | 1.32 | 1.39 |
| 1 | J | 99 | VAL | CB-CG1 | -5.20 | 1.42 | 1.52 |
| 1 | M | 284 | ALA | CA-C | -5.20 | 1.39 | 1.52 |
| 1 | D | 365 | ARG | CA-CB | 5.20 | 1.65 | 1.53 |
| 1 | K | 262 | ASN | CG-OD1 | 5.20 | 1.35 | 1.24 |
| 1 | A | 374 | PHE | CD1-CE1 | -5.20 | 1.28 | 1.39 |
| 1 | O | 29 | ALA | C-O | 5.20 | 1.33 | 1.23 |
| 1 | B | 21 | VAL | CB-CG2 | 5.20 | 1.63 | 1.52 |
| 1 | D | 216 | ASN | C-O | 5.20 | 1.33 | 1.23 |
| 1 | H | 459 | LEU | CG-CD1 | -5.20 | 1.32 | 1.51 |
| 1 | J | 27 | TYR | CG-CD1 | 5.20 | 1.46 | 1.39 |
| 1 | O | 179 | ALA | CA-CB | 5.20 | 1.63 | 1.52 |
| 1 | J | 387 | VAL | CB-CG1 | 5.19 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 249 | TYR | CE1-CZ | -5.19 | 1.31 | 1.38 |
| 1 | J | 83 | PHE | CB-CG | 5.19 | 1.60 | 1.51 |
| 1 | N | 467 | LYS | CB-CG | 5.19 | 1.66 | 1.52 |
| 1 | O | 299 | MET | C-O | -5.19 | 1.13 | 1.23 |
| 1 | O | 462 | PHE | CG-CD2 | 5.19 | 1.46 | 1.38 |
| 1 | F | 291 | TYR | CG-CD1 | -5.19 | 1.32 | 1.39 |
| 1 | G | 314 | GLN | CB-CG | 5.19 | 1.66 | 1.52 |
| 1 | H | 292 | PHE | CG-CD1 | 5.19 | 1.46 | 1.38 |
| 1 | J | 49 | TYR | CD2-CE2 | 5.19 | 1.47 | 1.39 |
| 1 | O | 195 | ILE | CA-CB | -5.19 | 1.43 | 1.54 |
| 1 | O | 231 | TYR | CG-CD1 | 5.19 | 1.45 | 1.39 |
| 1 | B | 73 | PHE | CB-CG | -5.19 | 1.42 | 1.51 |
| 1 | D | 292 | PHE | CD2-CE2 | 5.19 | 1.49 | 1.39 |
| 1 | I | 85 | PHE | CE1-CZ | 5.19 | 1.47 | 1.37 |
| 1 | N | 376 | PHE | C-O | 5.19 | 1.33 | 1.23 |
| 1 | C | 234 | TYR | CG-CD1 | -5.19 | 1.32 | 1.39 |
| 1 | E | 365 | ARG | CZ-NH1 | 5.19 | 1.39 | 1.33 |
| 1 | A | 242 | TYR | CD1-CE1 | 5.19 | 1.47 | 1.39 |
| 1 | H | 205 | PHE | CD2-CE2 | 5.19 | 1.49 | 1.39 |
| 1 | I | 359 | ASN | CB-CG | 5.19 | 1.62 | 1.51 |
| 1 | J | 200 | MET | C-O | 5.19 | 1.33 | 1.23 |
| 1 | H | 258 | ARG | CZ-NH1 | -5.18 | 1.26 | 1.33 |
| 1 | K | 447 | TRP | CB-CG | -5.18 | 1.41 | 1.50 |
| 1 | L | 162 | LYS | CE-NZ | 5.18 | 1.62 | 1.49 |
| 1 | H | 56 | ASN | CG-OD1 | 5.18 | 1.35 | 1.24 |
| 1 | I | 376 | PHE | CE2-CZ | 5.18 | 1.47 | 1.37 |
| 1 | J | 261 | PHE | CD2-CE2 | -5.18 | 1.28 | 1.39 |
| 1 | K | 281 | GLY | CA-C | 5.18 | 1.60 | 1.51 |
| 1 | O | 73 | PHE | CD1-CE1 | 5.18 | 1.49 | 1.39 |
| 1 | O | 189 | GLU | CD-OE1 | 5.18 | 1.31 | 1.25 |
| 1 | F | 164 | PRO | N-CA | -5.18 | 1.38 | 1.47 |
| 1 | F | 99 | VAL | CA-CB | 5.18 | 1.65 | 1.54 |
| 1 | G | 353 | THR | CB-CG2 | 5.18 | 1.69 | 1.52 |
| 1 | I | 41 | ARG | NE-CZ | 5.18 | 1.39 | 1.33 |
| 1 | O | 259 | HIS | C-O | 5.18 | 1.33 | 1.23 |
| 1 | H | 100 | TRP | CB-CG | -5.18 | 1.41 | 1.50 |
| 1 | H | 311 | TYR | CZ-OH | -5.18 | 1.29 | 1.37 |
| 1 | L | 389 | THR | CB-CG2 | 5.18 | 1.69 | 1.52 |
| 1 | O | 49 | TYR | CE2-CZ | 5.18 | 1.45 | 1.38 |
| 1 | E | 210 | PHE | CD1-CE1 | -5.18 | 1.28 | 1.39 |
| 1 | G | 70 | TYR | CB-CG | -5.18 | 1.43 | 1.51 |
| 1 | J | 394 | MET | CG-SD | 5.18 | 1.94 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 27 | TYR | CG-CD1 | 5.18 | 1.45 | 1.39 |
| 1 | M | 282 | SER | C-O | 5.18 | 1.33 | 1.23 |
| 1 | G | 358 | THR | C-O | 5.17 | 1.33 | 1.23 |
| 1 | H | 151 | TYR | N-CA | -5.17 | 1.35 | 1.46 |
| 1 | I | 310 | PRO | CG-CD | -5.17 | 1.33 | 1.50 |
| 1 | J | 86 | PRO | N-CA | 5.17 | 1.56 | 1.47 |
| 1 | K | 50 | PHE | CD1-CE1 | -5.17 | 1.28 | 1.39 |
| 1 | O | 449 | VAL | CA-CB | 5.17 | 1.65 | 1.54 |
| 1 | D | 295 | PRO | N-CD | -5.17 | 1.40 | 1.47 |
| 1 | G | 78 | PRO | C-O | 5.17 | 1.33 | 1.23 |
| 1 | G | 205 | PHE | C-O | 5.17 | 1.33 | 1.23 |
| 1 | F | 261 | PHE | CG-CD2 | -5.17 | 1.30 | 1.38 |
| 1 | H | 111 | GLN | N-CA | -5.17 | 1.36 | 1.46 |
| 1 | E | 364 | LEU | C-O | 5.17 | 1.33 | 1.23 |
| 1 | F | 54 | LYS | CD-CE | 5.17 | 1.64 | 1.51 |
| 1 | I | 95 | THR | CB-CG2 | 5.17 | 1.69 | 1.52 |
| 1 | M | 180 | VAL | C-O | 5.17 | 1.33 | 1.23 |
| 1 | B | 93 | PRO | N-CD | 5.17 | 1.55 | 1.47 |
| 1 | N | 365 | ARG | CG-CD | 5.17 | 1.64 | 1.51 |
| 1 | O | 85 | PHE | CE2-CZ | 5.17 | 1.47 | 1.37 |
| 1 | D | 214 | GLN | CD-NE2 | -5.17 | 1.20 | 1.32 |
| 1 | C | 58 | ASN | CB-CG | 5.16 | 1.62 | 1.51 |
| 1 | C | 121 | PRO | C-O | -5.16 | 1.12 | 1.23 |
| 1 | C | 239 | SER | CA-CB | 5.16 | 1.60 | 1.52 |
| 1 | F | 278 | LYS | CB-CG | 5.16 | 1.66 | 1.52 |
| 1 | H | 358 | THR | CB-CG2 | 5.16 | 1.69 | 1.52 |
| 1 | J | 231 | TYR | CZ-OH | 5.16 | 1.46 | 1.37 |
| 1 | O | 100 | TRP | CD2-CE2 | 5.16 | 1.47 | 1.41 |
| 1 | F | 205 | PHE | CG-CD2 | -5.16 | 1.31 | 1.38 |
| 1 | G | 328 | GLN | C-O | 5.16 | 1.33 | 1.23 |
| 1 | O | 368 | GLU | CB-CG | -5.16 | 1.42 | 1.52 |
| 1 | A | 468 | PHE | CB-CG | -5.16 | 1.42 | 1.51 |
| 1 | D | 355 | TYR | CG-CD2 | 5.16 | 1.45 | 1.39 |
| 1 | G | 463 | PRO | CA-CB | -5.16 | 1.43 | 1.53 |
| 1 | H | 467 | LYS | C-O | -5.16 | 1.13 | 1.23 |
| 1 | A | 176 | THR | CA-CB | 5.16 | 1.66 | 1.53 |
| 1 | L | 61 | LEU | CG-CD2 | 5.16 | 1.71 | 1.51 |
| 1 | E | 45 | VAL | CB-CG1 | -5.16 | 1.42 | 1.52 |
| 1 | G | 89 | SER | CB-OG | 5.16 | 1.49 | 1.42 |
| 1 | G | 137 | ALA | CA-CB | 5.16 | 1.63 | 1.52 |
| 1 | J | 313 | LEU | C-O | 5.16 | 1.33 | 1.23 |
| 1 | C | 22 | VAL | CA-CB | -5.15 | 1.44 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 173 | SER | C-N | 5.15 | 1.44 | 1.34 |
| 1 | A | 58 | ASN | C-O | 5.15 | 1.33 | 1.23 |
| 1 | A | 216 | ASN | N-CA | -5.15 | 1.36 | 1.46 |
| 1 | B | 91 | TYR | CD1-CE1 | 5.15 | 1.47 | 1.39 |
| 1 | G | 269 | GLU | CG-CD | 5.15 | 1.59 | 1.51 |
| 1 | K | 61 | LEU | CG-CD1 | 5.15 | 1.71 | 1.51 |
| 1 | O | 276 | TYR | CZ-OH | -5.15 | 1.29 | 1.37 |
| 1 | B | 214 | GLN | CA-CB | 5.15 | 1.65 | 1.53 |
| 1 | A | 133 | SER | CA-CB | 5.15 | 1.60 | 1.52 |
| 1 | D | 91 | TYR | CD2-CE2 | 5.15 | 1.47 | 1.39 |
| 1 | G | 462 | PHE | CD1-CE1 | 5.15 | 1.49 | 1.39 |
| 1 | J | 148 | SER | N-CA | 5.15 | 1.56 | 1.46 |
| 1 | B | 227 | SER | C-O | 5.15 | 1.33 | 1.23 |
| 1 | B | 300 | VAL | CA-CB | 5.15 | 1.65 | 1.54 |
| 1 | G | 442 | LYS | CD-CE | 5.15 | 1.64 | 1.51 |
| 1 | A | 95 | THR | CB-OG1 | 5.14 | 1.53 | 1.43 |
| 1 | A | 312 | TRP | NE1-CE2 | -5.14 | 1.30 | 1.37 |
| 1 | O | 108 | GLY | CA-C | 5.14 | 1.60 | 1.51 |
| 1 | E | 176 | THR | CA-CB | 5.14 | 1.66 | 1.53 |
| 1 | F | 259 | HIS | C-O | 5.14 | 1.33 | 1.23 |
| 1 | J | 142 | ASP | CG-OD1 | 5.14 | 1.37 | 1.25 |
| 1 | J | 214 | GLN | N-CA | -5.14 | 1.36 | 1.46 |
| 1 | C | 263 | ARG | CD-NE | -5.14 | 1.37 | 1.46 |
| 1 | D | 341 | ASN | CG-OD1 | 5.14 | 1.35 | 1.24 |
| 1 | F | 115 | VAL | CB-CG2 | -5.14 | 1.42 | 1.52 |
| 1 | F | 230 | LYS | CD-CE | 5.14 | 1.64 | 1.51 |
| 1 | I | 327 | ASN | CB-CG | 5.14 | 1.62 | 1.51 |
| 1 | K | 296 | SER | CB-OG | -5.14 | 1.35 | 1.42 |
| 1 | B | 472 | LEU | CA-C | 5.14 | 1.66 | 1.52 |
| 1 | F | 115 | VAL | CA-C | -5.14 | 1.39 | 1.52 |
| 1 | J | 326 | GLY | CA-C | 5.14 | 1.60 | 1.51 |
| 1 | B | 165 | ILE | CG1-CD1 | 5.14 | 1.85 | 1.50 |
| 1 | C | 112 | PRO | N-CD | -5.14 | 1.40 | 1.47 |
| 1 | I | 236 | LYS | CE-NZ | 5.14 | 1.61 | 1.49 |
| 1 | I | 373 | GLN | C-O | 5.14 | 1.33 | 1.23 |
| 1 | J | 242 | TYR | CG-CD1 | 5.14 | 1.45 | 1.39 |
| 1 | B | 280 | SER | CA-CB | -5.13 | 1.45 | 1.52 |
| 1 | D | 389 | THR | N-CA | 5.13 | 1.56 | 1.46 |
| 1 | E | 327 | ASN | C-O | 5.13 | 1.33 | 1.23 |
| 1 | G | 443 | LYS | CD-CE | 5.13 | 1.64 | 1.51 |
| 1 | E | 179 | ALA | CA-CB | 5.13 | 1.63 | 1.52 |
| 1 | F | 216 | ASN | CB-CG | -5.13 | 1.39 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 380 | LYS | N-CA | -5.13 | 1.36 | 1.46 |
| 1 | O | 240 | GLU | CB-CG | 5.13 | 1.61 | 1.52 |
| 1 | F | 446 | PHE | CA-CB | -5.13 | 1.42 | 1.53 |
| 1 | I | 177 | GLN | CB-CG | 5.13 | 1.66 | 1.52 |
| 1 | J | 153 | GLN | CG-CD | -5.13 | 1.39 | 1.51 |
| 1 | M | 56 | ASN | CG-OD1 | 5.13 | 1.35 | 1.24 |
| 1 | M | 444 | TYR | CE2-CZ | 5.13 | 1.45 | 1.38 |
| 1 | A | 168 | HIS | N-CA | 5.13 | 1.56 | 1.46 |
| 1 | H | 88 | THR | CB-CG2 | 5.13 | 1.69 | 1.52 |
| 1 | I | 152 | LYS | CE-NZ | -5.13 | 1.36 | 1.49 |
| 1 | K | 82 | LYS | CE-NZ | 5.13 | 1.61 | 1.49 |
| 1 | G | 311 | TYR | CE1-CZ | -5.12 | 1.31 | 1.38 |
| 1 | I | 400 | GLU | CG-CD | 5.12 | 1.59 | 1.51 |
| 1 | K | 447 | TRP | CD2-CE2 | -5.12 | 1.35 | 1.41 |
| 1 | E | 250 | LEU | C-O | 5.12 | 1.33 | 1.23 |
| 1 | F | 28 | VAL | CB-CG2 | -5.12 | 1.42 | 1.52 |
| 1 | F | 135 | TYR | CD1-CE1 | -5.12 | 1.31 | 1.39 |
| 1 | I | 221 | PRO | CG-CD | 5.12 | 1.67 | 1.50 |
| 1 | A | 471 | GLN | CB-CG | -5.12 | 1.38 | 1.52 |
| 1 | F | 30 | ARG | C-O | -5.12 | 1.13 | 1.23 |
| 1 | J | 121 | PRO | N-CA | -5.12 | 1.38 | 1.47 |
| 1 | J | 288 | SER | CA-CB | 5.12 | 1.60 | 1.52 |
| 1 | J | 368 | GLU | CG-CD | 5.12 | 1.59 | 1.51 |
| 1 | M | 175 | CYS | C-O | 5.12 | 1.33 | 1.23 |
| 1 | J | 237 | MET | C-O | 5.12 | 1.33 | 1.23 |
| 1 | J | 295 | PRO | N-CA | -5.12 | 1.38 | 1.47 |
| 1 | B | 354 | THR | CB-CG2 | -5.12 | 1.35 | 1.52 |
| 1 | D | 400 | GLU | CD-OE1 | 5.12 | 1.31 | 1.25 |
| 1 | F | 135 | TYR | CD2-CE2 | -5.12 | 1.31 | 1.39 |
| 1 | G | 242 | TYR | CZ-OH | 5.12 | 1.46 | 1.37 |
| 1 | H | 240 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | N | 83 | PHE | CD2-CE2 | 5.12 | 1.49 | 1.39 |
| 1 | B | 151 | TYR | CD2-CE2 | -5.12 | 1.31 | 1.39 |
| 1 | D | 106 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | E | 345 | CYS | CB-SG | -5.12 | 1.73 | 1.81 |
| 1 | H | 253 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | I | 235 | ILE | C-O | -5.12 | 1.13 | 1.23 |
| 1 | K | 162 | LYS | C-O | -5.12 | 1.13 | 1.23 |
| 1 | N | 151 | TYR | CD1-CE1 | 5.12 | 1.47 | 1.39 |
| 1 | F | 352 | GLU | CG-CD | 5.11 | 1.59 | 1.51 |
| 1 | H | 145 | GLU | CB-CG | 5.11 | 1.61 | 1.52 |
| 1 | H | 386 | ASP | C-O | 5.11 | 1.33 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | J | 176 | THR | CB-CG2 | 5.11 | 1.69 | 1.52 |
| 1 | K | 312 | TRP | CD2-CE3 | -5.11 | 1.32 | 1.40 |
| 1 | A | 69 | GLN | CD-OE1 | 5.11 | 1.35 | 1.24 |
| 1 | C | 37 | ALA | C-O | 5.11 | 1.33 | 1.23 |
| 1 | D | 394 | MET | CG-SD | -5.11 | 1.67 | 1.81 |
| 1 | H | 281 | GLY | C-O | 5.11 | 1.31 | 1.23 |
| 1 | L | 248 | PHE | CD2-CE2 | -5.11 | 1.29 | 1.39 |
| 1 | M | 138 | ASN | N-CA | 5.11 | 1.56 | 1.46 |
| 1 | N | 72 | VAL | CA-CB | 5.11 | 1.65 | 1.54 |
| 1 | M | 86 | PRO | CB-CG | 5.11 | 1.75 | 1.50 |
| 1 | N | 379 | CYS | CB-SG | 5.11 | 1.91 | 1.82 |
| 1 | F | 35 | TYR | CE2-CZ | 5.11 | 1.45 | 1.38 |
| 1 | F | 131 | ASN | CG-ND2 | -5.11 | 1.20 | 1.32 |
| 1 | H | 251 | ARG | CG-CD | -5.11 | 1.39 | 1.51 |
| 1 | J | 356 | LYS | CA-C | -5.11 | 1.39 | 1.52 |
| 1 | N | 362 | GLU | CB-CG | -5.11 | 1.42 | 1.52 |
| 1 | A | 235 | ILE | CA-C | -5.11 | 1.39 | 1.52 |
| 1 | C | 363 | TYR | CG-CD1 | 5.11 | 1.45 | 1.39 |
| 1 | E | 20 | ALA | C-O | 5.11 | 1.33 | 1.23 |
| 1 | F | 106 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | F | 447 | TRP | C-O | 5.11 | 1.33 | 1.23 |
| 1 | G | 264 | ALA | C-O | 5.11 | 1.33 | 1.23 |
| 1 | E | 174 | PRO | CG-CD | 5.10 | 1.67 | 1.50 |
| 1 | L | 206 | GLY | N-CA | 5.10 | 1.53 | 1.46 |
| 1 | O | 112 | PRO | C-O | 5.10 | 1.33 | 1.23 |
| 1 | C | 460 | ASP | CA-C | -5.10 | 1.39 | 1.52 |
| 1 | F | 360 | PHE | CE1-CZ | 5.10 | 1.47 | 1.37 |
| 1 | G | 104 | GLY | CA-C | 5.10 | 1.60 | 1.51 |
| 1 | H | 356 | LYS | CB-CG | 5.10 | 1.66 | 1.52 |
| 1 | K | 320 | ASN | C-O | -5.10 | 1.13 | 1.23 |
| 1 | A | 93 | PRO | C-O | 5.10 | 1.33 | 1.23 |
| 1 | A | 455 | PHE | CD1-CE1 | -5.10 | 1.29 | 1.39 |
| 1 | E | 63 | PRO | CB-CG | 5.10 | 1.75 | 1.50 |
| 1 | H | 256 | PHE | CD2-CE2 | 5.10 | 1.49 | 1.39 |
| 1 | H | 403 | ASN | CG-ND2 | 5.10 | 1.45 | 1.32 |
| 1 | M | 321 | ASN | C-O | 5.10 | 1.33 | 1.23 |
| 1 | N | 111 | GLN | CG-CD | 5.10 | 1.62 | 1.51 |
| 1 | B | 468 | PHE | C-O | 5.10 | 1.33 | 1.23 |
| 1 | D | 325 | TRP | CE2-CZ2 | 5.10 | 1.48 | 1.39 |
| 1 | I | 113 | LEU | C-N | 5.10 | 1.42 | 1.33 |
| 1 | N | 39 | THR | CB-CG2 | -5.10 | 1.35 | 1.52 |
| 1 | B | 250 | LEU | C-O | 5.10 | 1.33 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 100 | TRP | CA-CB | -5.10 | 1.42 | 1.53 |
| 1 | M | 20 | ALA | CA-CB | 5.10 | 1.63 | 1.52 |
| 1 | H | 449 | VAL | CB-CG2 | -5.09 | 1.42 | 1.52 |
| 1 | O | 363 | TYR | CE1-CZ | 5.09 | 1.45 | 1.38 |
| 1 | A | 56 | ASN | CG-OD1 | 5.09 | 1.35 | 1.24 |
| 1 | H | 250 | LEU | C-O | 5.09 | 1.33 | 1.23 |
| 1 | B | 149 | MET | CA-CB | -5.09 | 1.42 | 1.53 |
| 1 | E | 325 | TRP | C-O | 5.09 | 1.33 | 1.23 |
| 1 | J | 321 | ASN | CG-OD1 | 5.09 | 1.35 | 1.24 |
| 1 | K | 91 | TYR | CE2-CZ | 5.09 | 1.45 | 1.38 |
| 1 | M | 99 | VAL | CB-CG1 | -5.09 | 1.42 | 1.52 |
| 1 | N | 210 | PHE | CD1-CE1 | -5.09 | 1.29 | 1.39 |
| 1 | G | 370 | TYR | CE1-CZ | 5.09 | 1.45 | 1.38 |
| 1 | A | 73 | PHE | CE1-CZ | -5.09 | 1.27 | 1.37 |
| 1 | E | 362 | GLU | C-O | 5.09 | 1.33 | 1.23 |
| 1 | M | 117 | ILE | CB-CG2 | -5.09 | 1.37 | 1.52 |
| 1 | D | 201 | VAL | C-O | 5.09 | 1.33 | 1.23 |
| 1 | K | 375 | ILE | CB-CG2 | -5.09 | 1.37 | 1.52 |
| 1 | M | 21 | VAL | C-O | -5.09 | 1.13 | 1.23 |
| 1 | B | 358 | THR | CA-C | -5.08 | 1.39 | 1.52 |
| 1 | I | 462 | PHE | CB-CG | -5.08 | 1.42 | 1.51 |
| 1 | C | 249 | TYR | CD2-CE2 | 5.08 | 1.47 | 1.39 |
| 1 | D | 208 | MET | CB-CG | 5.08 | 1.67 | 1.51 |
| 1 | E | 162 | LYS | CD-CE | 5.08 | 1.64 | 1.51 |
| 1 | F | 119 | GLY | C-O | -5.08 | 1.15 | 1.23 |
| 1 | F | 146 | CYS | C-O | -5.08 | 1.13 | 1.23 |
| 1 | J | 106 | GLU | CB-CG | 5.08 | 1.61 | 1.52 |
| 1 | K | 140 | GLY | CA-C | 5.08 | 1.59 | 1.51 |
| 1 | K | 192 | ASN | CG-ND2 | 5.08 | 1.45 | 1.32 |
| 1 | M | 336 | THR | CB-OG1 | 5.08 | 1.53 | 1.43 |
| 1 | A | 470 | LEU | CG-CD1 | 5.08 | 1.70 | 1.51 |
| 1 | F | 34 | TYR | C-O | 5.08 | 1.33 | 1.23 |
| 1 | O | 361 | LYS | CD-CE | 5.08 | 1.64 | 1.51 |
| 1 | A | 231 | TYR | CB-CG | -5.08 | 1.44 | 1.51 |
| 1 | A | 357 | ASN | CB-CG | 5.08 | 1.62 | 1.51 |
| 1 | A | 445 | THR | C-O | 5.08 | 1.33 | 1.23 |
| 1 | D | 367 | GLY | N-CA | 5.08 | 1.53 | 1.46 |
| 1 | H | 172 | GLY | C-O | 5.08 | 1.31 | 1.23 |
| 1 | M | 448 | GLU | CD-OE1 | -5.08 | 1.20 | 1.25 |
| 1 | N | 439 | ASP | N-CA | 5.08 | 1.56 | 1.46 |
| 1 | O | 447 | TRP | CD1-NE1 | 5.08 | 1.46 | 1.38 |
| 1 | A | 70 | TYR | CD2-CE2 | -5.08 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 140 | GLY | CA-C | 5.08 | 1.59 | 1.51 |
| 1 | E | 460 | ASP | C-O | -5.08 | 1.13 | 1.23 |
| 1 | F | 118 | SER | C-O | 5.08 | 1.32 | 1.23 |
| 1 | I | 86 | PRO | C-O | 5.08 | 1.33 | 1.23 |
| 1 | K | 106 | GLU | CB-CG | 5.08 | 1.61 | 1.52 |
| 1 | K | 307 | PHE | CG-CD1 | -5.08 | 1.31 | 1.38 |
| 1 | E | 472 | LEU | C-O | 5.08 | 1.32 | 1.23 |
| 1 | I | 245 | SER | CB-OG | 5.08 | 1.48 | 1.42 |
| 1 | N | 390 | TYR | CG-CD1 | 5.08 | 1.45 | 1.39 |
| 1 | A | 380 | LYS | CB-CG | -5.08 | 1.38 | 1.52 |
| 1 | B | 289 | SER | CB-OG | 5.08 | 1.48 | 1.42 |
| 1 | I | 328 | GLN | CG-CD | 5.08 | 1.62 | 1.51 |
| 1 | O | 100 | TRP | CB-CG | -5.08 | 1.41 | 1.50 |
| 1 | O | 127 | ASP | CB-CG | 5.08 | 1.62 | 1.51 |
| 1 | A | 171 | LYS | CG-CD | 5.07 | 1.69 | 1.52 |
| 1 | G | 114 | GLY | CA-C | -5.07 | 1.43 | 1.51 |
| 1 | H | 390 | TYR | CG-CD1 | 5.07 | 1.45 | 1.39 |
| 1 | J | 261 | PHE | CE1-CZ | -5.07 | 1.27 | 1.37 |
| 1 | K | 65 | VAL | CB-CG1 | -5.07 | 1.42 | 1.52 |
| 1 | M | 173 | SER | CA-CB | 5.07 | 1.60 | 1.52 |
| 1 | O | 247 | PHE | CE2-CZ | -5.07 | 1.27 | 1.37 |
| 1 | H | 394 | MET | CG-SD | -5.07 | 1.68 | 1.81 |
| 1 | N | 277 | ILE | CA-CB | -5.07 | 1.43 | 1.54 |
| 1 | C | 129 | THR | C-O | 5.07 | 1.32 | 1.23 |
| 1 | C | 449 | VAL | CB-CG1 | 5.07 | 1.63 | 1.52 |
| 1 | K | 181 | GLN | CD-OE1 | 5.07 | 1.35 | 1.24 |
| 1 | L | 370 | TYR | CD1-CE1 | -5.07 | 1.31 | 1.39 |
| 1 | B | 454 | LYS | CE-NZ | 5.07 | 1.61 | 1.49 |
| 1 | F | 45 | VAL | N-CA | 5.07 | 1.56 | 1.46 |
| 1 | G | 27 | TYR | CG-CD1 | 5.07 | 1.45 | 1.39 |
| 1 | N | 171 | LYS | CG-CD | 5.07 | 1.69 | 1.52 |
| 1 | B | 345 | CYS | CB-SG | 5.07 | 1.90 | 1.82 |
| 1 | C | 205 | PHE | CD1-CE1 | 5.07 | 1.49 | 1.39 |
| 1 | H | 20 | ALA | N-CA | 5.07 | 1.56 | 1.46 |
| 1 | H | 448 | GLU | CB-CG | 5.07 | 1.61 | 1.52 |
| 1 | B | 273 | ASP | C-O | 5.07 | 1.32 | 1.23 |
| 1 | E | 148 | SER | CA-CB | -5.07 | 1.45 | 1.52 |
| 1 | B | 188 | LEU | CG-CD2 | -5.06 | 1.33 | 1.51 |
| 1 | B | 401 | ASP | CG-OD1 | 5.06 | 1.36 | 1.25 |
| 1 | K | 332 | THR | C-O | -5.06 | 1.13 | 1.23 |
| 1 | B | 247 | PHE | CE1-CZ | 5.06 | 1.47 | 1.37 |
| 1 | B | 292 | PHE | CD2-CE2 | 5.06 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 450 | ASN | C-O | 5.06 | 1.32 | 1.23 |
| 1 | H | 70 | TYR | CE1-CZ | 5.06 | 1.45 | 1.38 |
| 1 | J | 362 | GLU | CB-CG | 5.06 | 1.61 | 1.52 |
| 1 | K | 115 | VAL | CA-CB | 5.06 | 1.65 | 1.54 |
| 1 | M | 210 | PHE | CD2-CE2 | -5.06 | 1.29 | 1.39 |
| 1 | O | 355 | TYR | CB-CG | -5.06 | 1.44 | 1.51 |
| 1 | G | 362 | GLU | CB-CG | -5.06 | 1.42 | 1.52 |
| 1 | L | 245 | SER | CA-CB | 5.06 | 1.60 | 1.52 |
| 1 | M | 338 | ARG | CB-CG | 5.06 | 1.66 | 1.52 |
| 1 | A | 261 | PHE | CE1-CZ | 5.06 | 1.47 | 1.37 |
| 1 | B | 42 | LEU | CG-CD2 | 5.06 | 1.70 | 1.51 |
| 1 | D | 276 | TYR | CB-CG | -5.06 | 1.44 | 1.51 |
| 1 | F | 338 | ARG | CG-CD | 5.06 | 1.64 | 1.51 |
| 1 | N | 367 | GLY | N-CA | 5.06 | 1.53 | 1.46 |
| 1 | F | 105 | VAL | CB-CG1 | -5.06 | 1.42 | 1.52 |
| 1 | F | 169 | TRP | CD2-CE2 | -5.06 | 1.35 | 1.41 |
| 1 | K | 451 | LEU | CG-CD1 | -5.06 | 1.33 | 1.51 |
| 1 | B | 449 | VAL | C-O | 5.06 | 1.32 | 1.23 |
| 1 | C | 189 | GLU | CG-CD | 5.05 | 1.59 | 1.51 |
| 1 | E | 285 | ASN | C-O | 5.05 | 1.32 | 1.23 |
| 1 | F | 355 | TYR | CG-CD2 | 5.05 | 1.45 | 1.39 |
| 1 | H | 238 | VAL | CB-CG2 | 5.05 | 1.63 | 1.52 |
| 1 | I | 169 | TRP | CB-CG | -5.05 | 1.41 | 1.50 |
| 1 | J | 115 | VAL | CA-CB | -5.05 | 1.44 | 1.54 |
| 1 | K | 35 | TYR | CE2-CZ | 5.05 | 1.45 | 1.38 |
| 1 | M | 219 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | C | 440 | PRO | CB-CG | 5.05 | 1.75 | 1.50 |
| 1 | D | 24 | THR | CA-CB | -5.05 | 1.40 | 1.53 |
| 1 | J | 147 | ILE | CG1-CD1 | 5.05 | 1.85 | 1.50 |
| 1 | L | 403 | ASN | C-O | 5.05 | 1.32 | 1.23 |
| 1 | O | 134 | ALA | CA-CB | -5.05 | 1.41 | 1.52 |
| 1 | F | 22 | VAL | C-O | 5.05 | 1.32 | 1.23 |
| 1 | H | 206 | GLY | C-O | 5.05 | 1.31 | 1.23 |
| 1 | J | 255 | MET | N-CA | 5.05 | 1.56 | 1.46 |
| 1 | A | 116 | GLY | N-CA | -5.05 | 1.38 | 1.46 |
| 1 | D | 70 | TYR | CG-CD2 | -5.05 | 1.32 | 1.39 |
| 1 | N | 312 | TRP | CA-CB | -5.05 | 1.42 | 1.53 |
| 1 | A | 350 | THR | C-O | 5.05 | 1.32 | 1.23 |
| 1 | C | 402 | TRP | C-O | 5.05 | 1.32 | 1.23 |
| 1 | F | 340 | THR | CB-CG2 | 5.05 | 1.69 | 1.52 |
| 1 | F | 460 | ASP | C-O | 5.05 | 1.32 | 1.23 |
| 1 | M | 251 | ARG | CG-CD | -5.05 | 1.39 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 331 | VAL | CA-CB | -5.04 | 1.44 | 1.54 |
| 1 | L | 440 | PRO | C-O | 5.04 | 1.33 | 1.23 |
| 1 | B | 390 | TYR | CB-CG | -5.04 | 1.44 | 1.51 |
| 1 | C | 291 | TYR | CE2-CZ | -5.04 | 1.31 | 1.38 |
| 1 | I | 107 | VAL | CB-CG1 | -5.04 | 1.42 | 1.52 |
| 1 | J | 111 | GLN | CG-CD | 5.04 | 1.62 | 1.51 |
| 1 | J | 376 | PHE | CE2-CZ | 5.04 | 1.47 | 1.37 |
| 1 | N | 25 | ASP | CG-OD2 | 5.04 | 1.36 | 1.25 |
| 1 | A | 263 | ARG | N-CA | 5.04 | 1.56 | 1.46 |
| 1 | A | 459 | LEU | N-CA | -5.04 | 1.36 | 1.46 |
| 1 | D | 318 | GLY | CA-C | 5.04 | 1.59 | 1.51 |
| 1 | J | 95 | THR | N-CA | 5.04 | 1.56 | 1.46 |
| 1 | N | 105 | VAL | CA-CB | -5.04 | 1.44 | 1.54 |
| 1 | E | 295 | PRO | CG-CD | 5.04 | 1.67 | 1.50 |
| 1 | E | 329 | LEU | CG-CD2 | 5.04 | 1.70 | 1.51 |
| 1 | I | 236 | LYS | C-O | 5.04 | 1.32 | 1.23 |
| 1 | M | 178 | VAL | C-O | 5.04 | 1.32 | 1.23 |
| 1 | D | 346 | ALA | CA-CB | 5.04 | 1.63 | 1.52 |
| 1 | F | 249 | TYR | C-O | 5.04 | 1.32 | 1.23 |
| 1 | L | 400 | GLU | CD-OE2 | 5.04 | 1.31 | 1.25 |
| 1 | M | 230 | LYS | C-O | 5.04 | 1.32 | 1.23 |
| 1 | O | 131 | ASN | CA-C | -5.04 | 1.39 | 1.52 |
| 1 | B | 194 | VAL | C-O | 5.04 | 1.32 | 1.23 |
| 1 | C | 462 | PHE | CG-CD2 | -5.04 | 1.31 | 1.38 |
| 1 | D | 108 | GLY | N-CA | 5.04 | 1.53 | 1.46 |
| 1 | F | 189 | GLU | CD-OE2 | 5.04 | 1.31 | 1.25 |
| 1 | J | 57 | ASN | C-O | 5.04 | 1.32 | 1.23 |
| 1 | J | 375 | ILE | CB-CG2 | -5.04 | 1.37 | 1.52 |
| 1 | O | 234 | TYR | CG-CD1 | -5.04 | 1.32 | 1.39 |
| 1 | A | 390 | TYR | C-O | 5.03 | 1.32 | 1.23 |
| 1 | E | 70 | TYR | CB-CG | -5.03 | 1.44 | 1.51 |
| 1 | E | 253 | GLU | C-O | 5.03 | 1.32 | 1.23 |
| 1 | N | 63 | PRO | CB-CG | 5.03 | 1.75 | 1.50 |
| 1 | O | 214 | GLN | CD-OE1 | 5.03 | 1.35 | 1.24 |
| 1 | C | 51 | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 1 | C | 467 | LYS | CD-CE | 5.03 | 1.63 | 1.51 |
| 1 | A | 197 | ASP | C-O | -5.03 | 1.13 | 1.23 |
| 1 | B | 388 | MET | CG-SD | 5.03 | 1.94 | 1.81 |
| 1 | C | 470 | LEU | CA-CB | -5.03 | 1.42 | 1.53 |
| 1 | I | 22 | VAL | CB-CG1 | 5.03 | 1.63 | 1.52 |
| 1 | M | 249 | TYR | CE1-CZ | -5.03 | 1.32 | 1.38 |
| 1 | N | 116 | GLY | C-O | 5.03 | 1.31 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | O | 334 | VAL | CB-CG1 | 5.03 | 1.63 | 1.52 |
| 1 | O | 362 | GLU | C-O | 5.03 | 1.32 | 1.23 |
| 1 | C | 307 | PHE | CB-CG | -5.03 | 1.42 | 1.51 |
| 1 | L | 30 | ARG | CA-C | -5.03 | 1.39 | 1.52 |
| 1 | L | 216 | ASN | CB-CG | -5.03 | 1.39 | 1.51 |
| 1 | B | 364 | LEU | CG-CD1 | -5.03 | 1.33 | 1.51 |
| 1 | E | 400 | GLU | CG-CD | 5.03 | 1.59 | 1.51 |
| 1 | B | 100 | TRP | CB-CG | -5.02 | 1.41 | 1.50 |
| 1 | O | 231 | TYR | CE1-CZ | 5.02 | 1.45 | 1.38 |
| 1 | B | 248 | PHE | CD1-CE1 | 5.02 | 1.49 | 1.39 |
| 1 | B | 355 | TYR | CG-CD2 | -5.02 | 1.32 | 1.39 |
| 1 | F | 152 | LYS | C-O | 5.02 | 1.32 | 1.23 |
| 1 | F | 289 | SER | CB-OG | 5.02 | 1.48 | 1.42 |
| 1 | H | 312 | TRP | C-O | -5.02 | 1.13 | 1.23 |
| 1 | J | 96 | GLN | CG-CD | -5.02 | 1.39 | 1.51 |
| 1 | J | 471 | GLN | CA-CB | -5.02 | 1.43 | 1.53 |
| 1 | L | 439 | ASP | C-N | 5.02 | 1.43 | 1.34 |
| 1 | N | 170 | GLY | C-O | 5.02 | 1.31 | 1.23 |
| 1 | C | 359 | ASN | C-O | 5.02 | 1.32 | 1.23 |
| 1 | A | 376 | PHE | CA-CB | -5.02 | 1.43 | 1.53 |
| 1 | E | 135 | TYR | CG-CD2 | 5.02 | 1.45 | 1.39 |
| 1 | E | 162 | LYS | CE-NZ | 5.02 | 1.61 | 1.49 |
| 1 | J | 296 | SER | CA-CB | -5.02 | 1.45 | 1.52 |
| 1 | J | 472 | LEU | C-OXT | 5.02 | 1.32 | 1.23 |
| 1 | M | 397 | THR | CB-CG2 | 5.02 | 1.69 | 1.52 |
| 1 | O | 231 | TYR | CB-CG | -5.02 | 1.44 | 1.51 |
| 1 | C | 315 | ARG | NE-CZ | 5.02 | 1.39 | 1.33 |
| 1 | A | 447 | TRP | CE3-CZ3 | 5.01 | 1.47 | 1.38 |
| 1 | L | 143 | ASN | C-O | 5.01 | 1.32 | 1.23 |
| 1 | L | 314 | GLN | CB-CG | 5.01 | 1.66 | 1.52 |
| 1 | B | 131 | ASN | C-O | 5.01 | 1.32 | 1.23 |
| 1 | H | 292 | PHE | CD1-CE1 | 5.01 | 1.49 | 1.39 |
| 1 | H | 462 | PHE | CE2-CZ | 5.01 | 1.46 | 1.37 |
| 1 | J | 148 | SER | CB-OG | 5.01 | 1.48 | 1.42 |
| 1 | L | 333 | VAL | CB-CG2 | -5.01 | 1.42 | 1.52 |
| 1 | N | 251 | ARG | CZ-NH1 | 5.01 | 1.39 | 1.33 |
| 1 | D | 470 | LEU | CA-CB | -5.01 | 1.42 | 1.53 |
| 1 | M | 402 | TRP | C-O | 5.01 | 1.32 | 1.23 |
| 1 | N | 300 | VAL | CB-CG2 | 5.01 | 1.63 | 1.52 |
| 1 | B | 281 | GLY | C-O | 5.01 | 1.31 | 1.23 |
| 1 | L | 295 | PRO | CA-CB | -5.01 | 1.43 | 1.53 |
| 1 | L | 468 | PHE | CB-CG | -5.01 | 1.42 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 303 | ASP | CA-C | -5.01 | 1.40 | 1.52 |
| 1 | D | 253 | GLU | CG-CD | 5.01 | 1.59 | 1.51 |
| 1 | F | 266 | THR | CA-CB | -5.01 | 1.40 | 1.53 |
| 1 | J | 171 | LYS | CG-CD | 5.01 | 1.69 | 1.52 |
| 1 | N | 307 | PHE | CE1-CZ | -5.01 | 1.27 | 1.37 |
| 1 | A | 446 | PHE | CA-C | -5.00 | 1.40 | 1.52 |
| 1 | A | 454 | LYS | CD-CE | 5.00 | 1.63 | 1.51 |
| 1 | H | 186 | PRO | C-N | 5.00 | 1.43 | 1.34 |
| 1 | D | 22 | VAL | CA-CB | -5.00 | 1.44 | 1.54 |
| 1 | D | 375 | ILE | CB-CG2 | -5.00 | 1.37 | 1.52 |
| 1 | G | 230 | LYS | CG-CD | 5.00 | 1.69 | 1.52 |
| 1 | E | 108 | GLY | N-CA | 5.00 | 1.53 | 1.46 |
| 1 | I | 83 | PHE | C-O | 5.00 | 1.32 | 1.23 |
| 1 | M | 328 | GLN | N-CA | 5.00 | 1.56 | 1.46 |

All (1779) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 71 | ARG | NE-CZ-NH2 | 23.80 | 132.20 | 120.30 |
| 1 | F | 365 | ARG | NE-CZ-NH1 | 21.93 | 131.26 | 120.30 |
| 1 | C | 144 | ARG | NE-CZ-NH1 | 21.91 | 131.25 | 120.30 |
| 1 | I | 258 | ARG | NE-CZ-NH1 | 20.20 | 130.40 | 120.30 |
| 1 | D | 251 | ARG | NE-CZ-NH2 | 19.49 | 130.04 | 120.30 |
| 1 | J | 97 | ARG | NE-CZ-NH2 | 19.16 | 129.88 | 120.30 |
| 1 | E | 144 | ARG | NE-CZ-NH2 | -18.23 | 111.19 | 120.30 |
| 1 | O | 109 | ARG | NE-CZ-NH2 | 17.99 | 129.29 | 120.30 |
| 1 | M | 150 | ASP | CB-CG-OD2 | 17.50 | 134.05 | 118.30 |
| 1 | I | 97 | ARG | NE-CZ-NH2 | -17.16 | 111.72 | 120.30 |
| 1 | I | 258 | ARG | NE-CZ-NH2 | -17.14 | 111.73 | 120.30 |
| 1 | H | 460 | ASP | CB-CG-OD1 | 16.77 | 133.39 | 118.30 |
| 1 | F | 144 | ARG | NE-CZ-NH1 | -16.47 | 112.06 | 120.30 |
| 1 | D | 263 | ARG | NE-CZ-NH2 | -16.37 | 112.11 | 120.30 |
| 1 | J | 251 | ARG | NE-CZ-NH2 | 16.16 | 128.38 | 120.30 |
| 1 | G | 71 | ARG | NE-CZ-NH2 | -15.82 | 112.39 | 120.30 |
| 1 | G | 71 | ARG | NE-CZ-NH1 | 15.58 | 128.09 | 120.30 |
| 1 | M | 150 | ASP | CB-CG-OD1 | -15.01 | 104.79 | 118.30 |
| 1 | F | 251 | ARG | NE-CZ-NH2 | -14.99 | 112.81 | 120.30 |
| 1 | O | 71 | ARG | NE-CZ-NH2 | -14.97 | 112.81 | 120.30 |
| 1 | I | 97 | ARG | NE-CZ-NH1 | 14.80 | 127.70 | 120.30 |
| 1 | O | 335 | ASP | CB-CG-OD1 | -14.73 | 105.04 | 118.30 |
| 1 | K | 25 | ASP | CB-CG-OD1 | -14.66 | 105.11 | 118.30 |
| 1 | J | 150 | ASP | CB-CG-OD2 | 14.64 | 131.47 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 71 | ARG | NE-CZ-NH1 | -14.38 | 113.11 | 120.30 |
| 1 | N | 365 | ARG | NE-CZ-NH2 | -14.37 | 113.11 | 120.30 |
| 1 | D | 251 | ARG | NE-CZ-NH1 | -14.32 | 113.14 | 120.30 |
| 1 | C | 365 | ARG | NE-CZ-NH1 | 14.24 | 127.42 | 120.30 |
| 1 | A | 364 | LEU | CB-CG-CD1 | -14.13 | 86.98 | 111.00 |
| 1 | K | 460 | ASP | CB-CG-OD2 | -14.12 | 105.59 | 118.30 |
| 1 | C | 464 | LEU | CB-CG-CD1 | 14.05 | 134.88 | 111.00 |
| 1 | C | 144 | ARG | NE-CZ-NH2 | -14.04 | 113.28 | 120.30 |
| 1 | M | 126 | LEU | CB-CG-CD1 | -14.02 | 87.17 | 111.00 |
| 1 | M | 144 | ARG | NE-CZ-NH1 | 13.81 | 127.20 | 120.30 |
| 1 | D | 460 | ASP | CB-CG-OD2 | -13.73 | 105.95 | 118.30 |
| 1 | H | 275 | LEU | CB-CG-CD2 | 13.72 | 134.32 | 111.00 |
| 1 | F | 365 | ARG | NE-CZ-NH2 | -13.68 | 113.46 | 120.30 |
| 1 | C | 365 | ARG | NE-CZ-NH2 | -13.65 | 113.48 | 120.30 |
| 1 | H | 460 | ASP | CB-CG-OD2 | -13.56 | 106.10 | 118.30 |
| 1 | M | 252 | ARG | NE-CZ-NH2 | -13.35 | 113.63 | 120.30 |
| 1 | L | 144 | ARG | NE-CZ-NH2 | -13.23 | 113.69 | 120.30 |
| 1 | J | 150 | ASP | CB-CG-OD1 | -13.12 | 106.50 | 118.30 |
| 1 | D | 365 | ARG | NE-CZ-NH1 | 13.01 | 126.81 | 120.30 |
| 1 | N | 144 | ARG | NE-CZ-NH1 | -12.99 | 113.80 | 120.30 |
| 1 | O | 123 | LEU | CB-CG-CD2 | -12.99 | 88.91 | 111.00 |
| 1 | C | 156 | LEU | CB-CG-CD2 | -12.90 | 89.07 | 111.00 |
| 1 | N | 313 | LEU | CB-CG-CD2 | 12.85 | 132.85 | 111.00 |
| 1 | J | 315 | ARG | NE-CZ-NH1 | -12.79 | 113.91 | 120.30 |
| 1 | L | 42 | LEU | CB-CG-CD2 | 12.74 | 132.66 | 111.00 |
| 1 | E | 338 | ARG | NE-CZ-NH2 | -12.63 | 113.98 | 120.30 |
| 1 | G | 263 | ARG | NE-CZ-NH2 | 12.46 | 126.53 | 120.30 |
| 1 | O | 144 | ARG | NE-CZ-NH1 | 12.45 | 126.52 | 120.30 |
| 1 | B | 365 | ARG | NE-CZ-NH1 | 12.41 | 126.51 | 120.30 |
| 1 | A | 439 | ASP | CB-CG-OD1 | -12.38 | 107.16 | 118.30 |
| 1 | C | 250 | LEU | CB-CG-CD1 | -12.37 | 89.97 | 111.00 |
| 1 | B | 460 | ASP | CB-CG-OD2 | -12.36 | 107.18 | 118.30 |
| 1 | C | 374 | PHE | CB-CG-CD2 | -12.28 | 112.20 | 120.80 |
| 1 | O | 378 | LEU | CB-CG-CD2 | -12.11 | 90.42 | 111.00 |
| 1 | C | 71 | ARG | NE-CZ-NH1 | 11.88 | 126.24 | 120.30 |
| 1 | L | 109 | ARG | NE-CZ-NH1 | 11.88 | 126.24 | 120.30 |
| 1 | A | 223 | ASP | CB-CG-OD2 | 11.85 | 128.96 | 118.30 |
| 1 | H | 466 | ARG | NE-CZ-NH1 | 11.84 | 126.22 | 120.30 |
| 1 | D | 71 | ARG | NE-CZ-NH1 | 11.70 | 126.15 | 120.30 |
| 1 | M | 71 | ARG | NE-CZ-NH1 | 11.62 | 126.11 | 120.30 |
| 1 | A | 258 | ARG | NE-CZ-NH1 | 11.55 | 126.08 | 120.30 |
| 1 | I | 291 | TYR | CD1-CE1-CZ | 11.52 | 130.17 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 294 | THR | CA-CB-CG2 | -11.50 | 96.29 | 112.40 |
| 1 | H | 361 | LYS | CD-CE-NZ | -11.49 | 85.27 | 111.70 |
| 1 | C | 466 | ARG | NE-CZ-NH1 | -11.48 | 114.56 | 120.30 |
| 1 | K | 258 | ARG | NE-CZ-NH1 | -11.48 | 114.56 | 120.30 |
| 1 | O | 25 | ASP | CB-CG-OD1 | -11.35 | 108.08 | 118.30 |
| 1 | A | 223 | ASP | CB-CG-OD1 | -11.23 | 108.19 | 118.30 |
| 1 | H | 109 | ARG | NE-CZ-NH1 | 11.20 | 125.90 | 120.30 |
| 1 | N | 113 | LEU | CB-CG-CD2 | -11.15 | 92.04 | 111.00 |
| 1 | O | 365 | ARG | NE-CZ-NH2 | -11.12 | 114.74 | 120.30 |
| 1 | B | 30 | ARG | NE-CZ-NH2 | -11.10 | 114.75 | 120.30 |
| 1 | A | 197 | ASP | CB-CG-OD2 | 11.05 | 128.24 | 118.30 |
| 1 | J | 41 | ARG | NE-CZ-NH1 | 11.04 | 125.82 | 120.30 |
| 1 | F | 144 | ARG | NE-CZ-NH2 | 11.02 | 125.81 | 120.30 |
| 1 | K | 97 | ARG | NE-CZ-NH1 | 11.02 | 125.81 | 120.30 |
| 1 | N | 365 | ARG | NE-CZ-NH1 | 10.99 | 125.80 | 120.30 |
| 1 | E | 252 | ARG | NE-CZ-NH2 | -10.96 | 114.82 | 120.30 |
| 1 | M | 25 | ASP | CB-CG-OD2 | -10.93 | 108.46 | 118.30 |
| 1 | I | 213 | LEU | CB-CG-CD1 | -10.90 | 92.47 | 111.00 |
| 1 | K | 74 | ARG | NE-CZ-NH2 | -10.89 | 114.85 | 120.30 |
| 1 | A | 41 | ARG | NE-CZ-NH2 | -10.87 | 114.86 | 120.30 |
| 1 | N | 128 | ASP | CB-CG-OD1 | -10.87 | 108.52 | 118.30 |
| 1 | M | 126 | LEU | CB-CG-CD2 | 10.86 | 129.47 | 111.00 |
| 1 | A | 184 | ASP | CB-CG-OD2 | 10.85 | 128.06 | 118.30 |
| 1 | C | 371 | ASP | CB-CG-OD1 | 10.83 | 128.05 | 118.30 |
| 1 | C | 68 | LEU | CA-CB-CG | -10.82 | 90.41 | 115.30 |
| 1 | C | 150 | ASP | CB-CG-OD2 | 10.82 | 128.03 | 118.30 |
| 1 | J | 197 | ASP | CB-CG-OD2 | 10.78 | 128.00 | 118.30 |
| 1 | J | 365 | ARG | NE-CZ-NH2 | -10.74 | 114.93 | 120.30 |
| 1 | G | 286 | LEU | CB-CG-CD2 | -10.74 | 92.74 | 111.00 |
| 1 | J | 147 | ILE | CG1-CB-CG2 | -10.72 | 87.81 | 111.40 |
| 1 | O | 127 | ASP | CB-CG-OD2 | 10.72 | 127.95 | 118.30 |
| 1 | M | 338 | ARG | NE-CZ-NH2 | -10.70 | 114.95 | 120.30 |
| 1 | J | 97 | ARG | NH1-CZ-NH2 | -10.68 | 107.65 | 119.40 |
| 1 | C | 274 | ASP | CB-CG-OD1 | -10.66 | 108.70 | 118.30 |
| 1 | N | 30 | ARG | NE-CZ-NH2 | -10.63 | 114.98 | 120.30 |
| 1 | E | 144 | ARG | NE-CZ-NH1 | 10.62 | 125.61 | 120.30 |
| 1 | B | 223 | ASP | CB-CG-OD2 | 10.58 | 127.82 | 118.30 |
| 1 | C | 258 | ARG | NE-CZ-NH2 | -10.52 | 115.04 | 120.30 |
| 1 | L | 338 | ARG | NE-CZ-NH2 | 10.51 | 125.56 | 120.30 |
| 1 | C | 30 | ARG | NE-CZ-NH2 | -10.51 | 115.05 | 120.30 |
| 1 | M | 147 | ILE | CG1-CB-CG2 | -10.51 | 88.28 | 111.40 |
| 1 | D | 97 | ARG | NE-CZ-NH1 | 10.48 | 125.54 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 255 | MET | CG-SD-CE | 10.46 | 116.94 | 100.20 |
| 1 | K | 273 | ASP | CB-CG-OD1 | -10.41 | 108.93 | 118.30 |
| 1 | J | 365 | ARG | NE-CZ-NH1 | 10.37 | 125.49 | 120.30 |
| 1 | L | 159 | ILE | CG1-CB-CG2 | -10.37 | 88.58 | 111.40 |
| 1 | J | 113 | LEU | CB-CG-CD2 | -10.35 | 93.41 | 111.00 |
| 1 | D | 297 | GLY | N-CA-C | -10.31 | 87.33 | 113.10 |
| 1 | F | 97 | ARG | NE-CZ-NH1 | 10.27 | 125.43 | 120.30 |
| 1 | N | 68 | LEU | CA-CB-CG | -10.23 | 91.78 | 115.30 |
| 1 | O | 335 | ASP | CB-CG-OD2 | 10.21 | 127.49 | 118.30 |
| 1 | C | 255 | MET | CG-SD-CE | 10.19 | 116.50 | 100.20 |
| 1 | I | 208 | MET | CG-SD-CE | 10.18 | 116.49 | 100.20 |
| 1 | O | 222 | LEU | CB-CG-CD2 | -10.15 | 93.75 | 111.00 |
| 1 | O | 263 | ARG | NE-CZ-NH1 | 10.10 | 125.35 | 120.30 |
| 1 | F | 379 | CYS | CA-CB-SG | -10.10 | 95.83 | 114.00 |
| 1 | N | 335 | ASP | CB-CG-OD1 | -10.08 | 109.23 | 118.30 |
| 1 | K | 464 | LEU | CB-CG-CD1 | -10.07 | 93.87 | 111.00 |
| 1 | L | 122 | LEU | CB-CG-CD2 | -10.07 | 93.87 | 111.00 |
| 1 | K | 188 | LEU | CB-CG-CD2 | -10.05 | 93.91 | 111.00 |
| 1 | M | 41 | ARG | NE-CZ-NH1 | 10.05 | 125.33 | 120.30 |
| 1 | L | 208 | MET | CG-SD-CE | 10.04 | 116.27 | 100.20 |
| 1 | H | 464 | LEU | CB-CG-CD2 | 10.02 | 128.04 | 111.00 |
| 1 | A | 202 | ASP | CB-CG-OD1 | -10.01 | 109.29 | 118.30 |
| 1 | B | 144 | ARG | NE-CZ-NH1 | 10.00 | 125.30 | 120.30 |
| 1 | H | 74 | ARG | NE-CZ-NH1 | 10.00 | 125.30 | 120.30 |
| 1 | E | 365 | ARG | NE-CZ-NH2 | -9.98 | 115.31 | 120.30 |
| 1 | L | 365 | ARG | NE-CZ-NH2 | -9.96 | 115.32 | 120.30 |
| 1 | M | 75 | ILE | CG1-CB-CG2 | -9.95 | 89.52 | 111.40 |
| 1 | H | 470 | LEU | CB-CG-CD1 | -9.94 | 94.10 | 111.00 |
| 1 | J | 252 | ARG | NE-CZ-NH1 | 9.94 | 125.27 | 120.30 |
| 1 | D | 258 | ARG | NE-CZ-NH2 | -9.91 | 115.34 | 120.30 |
| 1 | G | 199 | ASP | CB-CG-OD2 | 9.91 | 127.22 | 118.30 |
| 1 | M | 68 | LEU | CA-CB-CG | -9.87 | 92.60 | 115.30 |
| 1 | L | 228 | ILE | CG1-CB-CG2 | -9.87 | 89.70 | 111.40 |
| 1 | A | 112 | PRO | N-CD-CG | -9.83 | 88.45 | 103.20 |
| 1 | H | 303 | ASP | CB-CG-OD1 | -9.83 | 109.45 | 118.30 |
| 1 | D | 197 | ASP | CB-CG-OD1 | 9.82 | 127.14 | 118.30 |
| 1 | F | 109 | ARG | NE-CZ-NH2 | -9.82 | 115.39 | 120.30 |
| 1 | L | 71 | ARG | NE-CZ-NH1 | -9.81 | 115.39 | 120.30 |
| 1 | M | 144 | ARG | NE-CZ-NH2 | -9.81 | 115.40 | 120.30 |
| 1 | L | 372 | LEU | CA-CB-CG | -9.76 | 92.86 | 115.30 |
| 1 | I | 388 | MET | CG-SD-CE | 9.75 | 115.80 | 100.20 |
| 1 | G | 209 | ASP | CB-CG-OD2 | 9.74 | 127.06 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | I | 255 | MET | CG-SD-CE | 9.73 | 115.77 | 100.20 |
| 1 | E | 109 | ARG | NE-CZ-NH2 | 9.72 | 125.16 | 120.30 |
| 1 | G | 331 | VAL | CA-CB-CG2 | -9.72 | 96.32 | 110.90 |
| 1 | C | 109 | ARG | NE-CZ-NH2 | 9.71 | 125.16 | 120.30 |
| 1 | G | 97 | ARG | NE-CZ-NH2 | -9.70 | 115.45 | 120.30 |
| 1 | N | 469 | LEU | CA-CB-CG | 9.67 | 137.54 | 115.30 |
| 1 | A | 297 | GLY | N-CA-C | -9.59 | 89.13 | 113.10 |
| 1 | G | 467 | LYS | CD-CE-NZ | 9.57 | 133.72 | 111.70 |
| 1 | I | 184 | ASP | CB-CG-OD2 | -9.55 | 109.70 | 118.30 |
| 1 | A | 441 | LEU | CB-CG-CD1 | -9.55 | 94.77 | 111.00 |
| 1 | H | 252 | ARG | NE-CZ-NH2 | -9.54 | 115.53 | 120.30 |
| 1 | L | 356 | LYS | CD-CE-NZ | -9.53 | 89.77 | 111.70 |
| 1 | D | 128 | ASP | CB-CG-OD2 | 9.53 | 126.88 | 118.30 |
| 1 | I | 142 | ASP | CB-CG-OD1 | 9.51 | 126.86 | 118.30 |
| 1 | A | 30 | ARG | NE-CZ-NH2 | -9.48 | 115.56 | 120.30 |
| 1 | M | 369 | GLU | OE1-CD-OE2 | 9.47 | 134.66 | 123.30 |
| 1 | D | 71 | ARG | NE-CZ-NH2 | -9.46 | 115.57 | 120.30 |
| 1 | N | 199 | ASP | CB-CG-OD2 | 9.46 | 126.81 | 118.30 |
| 1 | B | 286 | LEU | CB-CG-CD2 | -9.42 | 94.99 | 111.00 |
| 1 | B | 464 | LEU | CB-CG-CD1 | 9.42 | 127.02 | 111.00 |
| 1 | K | 335 | ASP | CB-CG-OD1 | -9.41 | 109.83 | 118.30 |
| 1 | A | 71 | ARG | NE-CZ-NH1 | -9.41 | 115.59 | 120.30 |
| 1 | K | 127 | ASP | CB-CG-OD2 | -9.39 | 109.85 | 118.30 |
| 1 | N | 159 | ILE | CG1-CB-CG2 | -9.39 | 90.75 | 111.40 |
| 1 | C | 286 | LEU | CB-CG-CD2 | -9.38 | 95.06 | 111.00 |
| 1 | J | 126 | LEU | CB-CG-CD1 | -9.38 | 95.06 | 111.00 |
| 1 | E | 469 | LEU | CA-CB-CG | 9.31 | 136.71 | 115.30 |
| 1 | L | 43 | LEU | CB-CG-CD2 | -9.29 | 95.20 | 111.00 |
| 1 | L | 209 | ASP | CB-CG-OD2 | 9.28 | 126.65 | 118.30 |
| 1 | L | 365 | ARG | NE-CZ-NH1 | 9.23 | 124.92 | 120.30 |
| 1 | D | 401 | ASP | CB-CG-OD1 | 9.22 | 126.59 | 118.30 |
| 1 | B | 144 | ARG | NE-CZ-NH2 | -9.21 | 115.69 | 120.30 |
| 1 | G | 260 | LEU | CB-CG-CD1 | -9.21 | 95.34 | 111.00 |
| 1 | D | 282 | SER | N-CA-CB | -9.20 | 96.70 | 110.50 |
| 1 | G | 365 | ARG | NE-CZ-NH2 | -9.20 | 115.70 | 120.30 |
| 1 | B | 400 | GLU | OE1-CD-OE2 | -9.19 | 112.27 | 123.30 |
| 1 | B | 71 | ARG | NE-CZ-NH1 | -9.19 | 115.70 | 120.30 |
| 1 | I | 74 | ARG | NE-CZ-NH1 | -9.19 | 115.70 | 120.30 |
| 1 | G | 202 | ASP | CB-CG-OD1 | -9.19 | 110.03 | 118.30 |
| 1 | E | 260 | LEU | CB-CG-CD2 | -9.14 | 95.47 | 111.00 |
| 1 | C | 113 | LEU | CB-CG-CD2 | -9.14 | 95.47 | 111.00 |
| 1 | C | 224 | ILE | CG1-CB-CG2 | -9.13 | 91.31 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 175 | CYS | CA-CB-SG | -9.08 | 97.66 | 114.00 |
| 1 | M | 113 | LEU | CB-CG-CD1 | -9.07 | 95.59 | 111.00 |
| 1 | N | 123 | LEU | CB-CG-CD2 | 9.06 | 126.40 | 111.00 |
| 1 | O | 144 | ARG | NE-CZ-NH2 | -9.05 | 115.77 | 120.30 |
| 1 | O | 42 | LEU | CB-CG-CD1 | -9.04 | 95.63 | 111.00 |
| 1 | N | 274 | ASP | CB-CG-OD2 | -9.02 | 110.18 | 118.30 |
| 1 | D | 77 | LEU | CB-CG-CD2 | -9.00 | 95.70 | 111.00 |
| 1 | O | 167 | GLU | OE1-CD-OE2 | 8.99 | 134.08 | 123.30 |
| 1 | D | 181 | GLN | N-CA-C | -8.97 | 86.78 | 111.00 |
| 1 | E | 255 | MET | CG-SD-CE | 8.95 | 114.52 | 100.20 |
| 1 | J | 62 | VAL | CG1-CB-CG2 | -8.93 | 96.61 | 110.90 |
| 1 | H | 297 | GLY | N-CA-C | -8.91 | 90.83 | 113.10 |
| 1 | K | 25 | ASP | CB-CG-OD2 | 8.91 | 126.32 | 118.30 |
| 1 | L | 144 | ARG | NH1-CZ-NH2 | 8.89 | 129.18 | 119.40 |
| 1 | B | 230 | LYS | CD-CE-NZ | -8.88 | 91.28 | 111.70 |
| 1 | H | 209 | ASP | CB-CG-OD2 | 8.88 | 126.29 | 118.30 |
| 1 | N | 128 | ASP | CB-CG-OD2 | 8.88 | 126.29 | 118.30 |
| 1 | H | 61 | LEU | CB-CG-CD1 | 8.87 | 126.07 | 111.00 |
| 1 | G | 332 | THR | CA-CB-CG2 | -8.86 | 99.99 | 112.40 |
| 1 | F | 159 | ILE | CG1-CB-CG2 | -8.84 | 91.95 | 111.40 |
| 1 | M | 202 | ASP | CB-CG-OD1 | -8.84 | 110.35 | 118.30 |
| 1 | B | 159 | ILE | CG1-CB-CG2 | -8.83 | 91.97 | 111.40 |
| 1 | K | 258 | ARG | NE-CZ-NH2 | 8.83 | 124.71 | 120.30 |
| 1 | C | 202 | ASP | CB-CG-OD2 | -8.80 | 110.38 | 118.30 |
| 1 | M | 68 | LEU | CB-CG-CD2 | 8.79 | 125.94 | 111.00 |
| 1 | M | 460 | ASP | CB-CG-OD1 | -8.77 | 110.41 | 118.30 |
| 1 | A | 313 | LEU | CB-CG-CD1 | 8.75 | 125.88 | 111.00 |
| 1 | K | 252 | ARG | NE-CZ-NH2 | -8.74 | 115.93 | 120.30 |
| 1 | K | 123 | LEU | CB-CG-CD1 | -8.73 | 96.15 | 111.00 |
| 1 | N | 71 | ARG | NE-CZ-NH1 | 8.73 | 124.67 | 120.30 |
| 1 | L | 372 | LEU | CB-CG-CD1 | 8.73 | 125.84 | 111.00 |
| 1 | N | 144 | ARG | NE-CZ-NH2 | 8.73 | 124.67 | 120.30 |
| 1 | O | 190 | LEU | CB-CG-CD1 | 8.71 | 125.81 | 111.00 |
| 1 | B | 442 | LYS | CD-CE-NZ | 8.69 | 131.70 | 111.70 |
| 1 | B | 202 | ASP | N-CA-C | -8.68 | 87.56 | 111.00 |
| 1 | B | 263 | ARG | NE-CZ-NH2 | -8.68 | 115.96 | 120.30 |
| 1 | L | 68 | LEU | CB-CG-CD1 | -8.68 | 96.24 | 111.00 |
| 1 | L | 364 | LEU | CB-CG-CD1 | 8.68 | 125.76 | 111.00 |
| 1 | I | 338 | ARG | NE-CZ-NH1 | 8.68 | 124.64 | 120.30 |
| 1 | H | 178 | VAL | CG1-CB-CG2 | 8.68 | 124.78 | 110.90 |
| 1 | L | 25 | ASP | CB-CG-OD1 | -8.67 | 110.50 | 118.30 |
| 1 | H | 277 | ILE | CG1-CB-CG2 | -8.67 | 92.33 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 226 | THR | CA-CB-CG2 | -8.66 | 100.27 | 112.40 |
| 1 | O | 398 | ILE | CG1-CB-CG2 | -8.66 | 92.35 | 111.40 |
| 1 | F | 107 | VAL | CA-CB-CG1 | -8.62 | 97.97 | 110.90 |
| 1 | D | 249 | TYR | CD1-CE1-CZ | 8.60 | 127.54 | 119.80 |
| 1 | G | 286 | LEU | CB-CG-CD1 | 8.59 | 125.60 | 111.00 |
| 1 | G | 383 | LEU | CB-CG-CD1 | 8.58 | 125.59 | 111.00 |
| 1 | C | 188 | LEU | CB-CG-CD2 | -8.58 | 96.42 | 111.00 |
| 1 | N | 202 | ASP | CB-CG-OD1 | -8.58 | 110.58 | 118.30 |
| 1 | L | 252 | ARG | NE-CZ-NH2 | 8.58 | 124.59 | 120.30 |
| 1 | I | 190 | LEU | CB-CG-CD1 | 8.56 | 125.56 | 111.00 |
| 1 | F | 344 | LEU | CB-CG-CD2 | 8.55 | 125.54 | 111.00 |
| 1 | O | 333 | VAL | CA-CB-CG2 | -8.56 | 98.07 | 110.90 |
| 1 | A | 162 | LYS | CD-CE-NZ | -8.55 | 92.03 | 111.70 |
| 1 | E | 458 | ASP | CB-CG-OD2 | -8.55 | 110.60 | 118.30 |
| 1 | F | 233 | ASP | CB-CG-OD2 | -8.53 | 110.62 | 118.30 |
| 1 | D | 156 | LEU | CB-CG-CD2 | -8.52 | 96.51 | 111.00 |
| 1 | J | 202 | ASP | CB-CG-OD1 | -8.52 | 110.63 | 118.30 |
| 1 | M | 52 | ILE | CG1-CB-CG2 | -8.52 | 92.65 | 111.40 |
| 1 | D | 365 | ARG | NE-CZ-NH2 | -8.50 | 116.05 | 120.30 |
| 1 | C | 278 | LYS | CD-CE-NZ | -8.49 | 92.16 | 111.70 |
| 1 | D | 315 | ARG | NE-CZ-NH1 | -8.48 | 116.06 | 120.30 |
| 1 | C | 237 | MET | CG-SD-CE | 8.47 | 113.76 | 100.20 |
| 1 | L | 41 | ARG | NE-CZ-NH2 | 8.45 | 124.53 | 120.30 |
| 1 | H | 371 | ASP | CB-CG-OD1 | 8.45 | 125.90 | 118.30 |
| 1 | M | 458 | ASP | CB-CG-OD1 | -8.43 | 110.71 | 118.30 |
| 1 | F | 109 | ARG | NE-CZ-NH1 | 8.43 | 124.51 | 120.30 |
| 1 | L | 33 | ILE | CG1-CB-CG2 | -8.43 | 92.86 | 111.40 |
| 1 | I | 209 | ASP | CB-CG-OD1 | 8.42 | 125.88 | 118.30 |
| 1 | C | 201 | VAL | CB-CA-C | -8.41 | 95.42 | 111.40 |
| 1 | B | 49 | TYR | CD1-CE1-CZ | 8.39 | 127.36 | 119.80 |
| 1 | O | 199 | ASP | CB-CG-OD1 | -8.39 | 110.75 | 118.30 |
| 1 | C | 338 | ARG | NE-CZ-NH2 | -8.38 | 116.11 | 120.30 |
| 1 | A | 335 | ASP | CB-CG-OD1 | -8.37 | 110.77 | 118.30 |
| 1 | O | 109 | ARG | NH1-CZ-NH2 | -8.37 | 110.20 | 119.40 |
| 1 | C | 233 | ASP | CB-CG-OD2 | 8.36 | 125.82 | 118.30 |
| 1 | C | 277 | ILE | CG1-CB-CG2 | -8.36 | 93.01 | 111.40 |
| 1 | J | 79 | ASP | CB-CG-OD2 | 8.36 | 125.82 | 118.30 |
| 1 | M | 464 | LEU | CB-CG-CD1 | 8.35 | 125.20 | 111.00 |
| 1 | G | 452 | LYS | CD-CE-NZ | 8.34 | 130.89 | 111.70 |
| 1 | N | 464 | LEU | CB-CG-CD1 | 8.34 | 125.18 | 111.00 |
| 1 | M | 113 | LEU | CB-CG-CD2 | -8.34 | 96.82 | 111.00 |
| 1 | H | 74 | ARG | NE-CZ-NH2 | -8.34 | 116.13 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | K | 365 | ARG | NE-CZ-NH1 | -8.34 | 116.13 | 120.30 |
| 1 | N | 378 | LEU | CB-CG-CD2 | -8.33 | 96.84 | 111.00 |
| 1 | M | 263 | ARG | CG-CD-NE | -8.31 | 94.36 | 111.80 |
| 1 | F | 256 | PHE | CB-CG-CD2 | 8.30 | 126.61 | 120.80 |
| 1 | D | 263 | ARG | NE-CZ-NH1 | 8.29 | 124.45 | 120.30 |
| 1 | J | 257 | VAL | CA-CB-CG2 | -8.29 | 98.46 | 110.90 |
| 1 | K | 460 | ASP | CB-CG-OD1 | 8.29 | 125.76 | 118.30 |
| 1 | B | 364 | LEU | CB-CG-CD2 | 8.29 | 125.09 | 111.00 |
| 1 | I | 217 | LYS | CD-CE-NZ | -8.29 | 92.64 | 111.70 |
| 1 | F | 74 | ARG | NE-CZ-NH2 | -8.28 | 116.16 | 120.30 |
| 1 | H | 222 | LEU | CB-CG-CD1 | -8.28 | 96.93 | 111.00 |
| 1 | G | 338 | ARG | NE-CZ-NH2 | 8.28 | 124.44 | 120.30 |
| 1 | I | 441 | LEU | CB-CG-CD1 | -8.27 | 96.94 | 111.00 |
| 1 | D | 379 | CYS | CA-CB-SG | -8.27 | 99.12 | 114.00 |
| 1 | G | 41 | ARG | NE-CZ-NH2 | 8.27 | 124.43 | 120.30 |
| 1 | G | 273 | ASP | CB-CG-OD1 | -8.26 | 110.87 | 118.30 |
| 1 | N | 60 | ILE | CG1-CB-CG2 | -8.26 | 93.23 | 111.40 |
| 1 | B | 208 | MET | CG-SD-CE | 8.25 | 113.40 | 100.20 |
| 1 | E | 274 | ASP | CB-CG-OD1 | -8.22 | 110.90 | 118.30 |
| 1 | G | 273 | ASP | CB-CG-OD2 | 8.22 | 125.70 | 118.30 |
| 1 | C | 79 | ASP | CB-CG-OD2 | 8.21 | 125.69 | 118.30 |
| 1 | K | 113 | LEU | CB-CG-CD2 | 8.21 | 124.96 | 111.00 |
| 1 | O | 365 | ARG | NE-CZ-NH1 | 8.21 | 124.41 | 120.30 |
| 1 | C | 178 | VAL | CG1-CB-CG2 | 8.21 | 124.03 | 110.90 |
| 1 | K | 97 | ARG | NE-CZ-NH2 | -8.21 | 116.20 | 120.30 |
| 1 | G | 74 | ARG | NE-CZ-NH1 | -8.20 | 116.20 | 120.30 |
| 1 | D | 141 | VAL | CA-CB-CG1 | -8.20 | 98.61 | 110.90 |
| 1 | C | 441 | LEU | CB-CG-CD1 | -8.18 | 97.09 | 111.00 |
| 1 | F | 213 | LEU | CB-CG-CD1 | -8.18 | 97.09 | 111.00 |
| 1 | M | 79 | ASP | CB-CG-OD2 | 8.18 | 125.66 | 118.30 |
| 1 | B | 111 | GLN | N-CA-CB | -8.18 | 95.88 | 110.60 |
| 1 | E | 43 | LEU | CB-CG-CD1 | 8.17 | 124.89 | 111.00 |
| 1 | K | 371 | ASP | CB-CG-OD2 | 8.16 | 125.65 | 118.30 |
| 1 | J | 77 | LEU | CB-CG-CD2 | -8.16 | 97.12 | 111.00 |
| 1 | N | 379 | CYS | CA-CB-SG | -8.15 | 99.32 | 114.00 |
| 1 | F | 458 | ASP | CB-CG-OD2 | -8.15 | 110.96 | 118.30 |
| 1 | M | 448 | GLU | OE1-CD-OE2 | -8.15 | 113.52 | 123.30 |
| 1 | F | 117 | ILE | CG1-CB-CG2 | 8.14 | 129.32 | 111.40 |
| 1 | M | 364 | LEU | CB-CG-CD2 | -8.14 | 97.16 | 111.00 |
| 1 | I | 144 | ARG | NE-CZ-NH2 | -8.13 | 116.23 | 120.30 |
| 1 | C | 234 | TYR | CB-CG-CD1 | -8.12 | 116.13 | 121.00 |
| 1 | A | 315 | ARG | NE-CZ-NH2 | -8.12 | 116.24 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | I | 68 | LEU | CA-CB-CG | -8.11 | 96.64 | 115.30 |
| 1 | K | 251 | ARG | NE-CZ-NH1 | -8.11 | 116.25 | 120.30 |
| 1 | A | 199 | ASP | CB-CG-OD1 | -8.10 | 111.01 | 118.30 |
| 1 | C | 111 | GLN | N-CA-CB | -8.10 | 96.03 | 110.60 |
| 1 | D | 391 | ILE | CG1-CB-CG2 | -8.10 | 93.59 | 111.40 |
| 1 | N | 389 | THR | CA-CB-CG2 | -8.10 | 101.07 | 112.40 |
| 1 | A | 365 | ARG | NE-CZ-NH1 | -8.09 | 116.25 | 120.30 |
| 1 | M | 441 | LEU | CB-CG-CD1 | -8.09 | 97.25 | 111.00 |
| 1 | N | 149 | MET | CA-CB-CG | -8.08 | 99.57 | 113.30 |
| 1 | C | 113 | LEU | CB-CG-CD1 | -8.06 | 97.30 | 111.00 |
| 1 | N | 460 | ASP | CB-CG-OD1 | 8.05 | 125.55 | 118.30 |
| 1 | F | 258 | ARG | NE-CZ-NH1 | 8.04 | 124.32 | 120.30 |
| 1 | K | 275 | LEU | CB-CG-CD1 | -8.04 | 97.34 | 111.00 |
| 1 | J | 181 | GLN | N-CA-C | -8.03 | 89.31 | 111.00 |
| 1 | O | 386 | ASP | CB-CG-OD1 | -8.03 | 111.07 | 118.30 |
| 1 | G | 107 | VAL | CG1-CB-CG2 | 8.03 | 123.75 | 110.90 |
| 1 | C | 184 | ASP | CB-CG-OD1 | -8.03 | 111.08 | 118.30 |
| 1 | G | 178 | VAL | CG1-CB-CG2 | 8.03 | 123.74 | 110.90 |
| 1 | L | 332 | THR | CA-CB-CG2 | -8.01 | 101.18 | 112.40 |
| 1 | L | 72 | VAL | CB-CA-C | -8.01 | 96.18 | 111.40 |
| 1 | C | 75 | ILE | CA-CB-CG2 | -8.00 | 94.91 | 110.90 |
| 1 | K | 79 | ASP | CB-CG-OD2 | -7.99 | 111.11 | 118.30 |
| 1 | B | 49 | TYR | CG-CD1-CE1 | -7.98 | 114.91 | 121.30 |
| 1 | H | 344 | LEU | CB-CG-CD2 | 7.98 | 124.57 | 111.00 |
| 1 | H | 61 | LEU | CB-CG-CD2 | -7.98 | 97.44 | 111.00 |
| 1 | C | 238 | VAL | CG1-CB-CG2 | -7.97 | 98.14 | 110.90 |
| 1 | J | 94 | ASP | CB-CG-OD1 | 7.96 | 125.46 | 118.30 |
| 1 | G | 252 | ARG | NE-CZ-NH2 | -7.95 | 116.33 | 120.30 |
| 1 | D | 331 | VAL | CA-CB-CG1 | -7.95 | 98.98 | 110.90 |
| 1 | A | 201 | VAL | CB-CA-C | -7.94 | 96.31 | 111.40 |
| 1 | A | 472 | LEU | CB-CG-CD2 | 7.92 | 124.47 | 111.00 |
| 1 | C | 332 | THR | CA-CB-CG2 | -7.92 | 101.31 | 112.40 |
| 1 | K | 115 | VAL | CG1-CB-CG2 | -7.91 | 98.25 | 110.90 |
| 1 | F | 71 | ARG | NE-CZ-NH2 | 7.90 | 124.25 | 120.30 |
| 1 | J | 96 | GLN | O-C-N | -7.90 | 110.06 | 122.70 |
| 1 | J | 128 | ASP | CB-CG-OD2 | 7.90 | 125.41 | 118.30 |
| 1 | I | 361 | LYS | CD-CE-NZ | -7.89 | 93.54 | 111.70 |
| 1 | O | 98 | LEU | CB-CG-CD2 | -7.89 | 97.58 | 111.00 |
| 1 | F | 68 | LEU | CB-CG-CD2 | -7.89 | 97.59 | 111.00 |
| 1 | N | 258 | ARG | NE-CZ-NH2 | -7.88 | 116.36 | 120.30 |
| 1 | E | 217 | LYS | CD-CE-NZ | -7.88 | 93.57 | 111.70 |
| 1 | H | 177 | GLN | CA-CB-CG | -7.88 | 96.06 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | M | 188 | LEU | CB-CG-CD2 | -7.88 | 97.60 | 111.00 |
| 1 | E | 260 | LEU | CB-CG-CD1 | -7.88 | 97.61 | 111.00 |
| 1 | E | 334 | VAL | CG1-CB-CG2 | -7.88 | 98.30 | 110.90 |
| 1 | I | 190 | LEU | CB-CG-CD2 | -7.88 | 97.61 | 111.00 |
| 1 | G | 222 | LEU | CB-CG-CD2 | -7.87 | 97.62 | 111.00 |
| 1 | H | 30 | ARG | NE-CZ-NH1 | -7.87 | 116.37 | 120.30 |
| 1 | C | 43 | LEU | CB-CG-CD2 | 7.87 | 124.37 | 111.00 |
| 1 | K | 105 | VAL | CA-CB-CG1 | -7.87 | 99.10 | 110.90 |
| 1 | E | 30 | ARG | NE-CZ-NH2 | -7.86 | 116.37 | 120.30 |
| 1 | H | 258 | ARG | NE-CZ-NH2 | 7.85 | 124.22 | 120.30 |
| 1 | K | 464 | LEU | CB-CG-CD2 | 7.85 | 124.34 | 111.00 |
| 1 | L | 28 | VAL | CB-CA-C | -7.84 | 96.50 | 111.40 |
| 1 | L | 222 | LEU | CB-CG-CD2 | -7.84 | 97.67 | 111.00 |
| 1 | O | 258 | ARG | NE-CZ-NH1 | -7.84 | 116.38 | 120.30 |
| 1 | A | 97 | ARG | NE-CZ-NH2 | -7.83 | 116.38 | 120.30 |
| 1 | M | 231 | TYR | CB-CG-CD2 | -7.83 | 116.30 | 121.00 |
| 1 | N | 263 | ARG | NE-CZ-NH1 | 7.83 | 124.21 | 120.30 |
| 1 | A | 171 | LYS | CD-CE-NZ | -7.83 | 93.70 | 111.70 |
| 1 | K | 338 | ARG | NE-CZ-NH1 | -7.82 | 116.39 | 120.30 |
| 1 | G | 74 | ARG | NE-CZ-NH2 | 7.82 | 124.21 | 120.30 |
| 1 | D | 470 | LEU | CB-CG-CD1 | -7.81 | 97.72 | 111.00 |
| 1 | L | 105 | VAL | CG1-CB-CG2 | -7.81 | 98.41 | 110.90 |
| 1 | D | 150 | ASP | CB-CG-OD1 | -7.81 | 111.28 | 118.30 |
| 1 | J | 294 | THR | CA-CB-CG2 | -7.80 | 101.47 | 112.40 |
| 1 | A | 263 | ARG | NE-CZ-NH1 | 7.80 | 124.20 | 120.30 |
| 1 | H | 70 | TYR | CG-CD2-CE2 | 7.80 | 127.54 | 121.30 |
| 1 | L | 39 | THR | OG1-CB-CG2 | -7.80 | 92.06 | 110.00 |
| 1 | E | 263 | ARG | NE-CZ-NH1 | 7.79 | 124.20 | 120.30 |
| 1 | A | 401 | ASP | CB-CG-OD2 | -7.79 | 111.29 | 118.30 |
| 1 | D | 30 | ARG | NE-CZ-NH1 | -7.79 | 116.40 | 120.30 |
| 1 | D | 103 | VAL | CA-CB-CG1 | -7.79 | 99.22 | 110.90 |
| 1 | E | 54 | LYS | CD-CE-NZ | 7.78 | 129.60 | 111.70 |
| 1 | L | 201 | VAL | CB-CA-C | -7.78 | 96.62 | 111.40 |
| 1 | B | 469 | LEU | CB-CG-CD1 | -7.78 | 97.78 | 111.00 |
| 1 | J | 74 | ARG | NE-CZ-NH1 | 7.77 | 124.19 | 120.30 |
| 1 | E | 472 | LEU | CB-CG-CD2 | 7.76 | 124.19 | 111.00 |
| 1 | K | 251 | ARG | NE-CZ-NH2 | 7.75 | 124.18 | 120.30 |
| 1 | M | 74 | ARG | NE-CZ-NH2 | 7.75 | 124.18 | 120.30 |
| 1 | N | 115 | VAL | CA-CB-CG1 | -7.75 | 99.27 | 110.90 |
| 1 | J | 229 | CYS | CA-CB-SG | -7.75 | 100.05 | 114.00 |
| 1 | I | 151 | TYR | CD1-CE1-CZ | -7.75 | 112.83 | 119.80 |
| 1 | O | 240 | GLU | CG-CD-OE2 | -7.74 | 102.83 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | J | 79 | ASP | CB-CG-OD1 | -7.74 | 111.34 | 118.30 |
| 1 | O | 146 | CYS | CA-CB-SG | -7.73 | 100.08 | 114.00 |
| 1 | A | 79 | ASP | CB-CG-OD2 | 7.73 | 125.25 | 118.30 |
| 1 | N | 142 | ASP | CB-CG-OD1 | 7.70 | 125.23 | 118.30 |
| 1 | L | 188 | LEU | CB-CG-CD2 | -7.69 | 97.93 | 111.00 |
| 1 | D | 60 | ILE | CG1-CB-CG2 | -7.68 | 94.51 | 111.40 |
| 1 | N | 297 | GLY | N-CA-C | -7.67 | 93.92 | 113.10 |
| 1 | C | 65 | VAL | CG1-CB-CG2 | -7.67 | 98.63 | 110.90 |
| 1 | K | 65 | VAL | CG1-CB-CG2 | -7.67 | 98.64 | 110.90 |
| 1 | K | 277 | ILE | CG1-CB-CG2 | -7.66 | 94.54 | 111.40 |
| 1 | D | 246 | LEU | CB-CG-CD1 | -7.66 | 97.98 | 111.00 |
| 1 | A | 21 | VAL | CB-CA-C | -7.66 | 96.85 | 111.40 |
| 1 | M | 331 | VAL | CA-CB-CG2 | -7.64 | 99.44 | 110.90 |
| 1 | C | 372 | LEU | CB-CG-CD2 | -7.64 | 98.02 | 111.00 |
| 1 | I | 113 | LEU | CB-CG-CD2 | -7.63 | 98.03 | 111.00 |
| 1 | A | 348 | ILE | CG1-CB-CG2 | -7.62 | 94.62 | 111.40 |
| 1 | D | 178 | VAL | CG1-CB-CG2 | 7.62 | 123.09 | 110.90 |
| 1 | K | 130 | GLU | OE1-CD-OE2 | 7.62 | 132.44 | 123.30 |
| 1 | G | 286 | LEU | CA-CB-CG | -7.62 | 97.77 | 115.30 |
| 1 | J | 300 | VAL | CA-CB-CG2 | -7.62 | 99.47 | 110.90 |
| 1 | E | 87 | ASP | CB-CG-OD2 | -7.62 | 111.44 | 118.30 |
| 1 | O | 260 | LEU | CB-CG-CD1 | -7.62 | 98.05 | 111.00 |
| 1 | F | 209 | ASP | CB-CG-OD1 | -7.61 | 111.45 | 118.30 |
| 1 | J | 329 | LEU | CB-CG-CD2 | -7.61 | 98.07 | 111.00 |
| 1 | J | 369 | GLU | OE1-CD-OE2 | 7.60 | 132.42 | 123.30 |
| 1 | K | 60 | ILE | CG1-CB-CG2 | -7.60 | 94.68 | 111.40 |
| 1 | O | 286 | LEU | CB-CG-CD2 | -7.59 | 98.09 | 111.00 |
| 1 | H | 274 | ASP | CB-CG-OD1 | -7.59 | 111.47 | 118.30 |
| 1 | N | 233 | ASP | CB-CG-OD1 | 7.59 | 125.13 | 118.30 |
| 1 | E | 34 | TYR | CG-CD1-CE1 | 7.59 | 127.37 | 121.30 |
| 1 | A | 52 | ILE | CG1-CB-CG2 | -7.59 | 94.71 | 111.40 |
| 1 | K | 472 | LEU | CA-CB-CG | 7.58 | 132.75 | 115.30 |
| 1 | F | 42 | LEU | CB-CG-CD2 | -7.58 | 98.11 | 111.00 |
| 1 | C | 97 | ARG | NE-CZ-NH2 | -7.57 | 116.52 | 120.30 |
| 1 | C | 275 | LEU | CB-CG-CD2 | 7.57 | 123.87 | 111.00 |
| 1 | M | 401 | ASP | CB-CG-OD1 | -7.55 | 111.50 | 118.30 |
| 1 | K | 128 | ASP | CB-CG-OD2 | 7.54 | 125.09 | 118.30 |
| 1 | H | 209 | ASP | CB-CG-OD1 | -7.54 | 111.52 | 118.30 |
| 1 | I | 25 | ASP | CB-CG-OD2 | -7.53 | 111.52 | 118.30 |
| 1 | L | 127 | ASP | CB-CG-OD1 | 7.53 | 125.08 | 118.30 |
| 1 | N | 109 | ARG | NE-CZ-NH1 | 7.53 | 124.06 | 120.30 |
| 1 | G | 105 | VAL | CA-CB-CG1 | -7.52 | 99.61 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | O | 41 | ARG | NE-CZ-NH1 | 7.52 | 124.06 | 120.30 |
| 1 | A | 264 | ALA | N-CA-CB | -7.51 | 99.58 | 110.10 |
| 1 | I | 231 | TYR | CD1-CE1-CZ | -7.51 | 113.04 | 119.80 |
| 1 | D | 70 | TYR | CB-CG-CD1 | 7.51 | 125.51 | 121.00 |
| 1 | D | 212 | THR | CA-CB-CG2 | -7.51 | 101.89 | 112.40 |
| 1 | F | 234 | TYR | CZ-CE2-CD2 | -7.51 | 113.04 | 119.80 |
| 1 | H | 294 | THR | CA-CB-CG2 | -7.50 | 101.89 | 112.40 |
| 1 | D | 123 | LEU | CB-CG-CD2 | 7.50 | 123.75 | 111.00 |
| 1 | F | 334 | VAL | CA-CB-CG1 | -7.50 | 99.65 | 110.90 |
| 1 | N | 26 | GLU | OE1-CD-OE2 | -7.49 | 114.31 | 123.30 |
| 1 | O | 230 | LYS | CD-CE-NZ | -7.49 | 94.48 | 111.70 |
| 1 | A | 106 | GLU | OE1-CD-OE2 | -7.48 | 114.32 | 123.30 |
| 1 | E | 383 | LEU | CB-CG-CD2 | -7.48 | 98.28 | 111.00 |
| 1 | A | 250 | LEU | CB-CG-CD2 | 7.48 | 123.72 | 111.00 |
| 1 | N | 77 | LEU | CB-CG-CD2 | -7.48 | 98.29 | 111.00 |
| 1 | B | 460 | ASP | CB-CG-OD1 | 7.47 | 125.03 | 118.30 |
| 1 | J | 251 | ARG | NH1-CZ-NH2 | -7.46 | 111.19 | 119.40 |
| 1 | G | 272 | PRO | N-CD-CG | -7.46 | 92.00 | 103.20 |
| 1 | D | 160 | GLY | CA-C-O | 7.45 | 134.01 | 120.60 |
| 1 | K | 364 | LEU | CB-CG-CD2 | -7.45 | 98.34 | 111.00 |
| 1 | M | 252 | ARG | NH1-CZ-NH2 | 7.45 | 127.59 | 119.40 |
| 1 | G | 274 | ASP | CB-CG-OD2 | 7.44 | 125.00 | 118.30 |
| 1 | E | 439 | ASP | CB-CG-OD2 | -7.44 | 111.61 | 118.30 |
| 1 | N | 256 | PHE | CB-CG-CD2 | 7.43 | 126.00 | 120.80 |
| 1 | L | 79 | ASP | CB-CG-OD1 | 7.43 | 124.98 | 118.30 |
| 1 | C | 286 | LEU | CB-CG-CD1 | 7.42 | 123.61 | 111.00 |
| 1 | K | 31 | THR | CA-CB-CG2 | -7.42 | 102.02 | 112.40 |
| 1 | L | 113 | LEU | CA-CB-CG | -7.42 | 98.24 | 115.30 |
| 1 | M | 213 | LEU | CB-CG-CD1 | -7.42 | 98.39 | 111.00 |
| 1 | K | 237 | MET | CG-SD-CE | 7.41 | 112.06 | 100.20 |
| 1 | H | 41 | ARG | NE-CZ-NH1 | -7.41 | 116.59 | 120.30 |
| 1 | D | 73 | PHE | CB-CG-CD1 | -7.41 | 115.62 | 120.80 |
| 1 | M | 365 | ARG | NE-CZ-NH2 | -7.40 | 116.60 | 120.30 |
| 1 | N | 25 | ASP | CB-CG-OD2 | 7.39 | 124.96 | 118.30 |
| 1 | E | 257 | VAL | CG1-CB-CG2 | 7.39 | 122.73 | 110.90 |
| 1 | H | 202 | ASP | CB-CG-OD1 | -7.38 | 111.65 | 118.30 |
| 1 | N | 399 | LEU | CA-CB-CG | -7.38 | 98.32 | 115.30 |
| 1 | I | 306 | ILE | CG1-CB-CG2 | -7.38 | 95.17 | 111.40 |
| 1 | J | 68 | LEU | CA-CB-CG | -7.37 | 98.34 | 115.30 |
| 1 | G | 97 | ARG | NE-CZ-NH1 | 7.37 | 123.98 | 120.30 |
| 1 | N | 25 | ASP | CB-CG-OD1 | -7.37 | 111.67 | 118.30 |
| 1 | E | 188 | LEU | CB-CG-CD2 | -7.37 | 98.48 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | I | 181 | GLN | N-CA-C | -7.37 | 91.11 | 111.00 |
| 1 | H | 338 | ARG | NE-CZ-NH1 | -7.36 | 116.62 | 120.30 |
| 1 | F | 25 | ASP | CB-CG-OD2 | -7.35 | 111.68 | 118.30 |
| 1 | F | 180 | VAL | CB-CA-C | -7.35 | 97.43 | 111.40 |
| 1 | N | 371 | ASP | CB-CG-OD2 | 7.35 | 124.92 | 118.30 |
| 1 | F | 202 | ASP | CB-CG-OD2 | -7.35 | 111.69 | 118.30 |
| 1 | N | 372 | LEU | CB-CG-CD2 | -7.34 | 98.52 | 111.00 |
| 1 | B | 97 | ARG | NE-CZ-NH1 | 7.34 | 123.97 | 120.30 |
| 1 | K | 244 | ASP | CB-CG-OD2 | -7.34 | 111.70 | 118.30 |
| 1 | J | 470 | LEU | CB-CG-CD1 | -7.34 | 98.53 | 111.00 |
| 1 | J | 95 | THR | OG1-CB-CG2 | 7.33 | 126.87 | 110.00 |
| 1 | A | 112 | PRO | CA-CB-CG | -7.33 | 90.07 | 104.00 |
| 1 | B | 251 | ARG | NE-CZ-NH1 | -7.33 | 116.63 | 120.30 |
| 1 | D | 292 | PHE | N-CA-CB | -7.33 | 97.41 | 110.60 |
| 1 | A | 326 | GLY | N-CA-C | -7.32 | 94.80 | 113.10 |
| 1 | M | 201 | VAL | CB-CA-C | -7.32 | 97.49 | 111.40 |
| 1 | G | 114 | GLY | CA-C-O | -7.32 | 107.43 | 120.60 |
| 1 | K | 315 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 |
| 1 | H | 159 | ILE | CG1-CB-CG2 | -7.32 | 95.31 | 111.40 |
| 1 | B | 123 | LEU | CB-CG-CD2 | 7.31 | 123.43 | 111.00 |
| 1 | M | 142 | ASP | CB-CG-OD1 | -7.31 | 111.72 | 118.30 |
| 1 | D | 260 | LEU | CB-CG-CD2 | -7.30 | 98.58 | 111.00 |
| 1 | F | 49 | TYR | CB-CG-CD1 | -7.30 | 116.62 | 121.00 |
| 1 | N | 28 | VAL | CG1-CB-CG2 | 7.30 | 122.58 | 110.90 |
| 1 | M | 209 | ASP | CB-CG-OD1 | -7.30 | 111.73 | 118.30 |
| 1 | K | 123 | LEU | CA-CB-CG | 7.29 | 132.06 | 115.30 |
| 1 | I | 251 | ARG | NE-CZ-NH2 | 7.28 | 123.94 | 120.30 |
| 1 | E | 472 | LEU | CB-CG-CD1 | -7.28 | 98.63 | 111.00 |
| 1 | C | 244 | ASP | CB-CG-OD1 | 7.27 | 124.84 | 118.30 |
| 1 | L | 340 | THR | CA-CB-CG2 | -7.26 | 102.23 | 112.40 |
| 1 | F | 467 | LYS | CD-CE-NZ | 7.26 | 128.41 | 111.70 |
| 1 | C | 209 | ASP | CB-CG-OD1 | -7.26 | 111.77 | 118.30 |
| 1 | O | 63 | PRO | N-CD-CG | -7.24 | 92.35 | 103.20 |
| 1 | J | 297 | GLY | N-CA-C | -7.21 | 95.08 | 113.10 |
| 1 | M | 276 | TYR | CZ-CE2-CD2 | 7.21 | 126.29 | 119.80 |
| 1 | I | 338 | ARG | NE-CZ-NH2 | -7.21 | 116.70 | 120.30 |
| 1 | L | 251 | ARG | NE-CZ-NH1 | 7.21 | 123.90 | 120.30 |
| 1 | I | 472 | LEU | CB-CG-CD1 | -7.20 | 98.76 | 111.00 |
| 1 | J | 370 | TYR | CB-CG-CD1 | 7.20 | 125.32 | 121.00 |
| 1 | L | 230 | LYS | CA-CB-CG | -7.20 | 97.57 | 113.40 |
| 1 | D | 136 | ALA | CB-CA-C | -7.19 | 99.32 | 110.10 |
| 1 | C | 269 | GLU | OE1-CD-OE2 | -7.18 | 114.68 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 365 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 1 | H | 293 | PRO | CA-N-CD | -7.17 | 101.46 | 111.50 |
| 1 | E | 246 | LEU | CB-CG-CD2 | -7.17 | 98.81 | 111.00 |
| 1 | G | 250 | LEU | CB-CG-CD1 | -7.17 | 98.81 | 111.00 |
| 1 | I | 365 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 1 | A | 64 | LYS | CD-CE-NZ | -7.17 | 95.22 | 111.70 |
| 1 | B | 222 | LEU | CB-CG-CD2 | 7.14 | 123.14 | 111.00 |
| 1 | B | 79 | ASP | CB-CG-OD2 | -7.14 | 111.88 | 118.30 |
| 1 | J | 52 | ILE | CG1-CB-CG2 | -7.13 | 95.71 | 111.40 |
| 1 | F | 364 | LEU | CB-CG-CD1 | -7.13 | 98.88 | 111.00 |
| 1 | K | 192 | ASN | N-CA-C | -7.12 | 91.77 | 111.00 |
| 1 | L | 206 | GLY | N-CA-C | -7.12 | 95.31 | 113.10 |
| 1 | B | 233 | ASP | CB-CG-OD2 | 7.10 | 124.69 | 118.30 |
| 1 | I | 291 | TYR | CB-CG-CD1 | 7.10 | 125.26 | 121.00 |
| 1 | N | 182 | PRO | CA-CB-CG | -7.10 | 90.51 | 104.00 |
| 1 | C | 194 | VAL | CG1-CB-CG2 | 7.10 | 122.26 | 110.90 |
| 1 | F | 294 | THR | CA-CB-CG2 | -7.10 | 102.46 | 112.40 |
| 1 | O | 332 | THR | CA-CB-CG2 | -7.09 | 102.47 | 112.40 |
| 1 | H | 275 | LEU | CB-CG-CD1 | -7.09 | 98.95 | 111.00 |
| 1 | J | 223 | ASP | CB-CG-OD1 | -7.09 | 111.92 | 118.30 |
| 1 | C | 159 | ILE | CG1-CB-CG2 | -7.08 | 95.81 | 111.40 |
| 1 | M | 383 | LEU | CB-CG-CD1 | 7.08 | 123.04 | 111.00 |
| 1 | F | 125 | LYS | CD-CE-NZ | -7.08 | 95.42 | 111.70 |
| 1 | H | 244 | ASP | CB-CG-OD1 | 7.07 | 124.67 | 118.30 |
| 1 | J | 275 | LEU | CB-CG-CD2 | 7.07 | 123.02 | 111.00 |
| 1 | K | 24 | THR | CA-CB-CG2 | -7.07 | 102.50 | 112.40 |
| 1 | J | 291 | TYR | CZ-CE2-CD2 | 7.07 | 126.16 | 119.80 |
| 1 | K | 463 | PRO | N-CD-CG | -7.06 | 92.61 | 103.20 |
| 1 | B | 383 | LEU | CB-CG-CD1 | 7.05 | 122.99 | 111.00 |
| 1 | L | 460 | ASP | CB-CG-OD1 | 7.05 | 124.65 | 118.30 |
| 1 | B | 162 | LYS | CD-CE-NZ | 7.05 | 127.91 | 111.70 |
| 1 | H | 289 | SER | N-CA-CB | -7.04 | 99.94 | 110.50 |
| 1 | K | 331 | VAL | CA-CB-CG2 | -7.04 | 100.34 | 110.90 |
| 1 | N | 362 | GLU | OE1-CD-OE2 | -7.04 | 114.86 | 123.30 |
| 1 | B | 355 | TYR | CG-CD1-CE1 | 7.03 | 126.92 | 121.30 |
| 1 | I | 174 | PRO | N-CA-C | 7.03 | 130.37 | 112.10 |
| 1 | J | 180 | VAL | CB-CA-C | -7.02 | 98.05 | 111.40 |
| 1 | L | 109 | ARG | NH1-CZ-NH2 | -7.02 | 111.67 | 119.40 |
| 1 | C | 128 | ASP | CB-CG-OD2 | -7.02 | 111.98 | 118.30 |
| 1 | F | 464 | LEU | CB-CG-CD2 | 7.02 | 122.93 | 111.00 |
| 1 | A | 194 | VAL | CB-CA-C | -7.01 | 98.08 | 111.40 |
| 1 | J | 260 | LEU | CB-CG-CD1 | -7.01 | 99.09 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | M | 25 | ASP | CB-CG-OD1 | 7.01 | 124.61 | 118.30 |
| 1 | M | 472 | LEU | CA-CB-CG | 7.00 | 131.41 | 115.30 |
| 1 | G | 274 | ASP | CB-CG-OD1 | -7.00 | 112.00 | 118.30 |
| 1 | H | 231 | TYR | CD1-CE1-CZ | -7.00 | 113.50 | 119.80 |
| 1 | L | 376 | PHE | CB-CG-CD1 | -6.99 | 115.91 | 120.80 |
| 1 | A | 244 | ASP | CB-CG-OD1 | 6.98 | 124.59 | 118.30 |
| 1 | B | 107 | VAL | CG1-CB-CG2 | -6.98 | 99.73 | 110.90 |
| 1 | N | 335 | ASP | CB-CG-OD2 | 6.98 | 124.58 | 118.30 |
| 1 | N | 64 | LYS | CD-CE-NZ | 6.98 | 127.75 | 111.70 |
| 1 | B | 97 | ARG | NE-CZ-NH2 | -6.98 | 116.81 | 120.30 |
| 1 | D | 335 | ASP | CB-CG-OD2 | 6.97 | 124.58 | 118.30 |
| 1 | G | 106 | GLU | OE1-CD-OE2 | -6.97 | 114.94 | 123.30 |
| 1 | N | 459 | LEU | CB-CG-CD1 | -6.97 | 99.16 | 111.00 |
| 1 | M | 42 | LEU | CB-CG-CD1 | -6.96 | 99.17 | 111.00 |
| 1 | K | 79 | ASP | CB-CG-OD1 | 6.95 | 124.56 | 118.30 |
| 1 | N | 292 | PHE | CB-CG-CD2 | -6.95 | 115.93 | 120.80 |
| 1 | O | 460 | ASP | CB-CG-OD1 | 6.95 | 124.56 | 118.30 |
| 1 | A | 266 | THR | CB-CA-C | -6.95 | 92.84 | 111.60 |
| 1 | G | 336 | THR | CA-CB-CG2 | -6.95 | 102.67 | 112.40 |
| 1 | C | 142 | ASP | CB-CG-OD2 | 6.95 | 124.55 | 118.30 |
| 1 | D | 144 | ARG | CG-CD-NE | -6.95 | 97.21 | 111.80 |
| 1 | E | 263 | ARG | NE-CZ-NH2 | 6.95 | 123.77 | 120.30 |
| 1 | L | 269 | GLU | N-CA-CB | -6.94 | 98.10 | 110.60 |
| 1 | B | 263 | ARG | NE-CZ-NH1 | 6.94 | 123.77 | 120.30 |
| 1 | A | 235 | ILE | CB-CA-C | -6.94 | 97.72 | 111.60 |
| 1 | J | 381 | ILE | CG1-CB-CG2 | 6.93 | 126.65 | 111.40 |
| 1 | E | 34 | TYR | CD1-CE1-CZ | -6.93 | 113.56 | 119.80 |
| 1 | H | 123 | LEU | CB-CG-CD1 | -6.93 | 99.22 | 111.00 |
| 1 | M | 72 | VAL | CG1-CB-CG2 | 6.92 | 121.98 | 110.90 |
| 1 | M | 299 | MET | CB-CG-SD | -6.92 | 91.65 | 112.40 |
| 1 | C | 181 | GLN | N-CA-C | -6.91 | 92.33 | 111.00 |
| 1 | F | 260 | LEU | CB-CG-CD2 | -6.91 | 99.25 | 111.00 |
| 1 | M | 332 | THR | CA-CB-CG2 | -6.91 | 102.73 | 112.40 |
| 1 | D | 223 | ASP | CB-CG-OD2 | -6.91 | 112.08 | 118.30 |
| 1 | K | 74 | ARG | NE-CZ-NH1 | 6.91 | 123.75 | 120.30 |
| 1 | I | 71 | ARG | NE-CZ-NH1 | 6.90 | 123.75 | 120.30 |
| 1 | H | 454 | LYS | CD-CE-NZ | 6.89 | 127.54 | 111.70 |
| 1 | N | 87 | ASP | C-N-CA | -6.89 | 104.48 | 121.70 |
| 1 | M | 90 | PHE | CB-CG-CD2 | -6.88 | 115.98 | 120.80 |
| 1 | J | 123 | LEU | CB-CG-CD1 | -6.88 | 99.31 | 111.00 |
| 1 | D | 160 | GLY | O-C-N | -6.87 | 111.70 | 122.70 |
| 1 | I | 344 | LEU | CB-CG-CD2 | 6.87 | 122.67 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | J | 377 | GLN | CA-CB-CG | 6.87 | 128.51 | 113.40 |
| 1 | B | 315 | ARG | NE-CZ-NH1 | 6.87 | 123.73 | 120.30 |
| 1 | F | 41 | ARG | NE-CZ-NH2 | 6.86 | 123.73 | 120.30 |
| 1 | H | 156 | LEU | CB-CG-CD1 | 6.86 | 122.66 | 111.00 |
| 1 | H | 391 | ILE | CA-CB-CG1 | -6.86 | 97.97 | 111.00 |
| 1 | I | 178 | VAL | CG1-CB-CG2 | -6.86 | 99.93 | 110.90 |
| 1 | J | 95 | THR | N-CA-C | 6.85 | 129.50 | 111.00 |
| 1 | E | 468 | PHE | CG-CD1-CE1 | 6.85 | 128.33 | 120.80 |
| 1 | M | 257 | VAL | CA-CB-CG2 | -6.85 | 100.63 | 110.90 |
| 1 | I | 197 | ASP | CB-CG-OD2 | -6.84 | 112.14 | 118.30 |
| 1 | H | 269 | GLU | OE1-CD-OE2 | -6.84 | 115.09 | 123.30 |
| 1 | B | 182 | PRO | CA-CB-CG | -6.84 | 91.00 | 104.00 |
| 1 | E | 252 | ARG | NH1-CZ-NH2 | 6.84 | 126.92 | 119.40 |
| 1 | H | 158 | LEU | CB-CG-CD2 | -6.84 | 99.38 | 111.00 |
| 1 | D | 235 | ILE | CB-CA-C | -6.83 | 97.93 | 111.60 |
| 1 | L | 230 | LYS | CD-CE-NZ | -6.83 | 95.99 | 111.70 |
| 1 | B | 214 | GLN | CA-CB-CG | -6.82 | 98.39 | 113.40 |
| 1 | J | 175 | CYS | CA-CB-SG | -6.82 | 101.72 | 114.00 |
| 1 | N | 165 | ILE | CA-CB-CG1 | -6.81 | 98.06 | 111.00 |
| 1 | I | 77 | LEU | CA-CB-CG | -6.81 | 99.64 | 115.30 |
| 1 | L | 195 | ILE | CG1-CB-CG2 | 6.81 | 126.38 | 111.40 |
| 1 | I | 466 | ARG | NE-CZ-NH2 | -6.80 | 116.90 | 120.30 |
| 1 | A | 449 | VAL | CG1-CB-CG2 | -6.80 | 100.02 | 110.90 |
| 1 | H | 201 | VAL | CB-CA-C | -6.80 | 98.47 | 111.40 |
| 1 | E | 98 | LEU | CB-CG-CD2 | -6.80 | 99.44 | 111.00 |
| 1 | L | 334 | VAL | CG1-CB-CG2 | -6.79 | 100.03 | 110.90 |
| 1 | M | 165 | ILE | CG1-CB-CG2 | -6.79 | 96.47 | 111.40 |
| 1 | D | 386 | ASP | CB-CG-OD2 | 6.78 | 124.40 | 118.30 |
| 1 | C | 126 | LEU | CA-CB-CG | -6.78 | 99.72 | 115.30 |
| 1 | F | 220 | VAL | CA-CB-CG1 | -6.78 | 100.74 | 110.90 |
| 1 | L | 22 | VAL | CB-CA-C | -6.77 | 98.53 | 111.40 |
| 1 | M | 49 | TYR | CB-CG-CD2 | 6.77 | 125.06 | 121.00 |
| 1 | D | 468 | PHE | CG-CD1-CE1 | 6.77 | 128.25 | 120.80 |
| 1 | H | 260 | LEU | CB-CG-CD1 | -6.77 | 99.49 | 111.00 |
| 1 | G | 159 | ILE | CG1-CB-CG2 | -6.77 | 96.51 | 111.40 |
| 1 | N | 201 | VAL | CA-CB-CG1 | -6.77 | 100.75 | 110.90 |
| 1 | G | 335 | ASP | CB-CG-OD2 | -6.77 | 112.21 | 118.30 |
| 1 | E | 150 | ASP | CB-CG-OD1 | -6.76 | 112.22 | 118.30 |
| 1 | D | 128 | ASP | CB-CG-OD1 | -6.75 | 112.22 | 118.30 |
| 1 | G | 180 | VAL | CB-CA-C | -6.75 | 98.57 | 111.40 |
| 1 | E | 335 | ASP | CB-CG-OD1 | -6.75 | 112.22 | 118.30 |
| 1 | O | 156 | LEU | CB-CG-CD1 | 6.75 | 122.48 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | M | 329 | LEU | CA-CB-CG | -6.75 | 99.78 | 115.30 |
| 1 | D | 277 | ILE | CG1-CB-CG2 | -6.75 | 96.56 | 111.40 |
| 1 | I | 74 | ARG | NE-CZ-NH2 | 6.74 | 123.67 | 120.30 |
| 1 | E | 263 | ARG | NH1-CZ-NH2 | -6.74 | 111.99 | 119.40 |
| 1 | O | 162 | LYS | CD-CE-NZ | 6.74 | 127.20 | 111.70 |
| 1 | F | 94 | ASP | CB-CG-OD1 | -6.73 | 112.25 | 118.30 |
| 1 | M | 281 | GLY | N-CA-C | -6.73 | 96.28 | 113.10 |
| 1 | A | 26 | GLU | OE1-CD-OE2 | -6.72 | 115.23 | 123.30 |
| 1 | D | 469 | LEU | CB-CG-CD2 | -6.72 | 99.58 | 111.00 |
| 1 | M | 363 | TYR | N-CA-CB | -6.72 | 98.50 | 110.60 |
| 1 | I | 237 | MET | CG-SD-CE | -6.72 | 89.45 | 100.20 |
| 1 | D | 438 | GLU | OE1-CD-OE2 | 6.71 | 131.36 | 123.30 |
| 1 | E | 300 | VAL | CA-CB-CG2 | -6.71 | 100.83 | 110.90 |
| 1 | G | 156 | LEU | CB-CG-CD2 | -6.71 | 99.59 | 111.00 |
| 1 | A | 181 | GLN | N-CA-C | -6.71 | 92.89 | 111.00 |
| 1 | I | 451 | LEU | CB-CG-CD2 | -6.71 | 99.60 | 111.00 |
| 1 | I | 390 | TYR | CB-CG-CD2 | -6.71 | 116.98 | 121.00 |
| 1 | H | 401 | ASP | CB-CG-OD2 | -6.70 | 112.27 | 118.30 |
| 1 | D | 66 | SER | C-N-CA | -6.70 | 108.24 | 122.30 |
| 1 | I | 112 | PRO | N-CD-CG | -6.70 | 93.16 | 103.20 |
| 1 | L | 247 | PHE | CG-CD1-CE1 | -6.69 | 113.44 | 120.80 |
| 1 | A | 390 | TYR | CB-CG-CD2 | -6.69 | 116.98 | 121.00 |
| 1 | D | 122 | LEU | CB-CG-CD1 | 6.69 | 122.38 | 111.00 |
| 1 | O | 322 | GLY | N-CA-C | -6.69 | 96.37 | 113.10 |
| 1 | A | 286 | LEU | CB-CG-CD1 | 6.69 | 122.38 | 111.00 |
| 1 | H | 212 | THR | CA-CB-CG2 | -6.69 | 103.03 | 112.40 |
| 1 | J | 195 | ILE | CG1-CB-CG2 | 6.68 | 126.10 | 111.40 |
| 1 | I | 105 | VAL | CA-CB-CG1 | -6.68 | 100.88 | 110.90 |
| 1 | A | 241 | PRO | CA-CB-CG | -6.67 | 91.32 | 104.00 |
| 1 | G | 30 | ARG | NE-CZ-NH2 | -6.67 | 116.96 | 120.30 |
| 1 | N | 199 | ASP | CB-CG-OD1 | -6.67 | 112.30 | 118.30 |
| 1 | H | 144 | ARG | CG-CD-NE | -6.67 | 97.80 | 111.80 |
| 1 | L | 398 | ILE | CB-CG1-CD1 | -6.67 | 95.23 | 113.90 |
| 1 | E | 458 | ASP | CB-CG-OD1 | 6.67 | 124.30 | 118.30 |
| 1 | J | 147 | ILE | CA-CB-CG1 | -6.66 | 98.34 | 111.00 |
| 1 | G | 365 | ARG | NE-CZ-NH1 | 6.66 | 123.63 | 120.30 |
| 1 | C | 374 | PHE | CB-CG-CD1 | 6.65 | 125.45 | 120.80 |
| 1 | M | 87 | ASP | CB-CG-OD1 | -6.64 | 112.32 | 118.30 |
| 1 | F | 390 | TYR | CB-CG-CD2 | -6.64 | 117.01 | 121.00 |
| 1 | N | 127 | ASP | CB-CG-OD2 | -6.64 | 112.32 | 118.30 |
| 1 | G | 371 | ASP | CB-CG-OD2 | -6.63 | 112.33 | 118.30 |
| 1 | F | 242 | TYR | CZ-CE2-CD2 | 6.63 | 125.76 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 49 | TYR | CZ-CE2-CD2 | -6.62 | 113.84 | 119.80 |
| 1 | H | 472 | LEU | CB-CG-CD2 | 6.62 | 122.25 | 111.00 |
| 1 | H | 235 | ILE | CB-CA-C | -6.61 | 98.38 | 111.60 |
| 1 | D | 115 | VAL | CA-CB-CG2 | -6.61 | 100.99 | 110.90 |
| 1 | E | 201 | VAL | CG1-CB-CG2 | -6.61 | 100.33 | 110.90 |
| 1 | L | 315 | ARG | NE-CZ-NH1 | -6.61 | 117.00 | 120.30 |
| 1 | L | 177 | GLN | N-CA-C | -6.60 | 93.18 | 111.00 |
| 1 | M | 42 | LEU | CB-CG-CD2 | 6.60 | 122.22 | 111.00 |
| 1 | M | 234 | TYR | CD1-CE1-CZ | 6.60 | 125.74 | 119.80 |
| 1 | D | 240 | GLU | OE1-CD-OE2 | 6.59 | 131.21 | 123.30 |
| 1 | H | 217 | LYS | CD-CE-NZ | -6.59 | 96.54 | 111.70 |
| 1 | N | 211 | THR | CA-CB-CG2 | -6.59 | 103.17 | 112.40 |
| 1 | E | 202 | ASP | CB-CG-OD2 | 6.59 | 124.23 | 118.30 |
| 1 | D | 75 | ILE | CG1-CB-CG2 | -6.59 | 96.91 | 111.40 |
| 1 | I | 72 | VAL | CA-CB-CG1 | -6.58 | 101.03 | 110.90 |
| 1 | N | 451 | LEU | CB-CG-CD1 | 6.58 | 122.18 | 111.00 |
| 1 | B | 463 | PRO | CA-CB-CG | -6.58 | 91.51 | 104.00 |
| 1 | D | 98 | LEU | CB-CG-CD2 | -6.57 | 99.83 | 111.00 |
| 1 | F | 175 | CYS | CA-CB-SG | -6.57 | 102.17 | 114.00 |
| 1 | F | 383 | LEU | CB-CG-CD2 | 6.57 | 122.17 | 111.00 |
| 1 | A | 71 | ARG | NH1-CZ-NH2 | -6.57 | 112.17 | 119.40 |
| 1 | A | 147 | ILE | CB-CA-C | -6.57 | 98.47 | 111.60 |
| 1 | E | 71 | ARG | NE-CZ-NH2 | -6.56 | 117.02 | 120.30 |
| 1 | C | 362 | GLU | OE1-CD-OE2 | 6.56 | 131.18 | 123.30 |
| 1 | I | 372 | LEU | CB-CG-CD2 | -6.56 | 99.84 | 111.00 |
| 1 | D | 447 | TRP | N-CA-C | -6.56 | 93.29 | 111.00 |
| 1 | A | 269 | GLU | OE1-CD-OE2 | -6.56 | 115.43 | 123.30 |
| 1 | I | 170 | GLY | N-CA-C | -6.55 | 96.71 | 113.10 |
| 1 | G | 313 | LEU | CB-CG-CD1 | 6.55 | 122.14 | 111.00 |
| 1 | K | 313 | LEU | CB-CG-CD1 | 6.55 | 122.14 | 111.00 |
| 1 | F | 123 | LEU | N-CA-CB | -6.55 | 97.30 | 110.40 |
| 1 | I | 173 | SER | C-N-CD | -6.55 | 106.19 | 120.60 |
| 1 | C | 180 | VAL | CB-CA-C | -6.54 | 98.97 | 111.40 |
| 1 | D | 258 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 1 | F | 372 | LEU | CA-CB-CG | -6.54 | 100.25 | 115.30 |
| 1 | J | 452 | LYS | CD-CE-NZ | 6.54 | 126.75 | 111.70 |
| 1 | F | 203 | THR | CA-CB-CG2 | -6.54 | 103.25 | 112.40 |
| 1 | D | 201 | VAL | CG1-CB-CG2 | -6.53 | 100.44 | 110.90 |
| 1 | K | 389 | THR | CA-CB-CG2 | -6.53 | 103.26 | 112.40 |
| 1 | F | 181 | GLN | N-CA-C | -6.53 | 93.37 | 111.00 |
| 1 | N | 274 | ASP | OD1-CG-OD2 | 6.53 | 135.70 | 123.30 |
| 1 | M | 457 | ALA | N-CA-CB | -6.52 | 100.97 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 263 | ARG | NH1-CZ-NH2 | -6.52 | 112.23 | 119.40 |
| 1 | I | 231 | TYR | CG-CD1-CE1 | 6.51 | 126.51 | 121.30 |
| 1 | L | 98 | LEU | CB-CG-CD2 | -6.51 | 99.94 | 111.00 |
| 1 | C | 274 | ASP | CB-CG-OD2 | 6.51 | 124.16 | 118.30 |
| 1 | E | 337 | THR | CA-CB-CG2 | -6.50 | 103.30 | 112.40 |
| 1 | I | 299 | MET | CG-SD-CE | 6.50 | 110.60 | 100.20 |
| 1 | M | 71 | ARG | NH1-CZ-NH2 | -6.50 | 112.25 | 119.40 |
| 1 | J | 230 | LYS | CD-CE-NZ | -6.49 | 96.77 | 111.70 |
| 1 | L | 144 | ARG | NE-CZ-NH1 | -6.49 | 117.06 | 120.30 |
| 1 | F | 297 | GLY | N-CA-C | -6.49 | 96.88 | 113.10 |
| 1 | F | 389 | THR | OG1-CB-CG2 | 6.49 | 124.92 | 110.00 |
| 1 | D | 175 | CYS | N-CA-C | -6.48 | 93.49 | 111.00 |
| 1 | G | 145 | GLU | OE1-CD-OE2 | 6.48 | 131.08 | 123.30 |
| 1 | G | 278 | LYS | CD-CE-NZ | -6.48 | 96.79 | 111.70 |
| 1 | H | 310 | PRO | N-CA-CB | -6.48 | 95.47 | 102.60 |
| 1 | F | 361 | LYS | CD-CE-NZ | -6.48 | 96.80 | 111.70 |
| 1 | G | 388 | MET | CG-SD-CE | 6.48 | 110.56 | 100.20 |
| 1 | N | 386 | ASP | CB-CG-OD2 | 6.48 | 124.13 | 118.30 |
| 1 | G | 72 | VAL | CG1-CB-CG2 | 6.47 | 121.26 | 110.90 |
| 1 | G | 363 | TYR | CG-CD1-CE1 | -6.47 | 116.12 | 121.30 |
| 1 | C | 295 | PRO | N-CD-CG | -6.47 | 93.49 | 103.20 |
| 1 | G | 207 | ALA | N-CA-CB | -6.47 | 101.04 | 110.10 |
| 1 | M | 98 | LEU | CB-CG-CD2 | -6.47 | 100.00 | 111.00 |
| 1 | M | 299 | MET | CG-SD-CE | 6.47 | 110.55 | 100.20 |
| 1 | F | 49 | TYR | CB-CG-CD2 | 6.47 | 124.88 | 121.00 |
| 1 | D | 72 | VAL | CA-CB-CG1 | -6.46 | 101.20 | 110.90 |
| 1 | M | 86 | PRO | C-N-CA | 6.46 | 137.86 | 121.70 |
| 1 | M | 269 | GLU | CG-CD-OE2 | 6.46 | 131.22 | 118.30 |
| 1 | C | 291 | TYR | CB-CG-CD2 | 6.46 | 124.88 | 121.00 |
| 1 | M | 323 | ILE | CG1-CB-CG2 | -6.46 | 97.20 | 111.40 |
| 1 | F | 199 | ASP | CB-CG-OD2 | -6.45 | 112.49 | 118.30 |
| 1 | G | 453 | GLU | OE1-CD-OE2 | -6.45 | 115.56 | 123.30 |
| 1 | H | 466 | ARG | NH1-CZ-NH2 | -6.45 | 112.30 | 119.40 |
| 1 | A | 315 | ARG | NH1-CZ-NH2 | 6.45 | 126.49 | 119.40 |
| 1 | H | 220 | VAL | CG1-CB-CG2 | -6.44 | 100.60 | 110.90 |
| 1 | H | 315 | ARG | NE-CZ-NH1 | -6.44 | 117.08 | 120.30 |
| 1 | L | 194 | VAL | O-C-N | -6.44 | 112.39 | 122.70 |
| 1 | H | 183 | GLY | O-C-N | 6.44 | 133.00 | 122.70 |
| 1 | J | 252 | ARG | NE-CZ-NH2 | -6.43 | 117.08 | 120.30 |
| 1 | J | 442 | LYS | N-CA-C | -6.43 | 93.63 | 111.00 |
| 1 | O | 68 | LEU | CA-CB-CG | -6.43 | 100.51 | 115.30 |
| 1 | G | 181 | GLN | N-CA-C | -6.43 | 93.64 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 277 | ILE | CG1-CB-CG2 | -6.43 | 97.26 | 111.40 |
| 1 | A | 233 | ASP | CB-CG-OD2 | -6.43 | 112.52 | 118.30 |
| 1 | C | 51 | PRO | CB-CG-CD | -6.43 | 81.43 | 106.50 |
| 1 | H | 338 | ARG | N-CA-C | -6.42 | 93.65 | 111.00 |
| 1 | K | 113 | LEU | CA-CB-CG | -6.42 | 100.53 | 115.30 |
| 1 | N | 201 | VAL | CB-CA-C | -6.42 | 99.19 | 111.40 |
| 1 | A | 241 | PRO | N-CD-CG | -6.42 | 93.57 | 103.20 |
| 1 | H | 59 | LYS | CD-CE-NZ | 6.41 | 126.45 | 111.70 |
| 1 | C | 41 | ARG | NE-CZ-NH1 | 6.41 | 123.50 | 120.30 |
| 1 | N | 460 | ASP | CB-CG-OD2 | -6.41 | 112.53 | 118.30 |
| 1 | C | 145 | GLU | OE1-CD-OE2 | 6.41 | 130.99 | 123.30 |
| 1 | L | 299 | MET | CA-CB-CG | 6.41 | 124.19 | 113.30 |
| 1 | L | 323 | ILE | CG1-CB-CG2 | -6.40 | 97.31 | 111.40 |
| 1 | H | 158 | LEU | CA-CB-CG | 6.40 | 130.03 | 115.30 |
| 1 | N | 191 | ILE | CB-CA-C | -6.40 | 98.80 | 111.60 |
| 1 | B | 331 | VAL | CG1-CB-CG2 | 6.40 | 121.14 | 110.90 |
| 1 | E | 177 | GLN | N-CA-C | -6.39 | 93.73 | 111.00 |
| 1 | M | 195 | ILE | N-CA-C | -6.39 | 93.75 | 111.00 |
| 1 | C | 383 | LEU | CB-CG-CD1 | 6.39 | 121.86 | 111.00 |
| 1 | K | 263 | ARG | NE-CZ-NH2 | -6.38 | 117.11 | 120.30 |
| 1 | L | 72 | VAL | CA-CB-CG1 | -6.38 | 101.33 | 110.90 |
| 1 | I | 87 | ASP | CB-CG-OD1 | 6.38 | 124.04 | 118.30 |
| 1 | J | 201 | VAL | CA-CB-CG1 | -6.38 | 101.34 | 110.90 |
| 1 | F | 222 | LEU | CB-CG-CD2 | 6.37 | 121.84 | 111.00 |
| 1 | D | 60 | ILE | CA-CB-CG1 | -6.37 | 98.89 | 111.00 |
| 1 | H | 233 | ASP | CB-CG-OD1 | 6.37 | 124.03 | 118.30 |
| 1 | C | 244 | ASP | CB-CG-OD2 | -6.37 | 112.57 | 118.30 |
| 1 | E | 468 | PHE | CD1-CE1-CZ | -6.37 | 112.46 | 120.10 |
| 1 | G | 439 | ASP | CB-CG-OD2 | 6.37 | 124.03 | 118.30 |
| 1 | B | 272 | PRO | CA-N-CD | 6.36 | 120.61 | 111.70 |
| 1 | L | 260 | LEU | CB-CG-CD1 | -6.36 | 100.19 | 111.00 |
| 1 | H | 99 | VAL | CG1-CB-CG2 | -6.36 | 100.73 | 110.90 |
| 1 | O | 190 | LEU | CB-CG-CD2 | -6.36 | 100.19 | 111.00 |
| 1 | O | 43 | LEU | CB-CG-CD1 | 6.35 | 121.80 | 111.00 |
| 1 | N | 203 | THR | CA-CB-CG2 | -6.35 | 103.51 | 112.40 |
| 1 | E | 368 | GLU | CA-CB-CG | -6.35 | 99.43 | 113.40 |
| 1 | G | 398 | ILE | CG1-CB-CG2 | -6.35 | 97.43 | 111.40 |
| 1 | J | 87 | ASP | CB-CG-OD2 | -6.35 | 112.59 | 118.30 |
| 1 | K | 180 | VAL | CG1-CB-CG2 | 6.34 | 121.05 | 110.90 |
| 1 | H | 298 | SER | N-CA-CB | -6.34 | 100.98 | 110.50 |
| 1 | I | 456 | SER | C-N-CA | -6.34 | 105.84 | 121.70 |
| 1 | L | 144 | ARG | CG-CD-NE | -6.34 | 98.49 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 240 | GLU | OE1-CD-OE2 | 6.34 | 130.90 | 123.30 |
| 1 | I | 275 | LEU | CB-CG-CD1 | 6.33 | 121.76 | 111.00 |
| 1 | C | 443 | LYS | CD-CE-NZ | 6.33 | 126.25 | 111.70 |
| 1 | E | 281 | GLY | N-CA-C | -6.32 | 97.29 | 113.10 |
| 1 | N | 33 | ILE | CG1-CB-CG2 | -6.32 | 97.49 | 111.40 |
| 1 | D | 28 | VAL | CA-CB-CG2 | -6.32 | 101.42 | 110.90 |
| 1 | I | 111 | GLN | CB-CG-CD | -6.32 | 95.17 | 111.60 |
| 1 | A | 306 | ILE | CA-CB-CG1 | -6.31 | 99.00 | 111.00 |
| 1 | D | 298 | SER | N-CA-CB | -6.31 | 101.03 | 110.50 |
| 1 | L | 344 | LEU | CB-CG-CD2 | -6.31 | 100.27 | 111.00 |
| 1 | F | 122 | LEU | CB-CG-CD2 | -6.31 | 100.27 | 111.00 |
| 1 | L | 263 | ARG | NE-CZ-NH1 | 6.30 | 123.45 | 120.30 |
| 1 | G | 199 | ASP | CB-CG-OD1 | -6.30 | 112.63 | 118.30 |
| 1 | C | 302 | SER | N-CA-CB | -6.29 | 101.06 | 110.50 |
| 1 | J | 180 | VAL | CG1-CB-CG2 | 6.29 | 120.97 | 110.90 |
| 1 | L | 213 | LEU | CB-CG-CD1 | -6.29 | 100.30 | 111.00 |
| 1 | O | 197 | ASP | CB-CG-OD1 | -6.29 | 112.64 | 118.30 |
| 1 | A | 299 | MET | CB-CA-C | -6.29 | 97.82 | 110.40 |
| 1 | B | 70 | TYR | CZ-CE2-CD2 | 6.29 | 125.46 | 119.80 |
| 1 | M | 300 | VAL | CA-CB-CG2 | -6.29 | 101.47 | 110.90 |
| 1 | B | 62 | VAL | CB-CA-C | -6.29 | 99.45 | 111.40 |
| 1 | A | 315 | ARG | NE-CZ-NH1 | -6.29 | 117.16 | 120.30 |
| 1 | A | 208 | MET | CG-SD-CE | 6.28 | 110.25 | 100.20 |
| 1 | M | 65 | VAL | CG1-CB-CG2 | -6.28 | 100.85 | 110.90 |
| 1 | D | 70 | TYR | CB-CG-CD2 | -6.28 | 117.23 | 121.00 |
| 1 | M | 184 | ASP | CB-CG-OD1 | -6.28 | 112.65 | 118.30 |
| 1 | A | 178 | VAL | CG1-CB-CG2 | 6.27 | 120.93 | 110.90 |
| 1 | O | 371 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | C | 441 | LEU | CB-CG-CD2 | 6.27 | 121.66 | 111.00 |
| 1 | G | 263 | ARG | CD-NE-CZ | -6.27 | 114.83 | 123.60 |
| 1 | H | 52 | ILE | CG1-CB-CG2 | -6.26 | 97.62 | 111.40 |
| 1 | C | 439 | ASP | CB-CG-OD1 | -6.26 | 112.67 | 118.30 |
| 1 | M | 313 | LEU | CB-CG-CD1 | 6.25 | 121.63 | 111.00 |
| 1 | G | 209 | ASP | CB-CG-OD1 | -6.25 | 112.67 | 118.30 |
| 1 | A | 334 | VAL | CA-CB-CG2 | 6.25 | 120.27 | 110.90 |
| 1 | B | 71 | ARG | NE-CZ-NH2 | 6.25 | 123.42 | 120.30 |
| 1 | N | 331 | VAL | CA-CB-CG2 | -6.24 | 101.54 | 110.90 |
| 1 | N | 399 | LEU | CB-CG-CD1 | -6.24 | 100.39 | 111.00 |
| 1 | L | 54 | LYS | CD-CE-NZ | 6.24 | 126.06 | 111.70 |
| 1 | D | 77 | LEU | CB-CG-CD1 | 6.23 | 121.60 | 111.00 |
| 1 | H | 35 | TYR | CZ-CE2-CD2 | 6.23 | 125.41 | 119.80 |
| 1 | C | 251 | ARG | NE-CZ-NH1 | 6.23 | 123.42 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 126 | LEU | CA-CB-CG | -6.23 | 100.97 | 115.30 |
| 1 | H | 123 | LEU | CB-CG-CD2 | 6.23 | 121.59 | 111.00 |
| 1 | O | 167 | GLU | CG-CD-OE1 | -6.23 | 105.84 | 118.30 |
| 1 | N | 212 | THR | CA-CB-CG2 | -6.23 | 103.68 | 112.40 |
| 1 | J | 372 | LEU | CA-CB-CG | -6.22 | 100.98 | 115.30 |
| 1 | L | 25 | ASP | CB-CG-OD2 | 6.22 | 123.90 | 118.30 |
| 1 | L | 291 | TYR | CG-CD1-CE1 | 6.22 | 126.28 | 121.30 |
| 1 | F | 52 | ILE | CG1-CB-CG2 | -6.22 | 97.72 | 111.40 |
| 1 | L | 123 | LEU | CB-CG-CD2 | -6.21 | 100.44 | 111.00 |
| 1 | C | 260 | LEU | CB-CG-CD1 | -6.21 | 100.44 | 111.00 |
| 1 | C | 249 | TYR | CG-CD1-CE1 | 6.21 | 126.27 | 121.30 |
| 1 | A | 64 | LYS | CB-CA-C | -6.21 | 97.99 | 110.40 |
| 1 | E | 460 | ASP | CB-CG-OD1 | 6.21 | 123.88 | 118.30 |
| 1 | I | 199 | ASP | CB-CG-OD1 | -6.20 | 112.72 | 118.30 |
| 1 | C | 122 | LEU | CB-CG-CD2 | -6.20 | 100.46 | 111.00 |
| 1 | D | 165 | ILE | CA-CB-CG1 | -6.19 | 99.23 | 111.00 |
| 1 | H | 383 | LEU | CB-CG-CD2 | -6.19 | 100.47 | 111.00 |
| 1 | L | 71 | ARG | NH1-CZ-NH2 | 6.19 | 126.21 | 119.40 |
| 1 | N | 282 | SER | N-CA-CB | -6.19 | 101.21 | 110.50 |
| 1 | H | 181 | GLN | N-CA-CB | -6.19 | 99.46 | 110.60 |
| 1 | H | 175 | CYS | N-CA-CB | -6.18 | 99.47 | 110.60 |
| 1 | N | 37 | ALA | C-N-CA | -6.18 | 109.33 | 122.30 |
| 1 | A | 255 | MET | CB-CA-C | -6.18 | 98.05 | 110.40 |
| 1 | F | 180 | VAL | N-CA-C | 6.17 | 127.67 | 111.00 |
| 1 | J | 388 | MET | CG-SD-CE | 6.17 | 110.08 | 100.20 |
| 1 | I | 266 | THR | CA-CB-CG2 | -6.17 | 103.76 | 112.40 |
| 1 | D | 159 | ILE | CA-CB-CG2 | -6.17 | 98.56 | 110.90 |
| 1 | H | 237 | MET | CA-CB-CG | 6.17 | 123.79 | 113.30 |
| 1 | K | 457 | ALA | CB-CA-C | -6.17 | 100.84 | 110.10 |
| 1 | B | 99 | VAL | CA-CB-CG2 | -6.17 | 101.64 | 110.90 |
| 1 | H | 43 | LEU | CB-CG-CD2 | -6.17 | 100.51 | 111.00 |
| 1 | G | 180 | VAL | N-CA-C | 6.17 | 127.65 | 111.00 |
| 1 | H | 365 | ARG | NE-CZ-NH1 | -6.17 | 117.22 | 120.30 |
| 1 | O | 299 | MET | CG-SD-CE | 6.17 | 110.07 | 100.20 |
| 1 | H | 336 | THR | CA-CB-CG2 | -6.16 | 103.78 | 112.40 |
| 1 | G | 90 | PHE | CB-CG-CD2 | -6.15 | 116.49 | 120.80 |
| 1 | G | 315 | ARG | NE-CZ-NH2 | -6.15 | 117.22 | 120.30 |
| 1 | E | 383 | LEU | CB-CG-CD1 | 6.15 | 121.45 | 111.00 |
| 1 | M | 123 | LEU | CB-CG-CD1 | 6.15 | 121.45 | 111.00 |
| 1 | B | 472 | LEU | CA-CB-CG | 6.15 | 129.44 | 115.30 |
| 1 | F | 209 | ASP | CB-CG-OD2 | 6.15 | 123.83 | 118.30 |
| 1 | I | 356 | LYS | CD-CE-NZ | -6.14 | 97.58 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | M | 113 | LEU | CA-CB-CG | 6.14 | 129.43 | 115.30 |
| 1 | B | 142 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | G | 115 | VAL | CB-CA-C | -6.14 | 99.73 | 111.40 |
| 1 | G | 225 | CYS | CA-CB-SG | -6.14 | 102.95 | 114.00 |
| 1 | H | 178 | VAL | CA-CB-CG2 | -6.14 | 101.69 | 110.90 |
| 1 | O | 262 | ASN | N-CA-CB | -6.14 | 99.55 | 110.60 |
| 1 | E | 141 | VAL | CA-CB-CG2 | -6.14 | 101.70 | 110.90 |
| 1 | G | 144 | ARG | NE-CZ-NH1 | -6.14 | 117.23 | 120.30 |
| 1 | L | 234 | TYR | CZ-CE2-CD2 | -6.14 | 114.28 | 119.80 |
| 1 | A | 144 | ARG | CG-CD-NE | -6.13 | 98.92 | 111.80 |
| 1 | B | 128 | ASP | CB-CG-OD1 | 6.13 | 123.82 | 118.30 |
| 1 | B | 68 | LEU | CA-CB-CG | -6.13 | 101.21 | 115.30 |
| 1 | D | 470 | LEU | CB-CG-CD2 | 6.12 | 121.41 | 111.00 |
| 1 | D | 144 | ARG | NE-CZ-NH1 | -6.12 | 117.24 | 120.30 |
| 1 | J | 156 | LEU | CB-CG-CD1 | -6.12 | 100.59 | 111.00 |
| 1 | M | 318 | GLY | N-CA-C | -6.12 | 97.79 | 113.10 |
| 1 | E | 125 | LYS | CD-CE-NZ | -6.12 | 97.62 | 111.70 |
| 1 | F | 72 | VAL | CA-CB-CG1 | -6.12 | 101.72 | 110.90 |
| 1 | B | 34 | TYR | CD1-CE1-CZ | -6.12 | 114.29 | 119.80 |
| 1 | C | 370 | TYR | CZ-CE2-CD2 | -6.12 | 114.30 | 119.80 |
| 1 | N | 54 | LYS | CD-CE-NZ | 6.12 | 125.77 | 111.70 |
| 1 | N | 464 | LEU | CB-CG-CD2 | 6.11 | 121.39 | 111.00 |
| 1 | H | 313 | LEU | CB-CG-CD1 | 6.11 | 121.39 | 111.00 |
| 1 | C | 156 | LEU | CB-CG-CD1 | 6.11 | 121.38 | 111.00 |
| 1 | G | 107 | VAL | CA-CB-CG1 | -6.11 | 101.74 | 110.90 |
| 1 | K | 142 | ASP | CB-CG-OD2 | 6.11 | 123.80 | 118.30 |
| 1 | J | 244 | ASP | CB-CG-OD2 | -6.10 | 112.81 | 118.30 |
| 1 | J | 378 | LEU | CB-CG-CD1 | 6.10 | 121.37 | 111.00 |
| 1 | D | 304 | ALA | N-CA-C | 6.10 | 127.47 | 111.00 |
| 1 | E | 156 | LEU | CB-CG-CD2 | -6.10 | 100.63 | 111.00 |
| 1 | G | 365 | ARG | CB-CG-CD | -6.09 | 95.76 | 111.60 |
| 1 | G | 439 | ASP | CB-CG-OD1 | -6.09 | 112.82 | 118.30 |
| 1 | J | 361 | LYS | O-C-N | -6.09 | 112.96 | 122.70 |
| 1 | M | 269 | GLU | OE1-CD-OE2 | -6.09 | 115.99 | 123.30 |
| 1 | D | 175 | CYS | CA-CB-SG | -6.09 | 103.04 | 114.00 |
| 1 | G | 180 | VAL | CA-C-N | -6.08 | 103.82 | 117.20 |
| 1 | F | 95 | THR | CA-CB-CG2 | -6.08 | 103.89 | 112.40 |
| 1 | D | 188 | LEU | CB-CG-CD1 | -6.08 | 100.67 | 111.00 |
| 1 | I | 172 | GLY | N-CA-C | -6.08 | 97.91 | 113.10 |
| 1 | M | 237 | MET | CG-SD-CE | 6.07 | 109.91 | 100.20 |
| 1 | E | 158 | LEU | CB-CG-CD1 | -6.07 | 100.68 | 111.00 |
| 1 | D | 269 | GLU | OE1-CD-OE2 | -6.06 | 116.02 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | M | 109 | ARG | NE-CZ-NH1 | -6.06 | 117.27 | 120.30 |
| 1 | H | 178 | VAL | CA-C-N | -6.06 | 103.87 | 117.20 |
| 1 | K | 45 | VAL | CA-CB-CG1 | -6.06 | 101.82 | 110.90 |
| 1 | K | 151 | TYR | CZ-CE2-CD2 | -6.05 | 114.35 | 119.80 |
| 1 | B | 386 | ASP | CB-CG-OD2 | 6.05 | 123.75 | 118.30 |
| 1 | F | 97 | ARG | CG-CD-NE | 6.05 | 124.51 | 111.80 |
| 1 | E | 234 | TYR | CZ-CE2-CD2 | -6.05 | 114.35 | 119.80 |
| 1 | F | 128 | ASP | CB-CG-OD2 | 6.05 | 123.74 | 118.30 |
| 1 | I | 194 | VAL | CG1-CB-CG2 | 6.05 | 120.58 | 110.90 |
| 1 | B | 278 | LYS | C-N-CA | -6.04 | 109.61 | 122.30 |
| 1 | G | 335 | ASP | OD1-CG-OD2 | 6.04 | 134.78 | 123.30 |
| 1 | M | 338 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | K | 333 | VAL | CB-CA-C | -6.04 | 99.93 | 111.40 |
| 1 | E | 25 | ASP | CB-CG-OD1 | -6.04 | 112.87 | 118.30 |
| 1 | I | 87 | ASP | CB-CG-OD2 | -6.03 | 112.87 | 118.30 |
| 1 | N | 88 | THR | CB-CA-C | 6.03 | 127.89 | 111.60 |
| 1 | G | 197 | ASP | CB-CG-OD1 | -6.03 | 112.87 | 118.30 |
| 1 | H | 33 | ILE | CG1-CB-CG2 | -6.03 | 98.13 | 111.40 |
| 1 | H | 65 | VAL | CG1-CB-CG2 | -6.03 | 101.25 | 110.90 |
| 1 | E | 122 | LEU | CA-CB-CG | -6.03 | 101.43 | 115.30 |
| 1 | D | 109 | ARG | NE-CZ-NH2 | 6.03 | 123.31 | 120.30 |
| 1 | G | 49 | TYR | CG-CD2-CE2 | -6.02 | 116.48 | 121.30 |
| 1 | B | 291 | TYR | CB-CG-CD2 | 6.02 | 124.61 | 121.00 |
| 1 | A | 209 | ASP | CB-CG-OD1 | -6.02 | 112.88 | 118.30 |
| 1 | F | 234 | TYR | CD1-CE1-CZ | 6.02 | 125.22 | 119.80 |
| 1 | B | 306 | ILE | CG1-CB-CG2 | -6.02 | 98.16 | 111.40 |
| 1 | A | 466 | ARG | NE-CZ-NH1 | 6.01 | 123.31 | 120.30 |
| 1 | L | 67 | GLY | O-C-N | -6.01 | 113.08 | 122.70 |
| 1 | N | 303 | ASP | CB-CG-OD1 | -6.01 | 112.89 | 118.30 |
| 1 | F | 49 | TYR | CD1-CE1-CZ | -6.01 | 114.39 | 119.80 |
| 1 | J | 112 | PRO | N-CD-CG | -6.00 | 94.19 | 103.20 |
| 1 | J | 457 | ALA | N-CA-CB | -6.00 | 101.69 | 110.10 |
| 1 | N | 277 | ILE | CG1-CB-CG2 | -6.00 | 98.19 | 111.40 |
| 1 | A | 258 | ARG | CG-CD-NE | -6.00 | 99.20 | 111.80 |
| 1 | F | 468 | PHE | CG-CD2-CE2 | -6.00 | 114.20 | 120.80 |
| 1 | G | 271 | VAL | CG1-CB-CG2 | 6.00 | 120.50 | 110.90 |
| 1 | D | 371 | ASP | CB-CG-OD2 | 6.00 | 123.70 | 118.30 |
| 1 | B | 292 | PHE | CG-CD2-CE2 | -5.99 | 114.21 | 120.80 |
| 1 | A | 33 | ILE | CB-CA-C | -5.99 | 99.62 | 111.60 |
| 1 | C | 128 | ASP | CB-CG-OD1 | 5.99 | 123.69 | 118.30 |
| 1 | I | 128 | ASP | CB-CG-OD2 | -5.99 | 112.91 | 118.30 |
| 1 | N | 469 | LEU | CB-CG-CD2 | -5.99 | 100.82 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 74 | ARG | NE-CZ-NH1 | -5.99 | 117.31 | 120.30 |
| 1 | D | 141 | VAL | CB-CA-C | -5.99 | 100.03 | 111.40 |
| 1 | E | 329 | LEU | CB-CG-CD1 | -5.99 | 100.82 | 111.00 |
| 1 | A | 64 | LYS | CA-CB-CG | -5.98 | 100.23 | 113.40 |
| 1 | A | 289 | SER | N-CA-CB | -5.98 | 101.52 | 110.50 |
| 1 | I | 206 | GLY | N-CA-C | -5.98 | 98.14 | 113.10 |
| 1 | L | 31 | THR | CB-CA-C | -5.98 | 95.44 | 111.60 |
| 1 | A | 222 | LEU | CB-CG-CD1 | 5.98 | 121.17 | 111.00 |
| 1 | M | 123 | LEU | CB-CG-CD2 | -5.98 | 100.84 | 111.00 |
| 1 | C | 256 | PHE | CB-CG-CD2 | 5.97 | 124.98 | 120.80 |
| 1 | F | 466 | ARG | NE-CZ-NH1 | -5.97 | 117.31 | 120.30 |
| 1 | G | 140 | GLY | CA-C-O | 5.97 | 131.35 | 120.60 |
| 1 | K | 98 | LEU | CA-CB-CG | 5.97 | 129.04 | 115.30 |
| 1 | G | 122 | LEU | CB-CG-CD1 | 5.97 | 121.15 | 111.00 |
| 1 | E | 338 | ARG | NE-CZ-NH1 | 5.97 | 123.28 | 120.30 |
| 1 | J | 144 | ARG | NE-CZ-NH1 | -5.97 | 117.32 | 120.30 |
| 1 | M | 158 | LEU | N-CA-CB | 5.97 | 122.34 | 110.40 |
| 1 | D | 374 | PHE | CB-CG-CD2 | -5.96 | 116.62 | 120.80 |
| 1 | M | 297 | GLY | N-CA-C | -5.96 | 98.19 | 113.10 |
| 1 | B | 266 | THR | CA-CB-CG2 | -5.96 | 104.05 | 112.40 |
| 1 | E | 177 | GLN | CB-CG-CD | 5.96 | 127.10 | 111.60 |
| 1 | K | 231 | TYR | CB-CA-C | -5.96 | 98.48 | 110.40 |
| 1 | E | 141 | VAL | CB-CA-C | -5.95 | 100.09 | 111.40 |
| 1 | E | 336 | THR | N-CA-CB | 5.95 | 121.61 | 110.30 |
| 1 | I | 102 | CYS | CA-CB-SG | -5.95 | 103.30 | 114.00 |
| 1 | F | 323 | ILE | CG1-CB-CG2 | -5.94 | 98.33 | 111.40 |
| 1 | E | 189 | GLU | OE1-CD-OE2 | 5.94 | 130.43 | 123.30 |
| 1 | G | 144 | ARG | CG-CD-NE | -5.94 | 99.33 | 111.80 |
| 1 | D | 306 | ILE | CG1-CB-CG2 | -5.94 | 98.33 | 111.40 |
| 1 | K | 344 | LEU | CB-CG-CD2 | 5.94 | 121.10 | 111.00 |
| 1 | K | 448 | GLU | N-CA-CB | -5.94 | 99.91 | 110.60 |
| 1 | A | 251 | ARG | NE-CZ-NH1 | -5.93 | 117.33 | 120.30 |
| 1 | G | 472 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 1 | I | 274 | ASP | CB-CG-OD2 | -5.93 | 112.96 | 118.30 |
| 1 | K | 297 | GLY | N-CA-C | -5.93 | 98.28 | 113.10 |
| 1 | K | 300 | VAL | CB-CA-C | -5.93 | 100.14 | 111.40 |
| 1 | L | 341 | ASN | N-CA-CB | 5.92 | 121.26 | 110.60 |
| 1 | J | 126 | LEU | CA-CB-CG | -5.92 | 101.68 | 115.30 |
| 1 | N | 205 | PHE | CG-CD1-CE1 | 5.92 | 127.31 | 120.80 |
| 1 | L | 466 | ARG | NE-CZ-NH2 | 5.92 | 123.26 | 120.30 |
| 1 | F | 383 | LEU | CB-CG-CD1 | 5.92 | 121.06 | 111.00 |
| 1 | M | 59 | LYS | CD-CE-NZ | -5.92 | 98.09 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 278 | LYS | C-N-CA | -5.91 | 109.89 | 122.30 |
| 1 | L | 398 | ILE | CG1-CB-CG2 | -5.91 | 98.40 | 111.40 |
| 1 | O | 77 | LEU | CB-CG-CD1 | 5.91 | 121.04 | 111.00 |
| 1 | C | 309 | LYS | CD-CE-NZ | 5.91 | 125.28 | 111.70 |
| 1 | D | 122 | LEU | CB-CG-CD2 | -5.91 | 100.96 | 111.00 |
| 1 | O | 71 | ARG | NE-CZ-NH1 | 5.91 | 123.25 | 120.30 |
| 1 | N | 244 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 1 | N | 157 | CYS | CA-CB-SG | 5.90 | 124.63 | 114.00 |
| 1 | B | 469 | LEU | O-C-N | -5.90 | 113.26 | 122.70 |
| 1 | A | 472 | LEU | N-CA-CB | 5.90 | 122.19 | 110.40 |
| 1 | N | 251 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | D | 62 | VAL | CA-CB-CG1 | -5.89 | 102.06 | 110.90 |
| 1 | D | 154 | THR | CA-CB-CG2 | 5.89 | 120.65 | 112.40 |
| 1 | K | 68 | LEU | CA-CB-CG | -5.89 | 101.74 | 115.30 |
| 1 | M | 112 | PRO | CA-CB-CG | -5.89 | 92.81 | 104.00 |
| 1 | G | 335 | ASP | CB-CG-OD1 | -5.89 | 113.00 | 118.30 |
| 1 | O | 72 | VAL | CG1-CB-CG2 | -5.89 | 101.48 | 110.90 |
| 1 | C | 53 | LYS | CD-CE-NZ | -5.89 | 98.16 | 111.70 |
| 1 | H | 208 | MET | CG-SD-CE | 5.89 | 109.62 | 100.20 |
| 1 | I | 234 | TYR | CG-CD1-CE1 | -5.89 | 116.59 | 121.30 |
| 1 | M | 275 | LEU | CB-CG-CD2 | 5.88 | 121.00 | 111.00 |
| 1 | F | 129 | THR | CA-CB-CG2 | -5.88 | 104.16 | 112.40 |
| 1 | J | 103 | VAL | CB-CA-C | -5.88 | 100.22 | 111.40 |
| 1 | K | 129 | THR | CA-CB-CG2 | -5.88 | 104.17 | 112.40 |
| 1 | A | 25 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | E | 27 | TYR | CG-CD1-CE1 | -5.88 | 116.60 | 121.30 |
| 1 | F | 256 | PHE | CB-CG-CD1 | -5.88 | 116.68 | 120.80 |
| 1 | D | 237 | MET | CB-CG-SD | -5.88 | 94.77 | 112.40 |
| 1 | F | 384 | THR | CB-CA-C | -5.87 | 95.76 | 111.60 |
| 1 | K | 274 | ASP | CB-CG-OD1 | -5.87 | 113.02 | 118.30 |
| 1 | G | 198 | GLY | N-CA-C | 5.86 | 127.76 | 113.10 |
| 1 | L | 247 | PHE | CG-CD2-CE2 | 5.86 | 127.25 | 120.80 |
| 1 | E | 470 | LEU | CB-CG-CD1 | -5.86 | 101.03 | 111.00 |
| 1 | E | 31 | THR | CA-CB-CG2 | -5.86 | 104.20 | 112.40 |
| 1 | C | 226 | THR | CA-CB-CG2 | -5.86 | 104.20 | 112.40 |
| 1 | N | 249 | TYR | CD1-CE1-CZ | 5.85 | 125.07 | 119.80 |
| 1 | A | 334 | VAL | N-CA-C | -5.85 | 95.20 | 111.00 |
| 1 | I | 190 | LEU | CA-CB-CG | -5.85 | 101.84 | 115.30 |
| 1 | K | 294 | THR | CA-CB-CG2 | -5.85 | 104.21 | 112.40 |
| 1 | L | 166 | GLY | N-CA-C | 5.85 | 127.72 | 113.10 |
| 1 | L | 361 | LYS | CD-CE-NZ | -5.85 | 98.25 | 111.70 |
| 1 | B | 439 | ASP | CB-CG-OD1 | -5.85 | 113.04 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | I | 68 | LEU | CB-CG-CD2 | 5.85 | 120.94 | 111.00 |
| 1 | H | 188 | LEU | CB-CG-CD1 | 5.85 | 120.94 | 111.00 |
| 1 | G | 22 | VAL | CG1-CB-CG2 | 5.84 | 120.25 | 110.90 |
| 1 | J | 360 | PHE | CB-CG-CD1 | 5.84 | 124.89 | 120.80 |
| 1 | A | 300 | VAL | CA-CB-CG2 | -5.84 | 102.14 | 110.90 |
| 1 | L | 195 | ILE | CB-CG1-CD1 | 5.84 | 130.26 | 113.90 |
| 1 | B | 141 | VAL | CB-CA-C | -5.84 | 100.31 | 111.40 |
| 1 | O | 25 | ASP | CB-CG-OD2 | 5.84 | 123.55 | 118.30 |
| 1 | D | 70 | TYR | CD1-CE1-CZ | -5.83 | 114.55 | 119.80 |
| 1 | I | 195 | ILE | CB-CG1-CD1 | 5.83 | 130.24 | 113.90 |
| 1 | B | 234 | TYR | CG-CD1-CE1 | -5.83 | 116.63 | 121.30 |
| 1 | O | 223 | ASP | CB-CG-OD2 | -5.83 | 113.05 | 118.30 |
| 1 | H | 107 | VAL | CA-CB-CG1 | -5.83 | 102.15 | 110.90 |
| 1 | M | 74 | ARG | NE-CZ-NH1 | -5.83 | 117.38 | 120.30 |
| 1 | J | 42 | LEU | CA-CB-CG | -5.83 | 101.89 | 115.30 |
| 1 | F | 31 | THR | O-C-N | 5.83 | 132.02 | 122.70 |
| 1 | J | 469 | LEU | O-C-N | -5.83 | 113.38 | 122.70 |
| 1 | C | 105 | VAL | CA-CB-CG1 | -5.82 | 102.16 | 110.90 |
| 1 | D | 355 | TYR | CD1-CE1-CZ | 5.82 | 125.04 | 119.80 |
| 1 | J | 341 | ASN | N-CA-C | -5.82 | 95.28 | 111.00 |
| 1 | G | 39 | THR | CA-CB-CG2 | -5.82 | 104.26 | 112.40 |
| 1 | H | 115 | VAL | CA-CB-CG1 | 5.82 | 119.62 | 110.90 |
| 1 | J | 334 | VAL | N-CA-C | -5.82 | 95.30 | 111.00 |
| 1 | F | 225 | CYS | CA-CB-SG | -5.81 | 103.54 | 114.00 |
| 1 | J | 291 | TYR | CB-CG-CD1 | 5.81 | 124.49 | 121.00 |
| 1 | I | 256 | PHE | CD1-CE1-CZ | 5.81 | 127.07 | 120.10 |
| 1 | N | 322 | GLY | N-CA-C | -5.81 | 98.57 | 113.10 |
| 1 | C | 291 | TYR | CG-CD2-CE2 | 5.81 | 125.95 | 121.30 |
| 1 | M | 181 | GLN | N-CA-C | -5.81 | 95.31 | 111.00 |
| 1 | C | 300 | VAL | CA-CB-CG2 | -5.80 | 102.20 | 110.90 |
| 1 | G | 61 | LEU | CB-CG-CD2 | 5.80 | 120.86 | 111.00 |
| 1 | K | 249 | TYR | CD1-CE1-CZ | 5.80 | 125.02 | 119.80 |
| 1 | E | 126 | LEU | CB-CG-CD2 | 5.80 | 120.86 | 111.00 |
| 1 | O | 202 | ASP | CB-CG-OD1 | -5.80 | 113.08 | 118.30 |
| 1 | N | 340 | THR | CA-CB-CG2 | -5.79 | 104.29 | 112.40 |
| 1 | F | 234 | TYR | CG-CD1-CE1 | -5.79 | 116.67 | 121.30 |
| 1 | G | 372 | LEU | CA-CB-CG | -5.79 | 101.98 | 115.30 |
| 1 | A | 244 | ASP | CB-CG-OD2 | -5.79 | 113.09 | 118.30 |
| 1 | N | 233 | ASP | CB-CG-OD2 | -5.79 | 113.09 | 118.30 |
| 1 | E | 258 | ARG | NE-CZ-NH1 | -5.79 | 117.41 | 120.30 |
| 1 | H | 380 | LYS | CD-CE-NZ | -5.79 | 98.39 | 111.70 |
| 1 | D | 448 | GLU | OE1-CD-OE2 | -5.79 | 116.36 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | M | 338 | ARG | CG-CD-NE | 5.79 | 123.95 | 111.80 |
| 1 | N | 158 | LEU | CB-CG-CD1 | -5.79 | 101.17 | 111.00 |
| 1 | D | 190 | LEU | CB-CG-CD2 | -5.78 | 101.17 | 111.00 |
| 1 | J | 83 | PHE | CB-CG-CD1 | 5.78 | 124.85 | 120.80 |
| 1 | G | 374 | PHE | CB-CG-CD2 | -5.78 | 116.75 | 120.80 |
| 1 | O | 150 | ASP | CB-CG-OD1 | -5.78 | 113.10 | 118.30 |
| 1 | K | 200 | MET | CA-CB-CG | -5.78 | 103.47 | 113.30 |
| 1 | L | 273 | ASP | CB-CG-OD2 | -5.78 | 113.10 | 118.30 |
| 1 | F | 141 | VAL | CA-CB-CG1 | -5.78 | 102.23 | 110.90 |
| 1 | F | 267 | VAL | CA-CB-CG2 | -5.78 | 102.23 | 110.90 |
| 1 | E | 370 | TYR | CB-CG-CD2 | 5.77 | 124.46 | 121.00 |
| 1 | O | 255 | MET | CG-SD-CE | 5.77 | 109.44 | 100.20 |
| 1 | J | 344 | LEU | CA-CB-CG | 5.77 | 128.57 | 115.30 |
| 1 | M | 323 | ILE | CB-CA-C | -5.77 | 100.06 | 111.60 |
| 1 | H | 446 | PHE | CB-CG-CD1 | 5.77 | 124.84 | 120.80 |
| 1 | M | 258 | ARG | NE-CZ-NH2 | -5.77 | 117.42 | 120.30 |
| 1 | N | 105 | VAL | CA-CB-CG2 | -5.77 | 102.25 | 110.90 |
| 1 | O | 464 | LEU | CB-CA-C | -5.77 | 99.24 | 110.20 |
| 1 | E | 68 | LEU | O-C-N | 5.77 | 131.93 | 122.70 |
| 1 | L | 222 | LEU | CA-CB-CG | 5.77 | 128.56 | 115.30 |
| 1 | L | 42 | LEU | CA-CB-CG | -5.76 | 102.04 | 115.30 |
| 1 | H | 105 | VAL | CG1-CB-CG2 | -5.76 | 101.69 | 110.90 |
| 1 | H | 315 | ARG | NE-CZ-NH2 | 5.76 | 123.18 | 120.30 |
| 1 | A | 330 | PHE | N-CA-CB | -5.76 | 100.24 | 110.60 |
| 1 | A | 370 | TYR | CZ-CE2-CD2 | -5.76 | 114.62 | 119.80 |
| 1 | I | 174 | PRO | O-C-N | 5.76 | 131.91 | 122.70 |
| 1 | L | 374 | PHE | CG-CD2-CE2 | 5.76 | 127.13 | 120.80 |
| 1 | N | 315 | ARG | NE-CZ-NH1 | -5.76 | 117.42 | 120.30 |
| 1 | A | 372 | LEU | CA-CB-CG | -5.75 | 102.06 | 115.30 |
| 1 | D | 194 | VAL | CB-CA-C | -5.75 | 100.47 | 111.40 |
| 1 | N | 197 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 1 | N | 316 | ALA | N-CA-CB | 5.75 | 118.15 | 110.10 |
| 1 | I | 458 | ASP | CB-CG-OD2 | -5.75 | 113.13 | 118.30 |
| 1 | B | 201 | VAL | CB-CA-C | -5.74 | 100.49 | 111.40 |
| 1 | B | 390 | TYR | CB-CG-CD2 | -5.74 | 117.55 | 121.00 |
| 1 | G | 98 | LEU | N-CA-C | 5.74 | 126.51 | 111.00 |
| 1 | I | 210 | PHE | CB-CG-CD1 | -5.74 | 116.78 | 120.80 |
| 1 | A | 335 | ASP | CB-CG-OD2 | 5.73 | 123.46 | 118.30 |
| 1 | I | 109 | ARG | NE-CZ-NH2 | 5.73 | 123.17 | 120.30 |
| 1 | N | 315 | ARG | NE-CZ-NH2 | -5.73 | 117.44 | 120.30 |
| 1 | A | 222 | LEU | CA-CB-CG | -5.73 | 102.13 | 115.30 |
| 1 | D | 296 | SER | N-CA-CB | -5.73 | 101.91 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 338 | ARG | CA-CB-CG | 5.73 | 126.00 | 113.40 |
| 1 | G | 289 | SER | N-CA-CB | -5.72 | 101.92 | 110.50 |
| 1 | C | 188 | LEU | CB-CG-CD1 | 5.72 | 120.72 | 111.00 |
| 1 | D | 355 | TYR | CB-CG-CD2 | 5.71 | 124.43 | 121.00 |
| 1 | G | 102 | CYS | CA-CB-SG | -5.71 | 103.71 | 114.00 |
| 1 | M | 234 | TYR | CB-CG-CD1 | -5.71 | 117.57 | 121.00 |
| 1 | I | 149 | MET | CB-CG-SD | 5.71 | 129.54 | 112.40 |
| 1 | I | 28 | VAL | CG1-CB-CG2 | -5.71 | 101.77 | 110.90 |
| 1 | O | 140 | GLY | CA-C-O | 5.71 | 130.88 | 120.60 |
| 1 | O | 151 | TYR | CB-CG-CD2 | 5.71 | 124.42 | 121.00 |
| 1 | B | 61 | LEU | CB-CG-CD1 | 5.70 | 120.69 | 111.00 |
| 1 | O | 257 | VAL | CA-CB-CG1 | -5.70 | 102.34 | 110.90 |
| 1 | A | 311 | TYR | CB-CG-CD2 | 5.70 | 124.42 | 121.00 |
| 1 | L | 321 | ASN | C-N-CA | -5.70 | 110.33 | 122.30 |
| 1 | N | 472 | LEU | CA-CB-CG | 5.70 | 128.40 | 115.30 |
| 1 | J | 111 | GLN | N-CA-CB | -5.70 | 100.35 | 110.60 |
| 1 | E | 388 | MET | CG-SD-CE | 5.69 | 109.31 | 100.20 |
| 1 | B | 315 | ARG | CD-NE-CZ | 5.69 | 131.57 | 123.60 |
| 1 | K | 112 | PRO | N-CD-CG | -5.69 | 94.66 | 103.20 |
| 1 | A | 252 | ARG | CD-NE-CZ | -5.69 | 115.63 | 123.60 |
| 1 | H | 286 | LEU | CB-CG-CD1 | 5.69 | 120.67 | 111.00 |
| 1 | M | 335 | ASP | C-N-CA | -5.69 | 107.47 | 121.70 |
| 1 | J | 43 | LEU | O-C-N | 5.69 | 131.80 | 122.70 |
| 1 | I | 256 | PHE | CG-CD1-CE1 | -5.68 | 114.55 | 120.80 |
| 1 | L | 247 | PHE | CZ-CE2-CD2 | -5.68 | 113.28 | 120.10 |
| 1 | I | 283 | THR | CA-CB-CG2 | 5.68 | 120.35 | 112.40 |
| 1 | E | 160 | GLY | N-CA-C | -5.68 | 98.90 | 113.10 |
| 1 | F | 176 | THR | OG1-CB-CG2 | 5.68 | 123.06 | 110.00 |
| 1 | H | 184 | ASP | CB-CG-OD1 | -5.68 | 113.19 | 118.30 |
| 1 | D | 70 | TYR | OH-CZ-CE2 | -5.67 | 104.78 | 120.10 |
| 1 | O | 462 | PHE | CZ-CE2-CD2 | -5.67 | 113.29 | 120.10 |
| 1 | C | 107 | VAL | CA-CB-CG1 | -5.67 | 102.39 | 110.90 |
| 1 | F | 194 | VAL | CG1-CB-CG2 | 5.67 | 119.97 | 110.90 |
| 1 | G | 112 | PRO | N-CD-CG | -5.67 | 94.69 | 103.20 |
| 1 | C | 296 | SER | O-C-N | -5.67 | 113.57 | 123.20 |
| 1 | O | 346 | ALA | CB-CA-C | -5.66 | 101.60 | 110.10 |
| 1 | F | 333 | VAL | CA-CB-CG2 | -5.66 | 102.41 | 110.90 |
| 1 | N | 303 | ASP | CB-CG-OD2 | 5.66 | 123.39 | 118.30 |
| 1 | J | 223 | ASP | CB-CG-OD2 | 5.66 | 123.39 | 118.30 |
| 1 | G | 463 | PRO | CB-CG-CD | -5.66 | 84.44 | 106.50 |
| 1 | J | 75 | ILE | CG1-CB-CG2 | -5.66 | 98.96 | 111.40 |
| 1 | D | 113 | LEU | CB-CG-CD1 | 5.65 | 120.61 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | K | 162 | LYS | CG-CD-CE | -5.65 | 94.96 | 111.90 |
| 1 | B | 158 | LEU | CD1-CG-CD2 | -5.64 | 93.57 | 110.50 |
| 1 | D | 364 | LEU | CB-CG-CD2 | -5.64 | 101.40 | 111.00 |
| 1 | F | 173 | SER | N-CA-CB | 5.64 | 118.97 | 110.50 |
| 1 | B | 151 | TYR | CB-CG-CD1 | -5.64 | 117.62 | 121.00 |
| 1 | J | 379 | CYS | CA-CB-SG | -5.64 | 103.85 | 114.00 |
| 1 | N | 390 | TYR | CB-CG-CD2 | -5.64 | 117.62 | 121.00 |
| 1 | B | 53 | LYS | CD-CE-NZ | -5.64 | 98.74 | 111.70 |
| 1 | E | 375 | ILE | CB-CA-C | -5.64 | 100.33 | 111.60 |
| 1 | J | 95 | THR | CB-CA-C | -5.63 | 96.39 | 111.60 |
| 1 | J | 149 | MET | N-CA-CB | -5.63 | 100.46 | 110.60 |
| 1 | N | 61 | LEU | CB-CG-CD1 | 5.63 | 120.58 | 111.00 |
| 1 | H | 199 | ASP | CB-CG-OD1 | 5.63 | 123.36 | 118.30 |
| 1 | O | 107 | VAL | CG1-CB-CG2 | 5.63 | 119.91 | 110.90 |
| 1 | H | 97 | ARG | O-C-N | 5.63 | 131.70 | 122.70 |
| 1 | J | 163 | PRO | CB-CG-CD | -5.62 | 84.57 | 106.50 |
| 1 | O | 201 | VAL | CB-CA-C | -5.62 | 100.72 | 111.40 |
| 1 | F | 231 | TYR | CZ-CE2-CD2 | 5.62 | 124.86 | 119.80 |
| 1 | K | 380 | LYS | CD-CE-NZ | -5.62 | 98.78 | 111.70 |
| 1 | M | 451 | LEU | CA-CB-CG | -5.62 | 102.38 | 115.30 |
| 1 | B | 209 | ASP | CB-CG-OD2 | 5.62 | 123.35 | 118.30 |
| 1 | E | 345 | CYS | CA-CB-SG | -5.62 | 103.89 | 114.00 |
| 1 | I | 315 | ARG | NE-CZ-NH1 | 5.61 | 123.11 | 120.30 |
| 1 | N | 200 | MET | CA-CB-CG | -5.61 | 103.76 | 113.30 |
| 1 | E | 117 | ILE | CG1-CB-CG2 | 5.61 | 123.75 | 111.40 |
| 1 | D | 275 | LEU | CB-CG-CD2 | 5.61 | 120.54 | 111.00 |
| 1 | N | 220 | VAL | CA-CB-CG1 | -5.61 | 102.48 | 110.90 |
| 1 | F | 61 | LEU | CB-CG-CD1 | 5.61 | 120.54 | 111.00 |
| 1 | M | 22 | VAL | CB-CA-C | -5.61 | 100.74 | 111.40 |
| 1 | G | 146 | CYS | CA-CB-SG | -5.61 | 103.91 | 114.00 |
| 1 | H | 300 | VAL | CA-CB-CG2 | -5.61 | 102.49 | 110.90 |
| 1 | H | 263 | ARG | NE-CZ-NH2 | 5.60 | 123.10 | 120.30 |
| 1 | N | 204 | GLY | O-C-N | 5.60 | 131.67 | 122.70 |
| 1 | F | 331 | VAL | CG1-CB-CG2 | 5.60 | 119.87 | 110.90 |
| 1 | I | 381 | ILE | CB-CG1-CD1 | -5.60 | 98.21 | 113.90 |
| 1 | G | 298 | SER | CB-CA-C | -5.60 | 99.47 | 110.10 |
| 1 | H | 249 | TYR | CB-CG-CD2 | 5.60 | 124.36 | 121.00 |
| 1 | B | 48 | PRO | N-CD-CG | -5.59 | 94.81 | 103.20 |
| 1 | N | 246 | LEU | CB-CG-CD2 | 5.59 | 120.51 | 111.00 |
| 1 | O | 354 | THR | CA-CB-CG2 | -5.59 | 104.58 | 112.40 |
| 1 | E | 177 | GLN | N-CA-CB | 5.59 | 120.66 | 110.60 |
| 1 | H | 219 | GLU | CG-CD-OE1 | -5.59 | 107.13 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | I | 363 | TYR | CB-CG-CD2 | -5.59 | 117.65 | 121.00 |
| 1 | A | 205 | PHE | CG-CD1-CE1 | 5.58 | 126.94 | 120.80 |
| 1 | B | 127 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | J | 147 | ILE | CB-CA-C | -5.58 | 100.44 | 111.60 |
| 1 | B | 33 | ILE | CG1-CB-CG2 | -5.58 | 99.13 | 111.40 |
| 1 | F | 34 | TYR | CD1-CE1-CZ | -5.58 | 114.78 | 119.80 |
| 1 | I | 41 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | B | 182 | PRO | CB-CG-CD | -5.57 | 84.77 | 106.50 |
| 1 | K | 151 | TYR | CD1-CE1-CZ | 5.57 | 124.81 | 119.80 |
| 1 | B | 242 | TYR | CB-CG-CD2 | 5.57 | 124.34 | 121.00 |
| 1 | A | 357 | ASN | N-CA-C | 5.57 | 126.04 | 111.00 |
| 1 | J | 326 | GLY | N-CA-C | -5.57 | 99.18 | 113.10 |
| 1 | H | 355 | TYR | CG-CD2-CE2 | 5.57 | 125.75 | 121.30 |
| 1 | K | 368 | GLU | OE1-CD-OE2 | 5.57 | 129.98 | 123.30 |
| 1 | L | 21 | VAL | CB-CA-C | -5.57 | 100.82 | 111.40 |
| 1 | A | 371 | ASP | CB-CG-OD1 | 5.56 | 123.31 | 118.30 |
| 1 | B | 241 | PRO | N-CD-CG | -5.56 | 94.86 | 103.20 |
| 1 | G | 77 | LEU | CB-CG-CD2 | -5.56 | 101.55 | 111.00 |
| 1 | M | 145 | GLU | CG-CD-OE1 | -5.56 | 107.19 | 118.30 |
| 1 | C | 65 | VAL | CA-CB-CG1 | 5.55 | 119.23 | 110.90 |
| 1 | F | 107 | VAL | CG1-CB-CG2 | 5.55 | 119.79 | 110.90 |
| 1 | N | 294 | THR | CA-CB-OG1 | 5.55 | 120.67 | 109.00 |
| 1 | D | 203 | THR | OG1-CB-CG2 | 5.55 | 122.77 | 110.00 |
| 1 | B | 71 | ARG | CB-CG-CD | -5.55 | 97.17 | 111.60 |
| 1 | G | 41 | ARG | NH1-CZ-NH2 | -5.55 | 113.30 | 119.40 |
| 1 | I | 22 | VAL | CG1-CB-CG2 | 5.55 | 119.78 | 110.90 |
| 1 | C | 149 | MET | CG-SD-CE | 5.55 | 109.08 | 100.20 |
| 1 | N | 280 | SER | C-N-CA | -5.55 | 110.65 | 122.30 |
| 1 | C | 73 | PHE | CD1-CE1-CZ | 5.54 | 126.75 | 120.10 |
| 1 | H | 356 | LYS | CB-CG-CD | -5.54 | 97.19 | 111.60 |
| 1 | I | 299 | MET | CB-CG-SD | -5.54 | 95.77 | 112.40 |
| 1 | K | 142 | ASP | CB-CG-OD1 | -5.54 | 113.31 | 118.30 |
| 1 | J | 206 | GLY | N-CA-C | -5.54 | 99.25 | 113.10 |
| 1 | L | 158 | LEU | CB-CG-CD2 | -5.54 | 101.58 | 111.00 |
| 1 | M | 94 | ASP | CB-CG-OD1 | -5.54 | 113.31 | 118.30 |
| 1 | M | 334 | VAL | N-CA-C | -5.54 | 96.04 | 111.00 |
| 1 | H | 201 | VAL | CG1-CB-CG2 | -5.54 | 102.04 | 110.90 |
| 1 | H | 180 | VAL | CA-CB-CG1 | -5.54 | 102.60 | 110.90 |
| 1 | J | 446 | PHE | CB-CG-CD2 | -5.54 | 116.92 | 120.80 |
| 1 | M | 26 | GLU | OE1-CD-OE2 | -5.53 | 116.66 | 123.30 |
| 1 | N | 235 | ILE | CG1-CB-CG2 | -5.53 | 99.23 | 111.40 |
| 1 | G | 347 | ALA | CB-CA-C | 5.53 | 118.39 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 207 | ALA | CB-CA-C | -5.53 | 101.81 | 110.10 |
| 1 | N | 375 | ILE | CB-CA-C | -5.53 | 100.54 | 111.60 |
| 1 | H | 30 | ARG | NE-CZ-NH2 | 5.53 | 123.06 | 120.30 |
| 1 | O | 189 | GLU | OE1-CD-OE2 | 5.53 | 129.93 | 123.30 |
| 1 | O | 331 | VAL | CA-CB-CG2 | -5.53 | 102.61 | 110.90 |
| 1 | A | 98 | LEU | CB-CG-CD2 | -5.53 | 101.61 | 111.00 |
| 1 | H | 151 | TYR | CD1-CE1-CZ | 5.52 | 124.77 | 119.80 |
| 1 | N | 378 | LEU | CB-CG-CD1 | 5.52 | 120.39 | 111.00 |
| 1 | K | 250 | LEU | CB-CG-CD1 | 5.52 | 120.39 | 111.00 |
| 1 | O | 375 | ILE | CG1-CB-CG2 | -5.52 | 99.25 | 111.40 |
| 1 | D | 361 | LYS | CD-CE-NZ | -5.52 | 99.00 | 111.70 |
| 1 | F | 176 | THR | CA-CB-CG2 | -5.52 | 104.67 | 112.40 |
| 1 | B | 73 | PHE | CB-CG-CD1 | -5.51 | 116.94 | 120.80 |
| 1 | D | 449 | VAL | CB-CA-C | -5.51 | 100.92 | 111.40 |
| 1 | N | 70 | TYR | CG-CD2-CE2 | 5.51 | 125.71 | 121.30 |
| 1 | A | 152 | LYS | CG-CD-CE | -5.51 | 95.37 | 111.90 |
| 1 | E | 332 | THR | CA-CB-CG2 | -5.51 | 104.69 | 112.40 |
| 1 | K | 45 | VAL | CA-CB-CG2 | 5.51 | 119.16 | 110.90 |
| 1 | F | 249 | TYR | CZ-CE2-CD2 | 5.51 | 124.76 | 119.80 |
| 1 | G | 201 | VAL | CB-CA-C | -5.51 | 100.94 | 111.40 |
| 1 | C | 303 | ASP | CB-CG-OD1 | -5.50 | 113.35 | 118.30 |
| 1 | M | 51 | PRO | CB-CG-CD | -5.50 | 85.04 | 106.50 |
| 1 | B | 43 | LEU | CB-CA-C | -5.50 | 99.75 | 110.20 |
| 1 | H | 300 | VAL | CB-CA-C | -5.50 | 100.95 | 111.40 |
| 1 | E | 167 | GLU | CB-CG-CD | -5.50 | 99.35 | 114.20 |
| 1 | G | 338 | ARG | CA-CB-CG | 5.50 | 125.49 | 113.40 |
| 1 | O | 449 | VAL | CG1-CB-CG2 | -5.50 | 102.11 | 110.90 |
| 1 | H | 265 | GLY | CA-C-N | -5.50 | 105.11 | 117.20 |
| 1 | O | 374 | PHE | CB-CG-CD2 | -5.50 | 116.95 | 120.80 |
| 1 | M | 101 | ALA | C-N-CA | -5.49 | 107.97 | 121.70 |
| 1 | F | 99 | VAL | CG1-CB-CG2 | -5.49 | 102.11 | 110.90 |
| 1 | E | 199 | ASP | CB-CG-OD1 | -5.49 | 113.36 | 118.30 |
| 1 | D | 383 | LEU | CB-CG-CD1 | 5.49 | 120.33 | 111.00 |
| 1 | O | 333 | VAL | CB-CA-C | -5.49 | 100.97 | 111.40 |
| 1 | E | 233 | ASP | CB-CG-OD2 | 5.48 | 123.23 | 118.30 |
| 1 | B | 389 | THR | CA-CB-CG2 | -5.48 | 104.73 | 112.40 |
| 1 | D | 266 | THR | CB-CA-C | -5.48 | 96.81 | 111.60 |
| 1 | I | 141 | VAL | CA-CB-CG2 | -5.48 | 102.69 | 110.90 |
| 1 | C | 97 | ARG | NE-CZ-NH1 | 5.47 | 123.04 | 120.30 |
| 1 | A | 152 | LYS | CD-CE-NZ | 5.47 | 124.29 | 111.70 |
| 1 | K | 468 | PHE | CG-CD1-CE1 | 5.47 | 126.82 | 120.80 |
| 1 | O | 103 | VAL | CA-CB-CG2 | 5.47 | 119.11 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 113 | LEU | CB-CG-CD2 | -5.47 | 101.70 | 111.00 |
| 1 | D | 176 | THR | O-C-N | 5.47 | 131.45 | 122.70 |
| 1 | B | 87 | ASP | CB-CG-OD2 | -5.47 | 113.38 | 118.30 |
| 1 | I | 252 | ARG | N-CA-CB | -5.47 | 100.76 | 110.60 |
| 1 | N | 66 | SER | C-N-CA | -5.47 | 110.82 | 122.30 |
| 1 | B | 286 | LEU | N-CA-C | 5.46 | 125.76 | 111.00 |
| 1 | I | 365 | ARG | NH1-CZ-NH2 | -5.46 | 113.39 | 119.40 |
| 1 | E | 268 | GLY | N-CA-C | -5.46 | 99.45 | 113.10 |
| 1 | L | 127 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 1 | C | 312 | TRP | N-CA-CB | -5.46 | 100.78 | 110.60 |
| 1 | J | 299 | MET | CG-SD-CE | 5.46 | 108.93 | 100.20 |
| 1 | J | 363 | TYR | CB-CG-CD2 | -5.46 | 117.72 | 121.00 |
| 1 | K | 180 | VAL | CB-CA-C | -5.46 | 101.03 | 111.40 |
| 1 | E | 189 | GLU | CG-CD-OE2 | -5.45 | 107.39 | 118.30 |
| 1 | E | 277 | ILE | CA-CB-CG2 | -5.45 | 100.00 | 110.90 |
| 1 | M | 250 | LEU | CB-CG-CD1 | -5.45 | 101.73 | 111.00 |
| 1 | B | 295 | PRO | CA-CB-CG | -5.45 | 93.65 | 104.00 |
| 1 | D | 151 | TYR | CB-CG-CD2 | -5.45 | 117.73 | 121.00 |
| 1 | L | 449 | VAL | CA-CB-CG1 | -5.45 | 102.73 | 110.90 |
| 1 | A | 95 | THR | CA-CB-CG2 | -5.45 | 104.78 | 112.40 |
| 1 | N | 300 | VAL | CB-CA-C | -5.44 | 101.06 | 111.40 |
| 1 | E | 445 | THR | CA-CB-CG2 | -5.44 | 104.78 | 112.40 |
| 1 | F | 469 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | G | 20 | ALA | N-CA-CB | 5.44 | 117.72 | 110.10 |
| 1 | G | 180 | VAL | CA-CB-CG1 | -5.44 | 102.74 | 110.90 |
| 1 | H | 68 | LEU | CB-CA-C | -5.44 | 99.86 | 110.20 |
| 1 | F | 226 | THR | CB-CA-C | -5.44 | 96.92 | 111.60 |
| 1 | F | 274 | ASP | CB-CG-OD1 | -5.44 | 113.41 | 118.30 |
| 1 | I | 126 | LEU | CB-CG-CD2 | 5.44 | 120.24 | 111.00 |
| 1 | J | 398 | ILE | CB-CA-C | -5.44 | 100.72 | 111.60 |
| 1 | F | 85 | PHE | CB-CG-CD2 | -5.43 | 117.00 | 120.80 |
| 1 | H | 372 | LEU | CB-CG-CD1 | 5.43 | 120.24 | 111.00 |
| 1 | O | 449 | VAL | CA-CB-CG1 | -5.43 | 102.75 | 110.90 |
| 1 | M | 28 | VAL | CA-CB-CG1 | 5.43 | 119.05 | 110.90 |
| 1 | H | 472 | LEU | CB-CG-CD1 | -5.43 | 101.77 | 111.00 |
| 1 | F | 219 | GLU | CA-CB-CG | -5.42 | 101.47 | 113.40 |
| 1 | K | 472 | LEU | CD1-CG-CD2 | 5.42 | 126.77 | 110.50 |
| 1 | M | 449 | VAL | CG1-CB-CG2 | -5.42 | 102.23 | 110.90 |
| 1 | D | 313 | LEU | CB-CG-CD1 | 5.42 | 120.21 | 111.00 |
| 1 | I | 334 | VAL | CA-CB-CG2 | -5.42 | 102.77 | 110.90 |
| 1 | E | 266 | THR | CA-CB-CG2 | -5.41 | 104.82 | 112.40 |
| 1 | H | 68 | LEU | CA-CB-CG | -5.41 | 102.85 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | I | 150 | ASP | CB-CA-C | -5.41 | 99.58 | 110.40 |
| 1 | L | 192 | ASN | O-C-N | -5.41 | 114.04 | 122.70 |
| 1 | N | 39 | THR | CA-CB-CG2 | -5.41 | 104.82 | 112.40 |
| 1 | B | 342 | MET | CA-CB-CG | 5.41 | 122.50 | 113.30 |
| 1 | D | 161 | CYS | CA-CB-SG | 5.41 | 123.74 | 114.00 |
| 1 | E | 145 | GLU | CG-CD-OE1 | -5.41 | 107.48 | 118.30 |
| 1 | H | 224 | ILE | CB-CA-C | -5.41 | 100.78 | 111.60 |
| 1 | J | 399 | LEU | CB-CG-CD2 | -5.41 | 101.80 | 111.00 |
| 1 | C | 187 | PRO | CA-N-CD | -5.41 | 103.93 | 111.50 |
| 1 | O | 42 | LEU | CA-CB-CG | -5.41 | 102.86 | 115.30 |
| 1 | K | 264 | ALA | N-CA-CB | -5.41 | 102.53 | 110.10 |
| 1 | A | 115 | VAL | CA-C-N | -5.40 | 105.41 | 116.20 |
| 1 | M | 208 | MET | CB-CA-C | -5.40 | 99.61 | 110.40 |
| 1 | D | 386 | ASP | OD1-CG-OD2 | -5.39 | 113.05 | 123.30 |
| 1 | H | 333 | VAL | CB-CA-C | -5.39 | 101.16 | 111.40 |
| 1 | D | 199 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 1 | G | 113 | LEU | C-N-CA | -5.39 | 110.98 | 122.30 |
| 1 | A | 149 | MET | CA-CB-CG | 5.39 | 122.46 | 113.30 |
| 1 | E | 59 | LYS | CD-CE-NZ | 5.39 | 124.09 | 111.70 |
| 1 | H | 472 | LEU | CA-C-O | -5.39 | 108.79 | 120.10 |
| 1 | J | 143 | ASN | N-CA-C | -5.39 | 96.46 | 111.00 |
| 1 | M | 279 | GLY | O-C-N | -5.39 | 114.08 | 122.70 |
| 1 | B | 31 | THR | OG1-CB-CG2 | 5.38 | 122.38 | 110.00 |
| 1 | M | 164 | PRO | N-CD-CG | -5.38 | 95.13 | 103.20 |
| 1 | A | 201 | VAL | CA-CB-CG1 | -5.38 | 102.83 | 110.90 |
| 1 | D | 99 | VAL | CB-CA-C | -5.38 | 101.17 | 111.40 |
| 1 | E | 362 | GLU | OE1-CD-OE2 | 5.38 | 129.76 | 123.30 |
| 1 | F | 297 | GLY | CA-C-O | 5.38 | 130.29 | 120.60 |
| 1 | K | 49 | TYR | CB-CG-CD1 | 5.38 | 124.23 | 121.00 |
| 1 | K | 470 | LEU | N-CA-CB | -5.38 | 99.64 | 110.40 |
| 1 | B | 291 | TYR | CE1-CZ-OH | -5.38 | 105.58 | 120.10 |
| 1 | F | 138 | ASN | CA-C-N | -5.38 | 105.37 | 117.20 |
| 1 | F | 386 | ASP | CB-CG-OD2 | 5.38 | 123.14 | 118.30 |
| 1 | N | 226 | THR | CB-CA-C | -5.38 | 97.08 | 111.60 |
| 1 | B | 70 | TYR | CE1-CZ-CE2 | -5.38 | 111.20 | 119.80 |
| 1 | G | 70 | TYR | CG-CD2-CE2 | 5.38 | 125.60 | 121.30 |
| 1 | D | 307 | PHE | CD1-CE1-CZ | 5.37 | 126.55 | 120.10 |
| 1 | E | 42 | LEU | CA-CB-CG | -5.37 | 102.94 | 115.30 |
| 1 | M | 394 | MET | CG-SD-CE | 5.37 | 108.80 | 100.20 |
| 1 | C | 263 | ARG | CD-NE-CZ | -5.37 | 116.08 | 123.60 |
| 1 | K | 49 | TYR | CD1-CG-CD2 | -5.37 | 111.99 | 117.90 |
| 1 | L | 35 | TYR | CB-CG-CD1 | -5.37 | 117.78 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | L | 372 | LEU | N-CA-CB | -5.37 | 99.66 | 110.40 |
| 1 | I | 178 | VAL | C-N-CA | 5.37 | 135.13 | 121.70 |
| 1 | O | 470 | LEU | CB-CG-CD1 | -5.37 | 101.87 | 111.00 |
| 1 | D | 97 | ARG | NE-CZ-NH2 | -5.37 | 117.62 | 120.30 |
| 1 | A | 172 | GLY | N-CA-C | -5.36 | 99.69 | 113.10 |
| 1 | J | 274 | ASP | CB-CG-OD1 | -5.36 | 113.47 | 118.30 |
| 1 | D | 231 | TYR | CD1-CE1-CZ | -5.36 | 114.98 | 119.80 |
| 1 | F | 75 | ILE | CG1-CB-CG2 | -5.36 | 99.61 | 111.40 |
| 1 | L | 117 | ILE | N-CA-CB | -5.36 | 98.48 | 110.80 |
| 1 | A | 70 | TYR | CG-CD2-CE2 | 5.36 | 125.58 | 121.30 |
| 1 | M | 201 | VAL | CA-CB-CG1 | -5.36 | 102.87 | 110.90 |
| 1 | E | 231 | TYR | CE1-CZ-OH | -5.35 | 105.65 | 120.10 |
| 1 | A | 71 | ARG | CB-CG-CD | -5.35 | 97.69 | 111.60 |
| 1 | C | 70 | TYR | CG-CD2-CE2 | 5.35 | 125.58 | 121.30 |
| 1 | D | 35 | TYR | CB-CG-CD2 | -5.35 | 117.79 | 121.00 |
| 1 | I | 283 | THR | OG1-CB-CG2 | -5.35 | 97.69 | 110.00 |
| 1 | A | 340 | THR | CA-CB-CG2 | -5.35 | 104.91 | 112.40 |
| 1 | I | 469 | LEU | CB-CG-CD1 | -5.35 | 101.91 | 111.00 |
| 1 | N | 344 | LEU | CA-CB-CG | -5.35 | 103.00 | 115.30 |
| 1 | I | 459 | LEU | CB-CG-CD1 | 5.35 | 120.09 | 111.00 |
| 1 | K | 293 | PRO | O-C-N | 5.35 | 131.25 | 122.70 |
| 1 | N | 295 | PRO | N-CD-CG | -5.35 | 95.18 | 103.20 |
| 1 | A | 331 | VAL | CA-CB-CG2 | -5.34 | 102.88 | 110.90 |
| 1 | E | 159 | ILE | CG1-CB-CG2 | -5.34 | 99.64 | 111.40 |
| 1 | F | 266 | THR | CB-CA-C | -5.34 | 97.17 | 111.60 |
| 1 | C | 451 | LEU | CB-CG-CD2 | -5.34 | 101.92 | 111.00 |
| 1 | M | 142 | ASP | CB-CG-OD2 | 5.34 | 123.11 | 118.30 |
| 1 | H | 103 | VAL | CB-CA-C | -5.34 | 101.26 | 111.40 |
| 1 | L | 203 | THR | CA-CB-CG2 | -5.34 | 104.93 | 112.40 |
| 1 | N | 87 | ASP | CB-CG-OD2 | -5.34 | 113.50 | 118.30 |
| 1 | A | 70 | TYR | N-CA-C | -5.33 | 96.60 | 111.00 |
| 1 | N | 309 | LYS | CD-CE-NZ | -5.33 | 99.43 | 111.70 |
| 1 | F | 355 | TYR | CZ-CE2-CD2 | -5.33 | 115.00 | 119.80 |
| 1 | J | 400 | GLU | OE1-CD-OE2 | -5.33 | 116.90 | 123.30 |
| 1 | N | 27 | TYR | N-CA-C | 5.33 | 125.40 | 111.00 |
| 1 | H | 129 | THR | CA-CB-CG2 | -5.33 | 104.94 | 112.40 |
| 1 | H | 251 | ARG | NE-CZ-NH1 | -5.33 | 117.64 | 120.30 |
| 1 | L | 70 | TYR | CG-CD2-CE2 | 5.33 | 125.56 | 121.30 |
| 1 | L | 271 | VAL | CG1-CB-CG2 | -5.33 | 102.37 | 110.90 |
| 1 | E | 262 | ASN | N-CA-CB | -5.33 | 101.01 | 110.60 |
| 1 | I | 383 | LEU | CB-CG-CD2 | -5.33 | 101.94 | 111.00 |
| 1 | K | 125 | LYS | CD-CE-NZ | -5.33 | 99.45 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 1 | O | 472 | LEU | CB-CG-CD1 | -5.33 | 101.94 | 111.00 |
| 1 | L | 238 | VAL | CA-CB-CG1 | 5.32 | 118.89 | 110.90 |
| 1 | N | 30 | ARG | NH1-CZ-NH2 | 5.32 | 125.25 | 119.40 |
| 1 | F | 219 | GLU | OE1-CD-OE2 | 5.32 | 129.69 | 123.30 |
| 1 | F | 356 | LYS | CD-CE-NZ | -5.32 | 99.48 | 111.70 |
| 1 | G | 306 | ILE | CA-CB-CG1 | -5.31 | 100.90 | 111.00 |
| 1 | H | 181 | GLN | N-CA-C | -5.31 | 96.67 | 111.00 |
| 1 | H | 197 | ASP | CB-CG-OD2 | 5.31 | 123.08 | 118.30 |
| 1 | A | 387 | VAL | CA-C-N | -5.30 | 105.53 | 117.20 |
| 1 | D | 64 | LYS | CB-CA-C | -5.30 | 99.80 | 110.40 |
| 1 | D | 68 | LEU | CA-CB-CG | -5.30 | 103.11 | 115.30 |
| 1 | J | 176 | THR | CA-CB-CG2 | -5.30 | 104.98 | 112.40 |
| 1 | C | 94 | ASP | CB-CG-OD1 | -5.30 | 113.53 | 118.30 |
| 1 | A | 257 | VAL | CA-CB-CG2 | -5.30 | 102.95 | 110.90 |
| 1 | N | 85 | PHE | CB-CG-CD1 | -5.29 | 117.09 | 120.80 |
| 1 | M | 115 | VAL | CA-CB-CG2 | -5.29 | 102.96 | 110.90 |
| 1 | A | 203 | THR | CA-C-N | -5.29 | 105.62 | 116.20 |
| 1 | G | 284 | ALA | CB-CA-C | 5.29 | 118.04 | 110.10 |
| 1 | C | 396 | SER | N-CA-CB | -5.29 | 102.57 | 110.50 |
| 1 | H | 22 | VAL | CB-CA-C | -5.29 | 101.35 | 111.40 |
| 1 | J | 145 | GLU | CG-CD-OE1 | -5.29 | 107.72 | 118.30 |
| 1 | L | 73 | PHE | CG-CD2-CE2 | 5.29 | 126.62 | 120.80 |
| 1 | I | 22 | VAL | CB-CA-C | -5.29 | 101.35 | 111.40 |
| 1 | E | 306 | ILE | CG1-CB-CG2 | -5.29 | 99.77 | 111.40 |
| 1 | H | 265 | GLY | CA-C-O | 5.29 | 130.11 | 120.60 |
| 1 | J | 209 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 1 | L | 103 | VAL | CA-CB-CG1 | -5.29 | 102.97 | 110.90 |
| 1 | D | 380 | LYS | CB-CG-CD | 5.28 | 125.33 | 111.60 |
| 1 | G | 194 | VAL | CB-CA-C | -5.28 | 101.37 | 111.40 |
| 1 | M | 312 | TRP | CD1-NE1-CE2 | -5.28 | 104.25 | 109.00 |
| 1 | I | 209 | ASP | N-CA-C | -5.28 | 96.75 | 111.00 |
| 1 | K | 277 | ILE | CA-CB-CG2 | -5.28 | 100.35 | 110.90 |
| 1 | O | 271 | VAL | CB-CA-C | -5.28 | 101.38 | 111.40 |
| 1 | D | 25 | ASP | CB-CG-OD2 | 5.27 | 123.05 | 118.30 |
| 1 | G | 256 | PHE | CD1-CE1-CZ | 5.27 | 126.43 | 120.10 |
| 1 | F | 208 | MET | CB-CG-SD | 5.27 | 128.22 | 112.40 |
| 1 | F | 467 | LYS | CG-CD-CE | -5.27 | 96.08 | 111.90 |
| 1 | M | 315 | ARG | CD-NE-CZ | 5.27 | 130.98 | 123.60 |
| 1 | C | 470 | LEU | CA-CB-CG | 5.27 | 127.42 | 115.30 |
| 1 | L | 209 | ASP | OD1-CG-OD2 | -5.27 | 113.29 | 123.30 |
| 1 | F | 21 | VAL | CB-CA-C | -5.27 | 101.39 | 111.40 |
| 1 | G | 105 | VAL | CA-CB-CG2 | 5.27 | 118.80 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | O | 122 | LEU | CA-CB-CG | -5.27 | 103.19 | 115.30 |
| 1 | D | 372 | LEU | CB-CG-CD2 | -5.26 | 102.05 | 111.00 |
| 1 | H | 172 | GLY | N-CA-C | -5.26 | 99.94 | 113.10 |
| 1 | B | 294 | THR | CA-CB-CG2 | 5.26 | 119.77 | 112.40 |
| 1 | C | 271 | VAL | CB-CA-C | -5.26 | 101.41 | 111.40 |
| 1 | C | 338 | ARG | CG-CD-NE | 5.26 | 122.84 | 111.80 |
| 1 | E | 390 | TYR | CD1-CG-CD2 | 5.26 | 123.68 | 117.90 |
| 1 | D | 238 | VAL | CA-CB-CG1 | -5.25 | 103.03 | 110.90 |
| 1 | N | 26 | GLU | CG-CD-OE1 | 5.25 | 128.80 | 118.30 |
| 1 | N | 122 | LEU | CB-CG-CD1 | 5.25 | 119.92 | 111.00 |
| 1 | O | 70 | TYR | CG-CD2-CE2 | 5.25 | 125.50 | 121.30 |
| 1 | I | 139 | ALA | C-N-CA | -5.25 | 111.28 | 122.30 |
| 1 | O | 397 | THR | CA-CB-CG2 | 5.25 | 119.74 | 112.40 |
| 1 | I | 178 | VAL | N-CA-C | 5.25 | 125.16 | 111.00 |
| 1 | I | 369 | GLU | OE1-CD-OE2 | -5.25 | 117.01 | 123.30 |
| 1 | J | 113 | LEU | CA-C-N | -5.24 | 105.72 | 116.20 |
| 1 | A | 274 | ASP | CB-CG-OD1 | -5.24 | 113.58 | 118.30 |
| 1 | N | 249 | TYR | CE1-CZ-CE2 | -5.24 | 111.42 | 119.80 |
| 1 | F | 41 | ARG | CG-CD-NE | 5.24 | 122.80 | 111.80 |
| 1 | K | 22 | VAL | CA-CB-CG1 | -5.24 | 103.05 | 110.90 |
| 1 | L | 162 | LYS | CD-CE-NZ | 5.24 | 123.74 | 111.70 |
| 1 | M | 87 | ASP | OD1-CG-OD2 | 5.24 | 133.25 | 123.30 |
| 1 | N | 71 | ARG | NH1-CZ-NH2 | -5.24 | 113.64 | 119.40 |
| 1 | E | 380 | LYS | CD-CE-NZ | 5.23 | 123.74 | 111.70 |
| 1 | J | 93 | PRO | N-CA-C | 5.23 | 125.71 | 112.10 |
| 1 | B | 107 | VAL | CA-CB-CG2 | 5.23 | 118.75 | 110.90 |
| 1 | C | 124 | ASN | O-C-N | -5.23 | 114.33 | 122.70 |
| 1 | F | 123 | LEU | CB-CA-C | 5.23 | 120.14 | 110.20 |
| 1 | F | 194 | VAL | CB-CA-C | -5.23 | 101.46 | 111.40 |
| 1 | J | 130 | GLU | CA-CB-CG | 5.23 | 124.91 | 113.40 |
| 1 | H | 222 | LEU | C-N-CA | -5.23 | 108.62 | 121.70 |
| 1 | I | 94 | ASP | CB-CG-OD1 | 5.23 | 123.01 | 118.30 |
| 1 | G | 444 | TYR | CB-CG-CD2 | -5.23 | 117.86 | 121.00 |
| 1 | B | 459 | LEU | CB-CG-CD2 | 5.23 | 119.89 | 111.00 |
| 1 | D | 390 | TYR | CG-CD1-CE1 | -5.23 | 117.12 | 121.30 |
| 1 | J | 76 | HIS | O-C-N | 5.23 | 131.06 | 122.70 |
| 1 | L | 35 | TYR | CD1-CE1-CZ | 5.23 | 124.50 | 119.80 |
| 1 | L | 283 | THR | O-C-N | -5.23 | 114.34 | 122.70 |
| 1 | A | 387 | VAL | CG1-CB-CG2 | -5.23 | 102.54 | 110.90 |
| 1 | G | 441 | LEU | CB-CG-CD1 | -5.23 | 102.12 | 111.00 |
| 1 | B | 447 | TRP | N-CA-C | -5.22 | 96.89 | 111.00 |
| 1 | D | 79 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 105 | VAL | CA-CB-CG1 | -5.22 | 103.06 | 110.90 |
| 1 | N | 362 | GLU | CG-CD-OE1 | 5.22 | 128.75 | 118.30 |
| 1 | A | 388 | MET | CB-CG-SD | 5.22 | 128.07 | 112.40 |
| 1 | M | 361 | LYS | CB-CG-CD | -5.22 | 98.02 | 111.60 |
| 1 | B | 74 | ARG | NE-CZ-NH2 | -5.22 | 117.69 | 120.30 |
| 1 | B | 113 | LEU | CB-CA-C | -5.22 | 100.28 | 110.20 |
| 1 | D | 208 | MET | CB-CG-SD | 5.22 | 128.06 | 112.40 |
| 1 | F | 63 | PRO | N-CD-CG | -5.22 | 95.37 | 103.20 |
| 1 | F | 193 | THR | OG1-CB-CG2 | -5.22 | 97.99 | 110.00 |
| 1 | L | 181 | GLN | N-CA-C | -5.22 | 96.91 | 111.00 |
| 1 | M | 223 | ASP | CB-CA-C | -5.22 | 99.96 | 110.40 |
| 1 | O | 212 | THR | CA-CB-CG2 | -5.22 | 105.09 | 112.40 |
| 1 | F | 247 | PHE | CB-CG-CD2 | -5.22 | 117.15 | 120.80 |
| 1 | L | 72 | VAL | CG1-CB-CG2 | -5.22 | 102.55 | 110.90 |
| 1 | L | 194 | VAL | CA-C-O | 5.22 | 131.05 | 120.10 |
| 1 | F | 253 | GLU | OE1-CD-OE2 | 5.21 | 129.56 | 123.30 |
| 1 | I | 179 | ALA | N-CA-CB | 5.21 | 117.40 | 110.10 |
| 1 | E | 234 | TYR | CG-CD2-CE2 | 5.21 | 125.47 | 121.30 |
| 1 | O | 390 | TYR | CZ-CE2-CD2 | -5.21 | 115.11 | 119.80 |
| 1 | A | 311 | TYR | OH-CZ-CE2 | 5.21 | 134.16 | 120.10 |
| 1 | I | 236 | LYS | CD-CE-NZ | -5.21 | 99.72 | 111.70 |
| 1 | B | 335 | ASP | CB-CG-OD2 | -5.21 | 113.61 | 118.30 |
| 1 | N | 21 | VAL | CB-CA-C | -5.21 | 101.51 | 111.40 |
| 1 | H | 374 | PHE | CZ-CE2-CD2 | -5.21 | 113.85 | 120.10 |
| 1 | I | 257 | VAL | CB-CA-C | -5.20 | 101.51 | 111.40 |
| 1 | J | 340 | THR | CA-CB-CG2 | -5.20 | 105.11 | 112.40 |
| 1 | L | 171 | LYS | CD-CE-NZ | -5.20 | 99.73 | 111.70 |
| 1 | N | 264 | ALA | C-N-CA | -5.20 | 111.37 | 122.30 |
| 1 | N | 468 | PHE | N-CA-C | 5.20 | 125.05 | 111.00 |
| 1 | A | 334 | VAL | CG1-CB-CG2 | -5.20 | 102.58 | 110.90 |
| 1 | N | 226 | THR | CA-CB-CG2 | -5.20 | 105.12 | 112.40 |
| 1 | B | 247 | PHE | CB-CG-CD1 | 5.20 | 124.44 | 120.80 |
| 1 | D | 337 | THR | CB-CA-C | -5.20 | 97.56 | 111.60 |
| 1 | G | 109 | ARG | NE-CZ-NH2 | 5.20 | 122.90 | 120.30 |
| 1 | I | 142 | ASP | OD1-CG-OD2 | -5.20 | 113.43 | 123.30 |
| 1 | K | 311 | TYR | CG-CD1-CE1 | -5.20 | 117.14 | 121.30 |
| 1 | L | 245 | SER | CB-CA-C | 5.20 | 119.97 | 110.10 |
| 1 | M | 283 | THR | C-N-CA | -5.20 | 108.71 | 121.70 |
| 1 | M | 460 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 1 | N | 250 | LEU | CB-CG-CD2 | 5.20 | 119.83 | 111.00 |
| 1 | E | 464 | LEU | CA-CB-CG | -5.19 | 103.36 | 115.30 |
| 1 | F | 220 | VAL | CA-CB-CG2 | 5.19 | 118.69 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 211 | THR | OG1-CB-CG2 | -5.19 | 98.06 | 110.00 |
| 1 | D | 462 | PHE | CB-CG-CD1 | -5.19 | 117.17 | 120.80 |
| 1 | A | 258 | ARG | NE-CZ-NH2 | -5.19 | 117.71 | 120.30 |
| 1 | K | 180 | VAL | N-CA-C | 5.19 | 125.00 | 111.00 |
| 1 | F | 213 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 1 | A | 180 | VAL | CB-CA-C | -5.18 | 101.55 | 111.40 |
| 1 | H | 147 | ILE | CA-CB-CG2 | 5.18 | 121.27 | 110.90 |
| 1 | N | 446 | PHE | N-CA-CB | -5.18 | 101.27 | 110.60 |
| 1 | H | 103 | VAL | CG1-CB-CG2 | 5.18 | 119.19 | 110.90 |
| 1 | J | 171 | LYS | CA-C-N | -5.18 | 105.84 | 116.20 |
| 1 | L | 184 | ASP | CB-CG-OD2 | -5.18 | 113.64 | 118.30 |
| 1 | A | 440 | PRO | CA-N-CD | 5.18 | 118.95 | 111.70 |
| 1 | B | 399 | LEU | CB-CG-CD2 | 5.18 | 119.80 | 111.00 |
| 1 | N | 292 | PHE | CA-C-O | -5.18 | 109.23 | 120.10 |
| 1 | H | 178 | VAL | O-C-N | 5.17 | 130.98 | 122.70 |
| 1 | J | 107 | VAL | CG1-CB-CG2 | 5.17 | 119.17 | 110.90 |
| 1 | B | 356 | LYS | CG-CD-CE | -5.17 | 96.40 | 111.90 |
| 1 | D | 337 | THR | N-CA-C | 5.17 | 124.95 | 111.00 |
| 1 | E | 400 | GLU | OE1-CD-OE2 | -5.17 | 117.10 | 123.30 |
| 1 | G | 333 | VAL | CA-CB-CG2 | -5.17 | 103.15 | 110.90 |
| 1 | M | 103 | VAL | CA-CB-CG2 | 5.17 | 118.65 | 110.90 |
| 1 | N | 292 | PHE | N-CA-CB | -5.17 | 101.30 | 110.60 |
| 1 | G | 49 | TYR | CB-CG-CD1 | -5.17 | 117.90 | 121.00 |
| 1 | B | 251 | ARG | CG-CD-NE | -5.16 | 100.95 | 111.80 |
| 1 | F | 151 | TYR | CB-CG-CD2 | -5.16 | 117.90 | 121.00 |
| 1 | F | 336 | THR | CA-CB-OG1 | -5.16 | 98.16 | 109.00 |
| 1 | G | 22 | VAL | CA-CB-CG2 | -5.16 | 103.16 | 110.90 |
| 1 | G | 65 | VAL | N-CA-CB | -5.16 | 100.15 | 111.50 |
| 1 | H | 41 | ARG | NH1-CZ-NH2 | 5.16 | 125.08 | 119.40 |
| 1 | M | 266 | THR | CB-CA-C | -5.16 | 97.67 | 111.60 |
| 1 | E | 62 | VAL | CG1-CB-CG2 | 5.16 | 119.15 | 110.90 |
| 1 | N | 383 | LEU | CB-CG-CD1 | 5.16 | 119.77 | 111.00 |
| 1 | B | 29 | ALA | N-CA-CB | -5.16 | 102.88 | 110.10 |
| 1 | I | 143 | ASN | CB-CA-C | -5.16 | 100.09 | 110.40 |
| 1 | E | 139 | ALA | C-N-CA | -5.15 | 111.48 | 122.30 |
| 1 | H | 126 | LEU | CB-CG-CD1 | 5.15 | 119.76 | 111.00 |
| 1 | L | 150 | ASP | CB-CG-OD1 | -5.15 | 113.66 | 118.30 |
| 1 | G | 383 | LEU | CB-CG-CD2 | -5.15 | 102.25 | 111.00 |
| 1 | L | 144 | ARG | N-CA-CB | -5.15 | 101.33 | 110.60 |
| 1 | J | 109 | ARG | NE-CZ-NH2 | -5.15 | 117.73 | 120.30 |
| 1 | O | 180 | VAL | CB-CA-C | -5.15 | 101.62 | 111.40 |
| 1 | E | 151 | TYR | CG-CD1-CE1 | -5.15 | 117.18 | 121.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | H | 215 | ALA | N-CA-CB | 5.15 | 117.30 | 110.10 |
| 1 | B | 292 | PHE | CB-CG-CD1 | 5.14 | 124.40 | 120.80 |
| 1 | N | 129 | THR | OG1-CB-CG2 | 5.14 | 121.83 | 110.00 |
| 1 | F | 202 | ASP | N-CA-C | -5.14 | 97.12 | 111.00 |
| 1 | G | 304 | ALA | CB-CA-C | -5.14 | 102.39 | 110.10 |
| 1 | H | 97 | ARG | CA-C-N | -5.14 | 105.89 | 117.20 |
| 1 | N | 452 | LYS | CD-CE-NZ | 5.14 | 123.52 | 111.70 |
| 1 | D | 45 | VAL | CG1-CB-CG2 | -5.14 | 102.68 | 110.90 |
| 1 | M | 253 | GLU | N-CA-CB | -5.14 | 101.35 | 110.60 |
| 1 | A | 381 | ILE | CB-CA-C | -5.14 | 101.33 | 111.60 |
| 1 | E | 74 | ARG | NE-CZ-NH2 | 5.13 | 122.87 | 120.30 |
| 1 | J | 32 | ASN | CB-CA-C | -5.13 | 100.13 | 110.40 |
| 1 | J | 157 | CYS | N-CA-CB | -5.13 | 101.36 | 110.60 |
| 1 | M | 311 | TYR | CG-CD1-CE1 | 5.13 | 125.41 | 121.30 |
| 1 | O | 346 | ALA | N-CA-CB | 5.13 | 117.29 | 110.10 |
| 1 | O | 177 | GLN | N-CA-C | -5.13 | 97.15 | 111.00 |
| 1 | F | 85 | PHE | CB-CG-CD1 | 5.13 | 124.39 | 120.80 |
| 1 | M | 175 | CYS | N-CA-C | -5.13 | 97.15 | 111.00 |
| 1 | C | 198 | GLY | N-CA-C | 5.13 | 125.91 | 113.10 |
| 1 | E | 49 | TYR | CD1-CE1-CZ | 5.13 | 124.41 | 119.80 |
| 1 | E | 98 | LEU | CB-CG-CD1 | 5.13 | 119.71 | 111.00 |
| 1 | H | 462 | PHE | CB-CG-CD1 | -5.13 | 117.21 | 120.80 |
| 1 | O | 240 | GLU | CG-CD-OE1 | 5.13 | 128.55 | 118.30 |
| 1 | H | 191 | ILE | CB-CG1-CD1 | -5.12 | 99.55 | 113.90 |
| 1 | F | 222 | LEU | C-N-CA | -5.12 | 108.90 | 121.70 |
| 1 | J | 455 | PHE | CB-CG-CD2 | -5.12 | 117.21 | 120.80 |
| 1 | B | 266 | THR | CB-CA-C | -5.12 | 97.78 | 111.60 |
| 1 | C | 396 | SER | CB-CA-C | 5.12 | 119.83 | 110.10 |
| 1 | J | 144 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 1 | L | 61 | LEU | CB-CG-CD2 | 5.12 | 119.70 | 111.00 |
| 1 | L | 219 | GLU | OE1-CD-OE2 | 5.12 | 129.44 | 123.30 |
| 1 | L | 383 | LEU | CB-CG-CD2 | -5.12 | 102.30 | 111.00 |
| 1 | K | 43 | LEU | CB-CG-CD2 | -5.12 | 102.30 | 111.00 |
| 1 | J | 93 | PRO | CA-N-CD | -5.12 | 104.34 | 111.50 |
| 1 | L | 152 | LYS | CD-CE-NZ | 5.12 | 123.47 | 111.70 |
| 1 | G | 364 | LEU | CB-CG-CD1 | -5.11 | 102.31 | 111.00 |
| 1 | N | 374 | PHE | CB-CG-CD1 | -5.11 | 117.22 | 120.80 |
| 1 | F | 33 | ILE | CG1-CB-CG2 | -5.11 | 100.16 | 111.40 |
| 1 | G | 94 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | I | 42 | LEU | CA-CB-CG | -5.11 | 103.55 | 115.30 |
| 1 | I | 113 | LEU | C-N-CA | -5.11 | 111.57 | 122.30 |
| 1 | L | 151 | TYR | N-CA-CB | -5.11 | 101.40 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | J | 439 | ASP | CB-CG-OD1 | -5.11 | 113.70 | 118.30 |
| 1 | K | 70 | TYR | CG-CD2-CE2 | 5.11 | 125.39 | 121.30 |
| 1 | C | 146 | CYS | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | D | 201 | VAL | CA-CB-CG1 | -5.11 | 103.24 | 110.90 |
| 1 | K | 179 | ALA | N-CA-CB | 5.11 | 117.25 | 110.10 |
| 1 | M | 164 | PRO | CA-N-CD | -5.11 | 104.35 | 111.50 |
| 1 | H | 277 | ILE | CB-CG1-CD1 | -5.10 | 99.61 | 113.90 |
| 1 | N | 315 | ARG | NH1-CZ-NH2 | 5.10 | 125.01 | 119.40 |
| 1 | O | 105 | VAL | CA-CB-CG1 | -5.10 | 103.25 | 110.90 |
| 1 | D | 402 | TRP | CA-C-N | -5.10 | 105.98 | 117.20 |
| 1 | I | 201 | VAL | CA-CB-CG1 | -5.10 | 103.25 | 110.90 |
| 1 | L | 44 | ALA | O-C-N | -5.10 | 114.54 | 122.70 |
| 1 | B | 22 | VAL | CB-CA-C | -5.10 | 101.71 | 111.40 |
| 1 | E | 223 | ASP | CB-CG-OD2 | -5.10 | 113.71 | 118.30 |
| 1 | E | 470 | LEU | N-CA-C | 5.10 | 124.77 | 111.00 |
| 1 | D | 304 | ALA | CB-CA-C | -5.09 | 102.46 | 110.10 |
| 1 | L | 333 | VAL | CA-CB-CG1 | -5.09 | 103.26 | 110.90 |
| 1 | M | 144 | ARG | CG-CD-NE | -5.09 | 101.10 | 111.80 |
| 1 | I | 219 | GLU | OE1-CD-OE2 | -5.09 | 117.19 | 123.30 |
| 1 | J | 234 | TYR | CB-CG-CD1 | -5.09 | 117.94 | 121.00 |
| 1 | B | 457 | ALA | CB-CA-C | 5.09 | 117.74 | 110.10 |
| 1 | G | 242 | TYR | CB-CG-CD1 | -5.09 | 117.95 | 121.00 |
| 1 | G | 251 | ARG | C-N-CA | -5.09 | 108.97 | 121.70 |
| 1 | M | 65 | VAL | CA-CB-CG1 | 5.09 | 118.54 | 110.90 |
| 1 | A | 398 | ILE | CB-CA-C | -5.09 | 101.42 | 111.60 |
| 1 | C | 285 | ASN | N-CA-CB | -5.09 | 101.44 | 110.60 |
| 1 | O | 220 | VAL | CG1-CB-CG2 | 5.09 | 119.04 | 110.90 |
| 1 | I | 242 | TYR | CB-CG-CD2 | 5.09 | 124.05 | 121.00 |
| 1 | B | 297 | GLY | N-CA-C | -5.09 | 100.38 | 113.10 |
| 1 | C | 315 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 |
| 1 | E | 258 | ARG | NE-CZ-NH2 | -5.09 | 117.76 | 120.30 |
| 1 | B | 363 | TYR | OH-CZ-CE2 | -5.08 | 106.37 | 120.10 |
| 1 | I | 250 | LEU | N-CA-CB | 5.08 | 120.56 | 110.40 |
| 1 | L | 338 | ARG | O-C-N | 5.08 | 130.82 | 122.70 |
| 1 | B | 214 | GLN | CB-CA-C | -5.08 | 100.25 | 110.40 |
| 1 | M | 263 | ARG | NE-CZ-NH2 | -5.08 | 117.76 | 120.30 |
| 1 | B | 195 | ILE | CG1-CB-CG2 | -5.07 | 100.24 | 111.40 |
| 1 | K | 260 | LEU | CB-CG-CD1 | -5.07 | 102.38 | 111.00 |
| 1 | F | 31 | THR | OG1-CB-CG2 | 5.07 | 121.66 | 110.00 |
| 1 | H | 240 | GLU | OE1-CD-OE2 | 5.07 | 129.38 | 123.30 |
| 1 | F | 319 | HIS | N-CA-C | 5.07 | 124.69 | 111.00 |
| 1 | I | 459 | LEU | CB-CG-CD2 | -5.07 | 102.38 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | J | 98 | LEU | CA-CB-CG | 5.07 | 126.96 | 115.30 |
| 1 | B | 226 | THR | CA-CB-CG2 | -5.07 | 105.31 | 112.40 |
| 1 | B | 186 | PRO | N-CD-CG | 5.06 | 110.79 | 103.20 |
| 1 | E | 390 | TYR | CG-CD2-CE2 | -5.06 | 117.25 | 121.30 |
| 1 | H | 286 | LEU | CB-CG-CD2 | -5.06 | 102.39 | 111.00 |
| 1 | I | 281 | GLY | N-CA-C | -5.06 | 100.44 | 113.10 |
| 1 | J | 217 | LYS | CD-CE-NZ | -5.06 | 100.06 | 111.70 |
| 1 | G | 174 | PRO | CA-C-N | -5.06 | 106.07 | 117.20 |
| 1 | G | 334 | VAL | N-CA-C | -5.06 | 97.34 | 111.00 |
| 1 | L | 156 | LEU | CB-CG-CD1 | 5.06 | 119.60 | 111.00 |
| 1 | I | 117 | ILE | CG1-CB-CG2 | 5.05 | 122.52 | 111.40 |
| 1 | N | 261 | PHE | CA-C-N | -5.05 | 106.08 | 117.20 |
| 1 | J | 213 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 1 | M | 175 | CYS | CA-CB-SG | -5.05 | 104.91 | 114.00 |
| 1 | O | 293 | PRO | CA-CB-CG | -5.05 | 94.40 | 104.00 |
| 1 | K | 261 | PHE | CB-CG-CD2 | 5.05 | 124.33 | 120.80 |
| 1 | M | 362 | GLU | CG-CD-OE2 | -5.05 | 108.20 | 118.30 |
| 1 | E | 459 | LEU | CB-CG-CD2 | -5.05 | 102.42 | 111.00 |
| 1 | A | 145 | GLU | CG-CD-OE1 | -5.04 | 108.21 | 118.30 |
| 1 | L | 277 | ILE | CG1-CB-CG2 | -5.04 | 100.30 | 111.40 |
| 1 | M | 277 | ILE | CG1-CB-CG2 | -5.04 | 100.30 | 111.40 |
| 1 | C | 248 | PHE | CB-CG-CD2 | -5.04 | 117.27 | 120.80 |
| 1 | I | 144 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | M | 99 | VAL | CG1-CB-CG2 | -5.04 | 102.83 | 110.90 |
| 1 | A | 231 | TYR | CZ-CE2-CD2 | 5.04 | 124.34 | 119.80 |
| 1 | L | 77 | LEU | CB-CG-CD1 | 5.04 | 119.57 | 111.00 |
| 1 | M | 115 | VAL | CG1-CB-CG2 | 5.04 | 118.97 | 110.90 |
| 1 | I | 193 | THR | N-CA-CB | -5.04 | 100.73 | 110.30 |
| 1 | L | 242 | TYR | CD1-CE1-CZ | -5.04 | 115.27 | 119.80 |
| 1 | K | 54 | LYS | CD-CE-NZ | 5.04 | 123.28 | 111.70 |
| 1 | E | 293 | PRO | N-CD-CG | -5.03 | 95.65 | 103.20 |
| 1 | K | 74 | ARG | N-CA-C | -5.03 | 97.41 | 111.00 |
| 1 | B | 238 | VAL | CA-CB-CG1 | 5.03 | 118.45 | 110.90 |
| 1 | I | 226 | THR | CB-CA-C | -5.03 | 98.02 | 111.60 |
| 1 | J | 70 | TYR | N-CA-C | -5.03 | 97.42 | 111.00 |
| 1 | E | 335 | ASP | CB-CG-OD2 | 5.03 | 122.83 | 118.30 |
| 1 | J | 380 | LYS | CD-CE-NZ | 5.03 | 123.27 | 111.70 |
| 1 | N | 338 | ARG | NE-CZ-NH2 | -5.03 | 117.79 | 120.30 |
| 1 | E | 165 | ILE | CG1-CB-CG2 | 5.03 | 122.46 | 111.40 |
| 1 | B | 142 | ASP | OD1-CG-OD2 | 5.03 | 132.85 | 123.30 |
| 1 | F | 45 | VAL | CG1-CB-CG2 | 5.03 | 118.94 | 110.90 |
| 1 | J | 294 | THR | CA-C-O | -5.03 | 109.55 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | K | 22 | VAL | CB-CA-C | -5.03 | 101.85 | 111.40 |
| 1 | C | 472 | LEU | CB-CG-CD2 | -5.02 | 102.46 | 111.00 |
| 1 | H | 87 | ASP | CB-CG-OD1 | -5.02 | 113.78 | 118.30 |
| 1 | D | 173 | SER | N-CA-CB | 5.02 | 118.03 | 110.50 |
| 1 | J | 42 | LEU | CB-CG-CD1 | -5.02 | 102.47 | 111.00 |
| 1 | E | 180 | VAL | CA-C-O | 5.02 | 130.64 | 120.10 |
| 1 | H | 472 | LEU | CA-CB-CG | 5.02 | 126.85 | 115.30 |
| 1 | F | 469 | LEU | CB-CG-CD1 | -5.02 | 102.47 | 111.00 |
| 1 | I | 230 | LYS | CA-CB-CG | -5.02 | 102.36 | 113.40 |
| 1 | J | 238 | VAL | CG1-CB-CG2 | -5.02 | 102.87 | 110.90 |
| 1 | L | 281 | GLY | N-CA-C | -5.02 | 100.56 | 113.10 |
| 1 | O | 156 | LEU | CB-CG-CD2 | -5.02 | 102.47 | 111.00 |
| 1 | E | 209 | ASP | N-CA-C | -5.02 | 97.46 | 111.00 |
| 1 | F | 205 | PHE | C-N-CA | -5.02 | 111.77 | 122.30 |
| 1 | H | 390 | TYR | CB-CG-CD1 | 5.02 | 124.01 | 121.00 |
| 1 | C | 102 | CYS | CA-CB-SG | -5.01 | 104.97 | 114.00 |
| 1 | F | 112 | PRO | N-CD-CG | -5.01 | 95.68 | 103.20 |
| 1 | J | 311 | TYR | CD1-CE1-CZ | -5.01 | 115.29 | 119.80 |
| 1 | O | 350 | THR | CA-CB-CG2 | -5.01 | 105.38 | 112.40 |
| 1 | A | 364 | LEU | CB-CG-CD2 | 5.01 | 119.52 | 111.00 |
| 1 | L | 276 | TYR | CB-CA-C | -5.01 | 100.38 | 110.40 |
| 1 | A | 103 | VAL | CB-CA-C | -5.01 | 101.88 | 111.40 |
| 1 | K | 224 | ILE | N-CA-C | 5.01 | 124.52 | 111.00 |
| 1 | L | 310 | PRO | CA-CB-CG | -5.01 | 94.48 | 104.00 |
| 1 | O | 312 | TRP | CD1-NE1-CE2 | -5.01 | 104.49 | 109.00 |
| 1 | O | 331 | VAL | CA-CB-CG1 | 5.01 | 118.42 | 110.90 |
| 1 | I | 456 | SER | CA-CB-OG | -5.01 | 97.68 | 111.20 |
| 1 | L | 49 | TYR | CZ-CE2-CD2 | -5.00 | 115.30 | 119.80 |
| 1 | J | 244 | ASP | CB-CG-OD1 | 5.00 | 122.80 | 118.30 |
| 1 | J | 323 | ILE | CB-CA-C | -5.00 | 101.60 | 111.60 |
| 1 | M | 176 | THR | CA-CB-CG2 | -5.00 | 105.40 | 112.40 |
| 1 | N | 260 | LEU | CB-CG-CD2 | -5.00 | 102.50 | 111.00 |
| 1 | O | 159 | ILE | CA-CB-CG2 | -5.00 | 100.90 | 110.90 |

There are no chirality outliers.

All (13) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | C | 292 | PHE | Sidechain |
| 1 | C | 390 | TYR | Sidechain |
| 1 | C | 70 | TYR | Sidechain |
| 1 | D | 294 | THR | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | E | 234 | TYR | Sidechain |
| 1 | F | 383 | LEU | Mainchain |
| 1 | G | 135 | TYR | Sidechain |
| 1 | L | 276 | TYR | Sidechain |
| 1 | L | 311 | TYR | Sidechain |
| 1 | L | 390 | TYR | Sidechain |
| 1 | M | 271 | VAL | Mainchain |
| 1 | N | 249 | TYR | Sidechain |
| 1 | O | 291 | TYR | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3310 | 0 | 3213 | 561 | 0 |
| 1 | B | 3310 | 0 | 3213 | 550 | 0 |
| 1 | C | 3310 | 0 | 3213 | 527 | 0 |
| 1 | D | 3310 | 0 | 3213 | 540 | 11 |
| 1 | E | 3310 | 0 | 3213 | 509 | 5 |
| 1 | F | 3310 | 0 | 3213 | 553 | 5 |
| 1 | G | 3310 | 0 | 3213 | 579 | 0 |
| 1 | H | 3310 | 0 | 3213 | 520 | 5 |
| 1 | I | 3310 | 0 | 3213 | 568 | 26 |
| 1 | J | 3310 | 0 | 3213 | 543 | 26 |
| 1 | K | 3310 | 0 | 3213 | 526 | 0 |
| 1 | L | 3310 | 0 | 3213 | 530 | 0 |
| 1 | M | 3310 | 0 | 3213 | 537 | 5 |
| 1 | N | 3310 | 0 | 3213 | 540 | 11 |
| 1 | O | 3310 | 0 | 3213 | 531 | 0 |
| All | All | 49650 | 0 | 48195 | 7270 | 47 |

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 74.

All (7270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:115:VAL:CG1 | 1:D:115:VAL:CB | 1.75 | 1.65 |
| 1:B:82:LYS:CB | 1:B:82:LYS:CG | 1.75 | 1.64 |
| 1:I:88:THR:CB | 1:I:88:THR:CG2 | 1.76 | 1.64 |
| 1:F:176:THR:CB | 1:F:176:THR:CG2 | 1.74 | 1.64 |
| 1:O:331:VAL:CB | 1:O:331:VAL:CG1 | 1.75 | 1.63 |
| 1:N:95:THR:CB | 1:N:95:THR:CG2 | 1.76 | 1.63 |
| 1:L:309:LYS:CD | 1:L:309:LYS:CE | 1.75 | 1.63 |
| 1:E:323:ILE:CB | 1:E:323:ILE:CG2 | 1.76 | 1.62 |
| 1:C:348:ILE:CD1 | 1:C:348:ILE:CG1 | 1.74 | 1.61 |
| 1:F:353:THR:CB | 1:F:353:THR:CG2 | 1.75 | 1.61 |
| 1:F:389:THR:CB | 1:F:389:THR:CG2 | 1.75 | 1.61 |
| 1:I:61:LEU:CG | 1:I:61:LEU:CD1 | 1.74 | 1.61 |
| 1:K:452:LYS:CG | 1:K:452:LYS:CD | 1.76 | 1.61 |
| 1:A:228:ILE:CD1 | 1:A:228:ILE:CG1 | 1.75 | 1.61 |
| 1:D:301:THR:CB | 1:D:301:THR:CG2 | 1.75 | 1.61 |
| 1:J:300:VAL:CB | 1:J:300:VAL:CG1 | 1.78 | 1.61 |
| 1:F:178:VAL:CG1 | 1:F:178:VAL:CB | 1.75 | 1.61 |
| 1:B:33:ILE:CG1 | 1:B:33:ILE:CD1 | 1.79 | 1.61 |
| 1:D:64:LYS:CB | 1:D:64:LYS:CG | 1.76 | 1.61 |
| 1:J:180:VAL:CB | 1:J:180:VAL:CG2 | 1.78 | 1.61 |
| 1:M:98:LEU:CG | 1:M:98:LEU:CD1 | 1.76 | 1.61 |
| 1:A:178:VAL:CG1 | 1:A:178:VAL:CB | 1.75 | 1.60 |
| 1:H:380:LYS:CE | 1:H:380:LYS:CD | 1.75 | 1.60 |
| 1:M:137:ALA:CA | 1:M:137:ALA:CB | 1.77 | 1.60 |
| 1:M:441:LEU:CD2 | 1:M:441:LEU:CG | 1.77 | 1.60 |
| 1:K:346:ALA:CA | 1:K:346:ALA:CB | 1.75 | 1.60 |
| 1:D:380:LYS:CD | 1:D:380:LYS:CE | 1.77 | 1.60 |
| 1:K:230:LYS:CG | 1:K:230:LYS:CD | 1.78 | 1.60 |
| 1:B:61:LEU:CD1 | 1:B:61:LEU:CG | 1.77 | 1.60 |
| 1:B:441:LEU:CD2 | 1:B:441:LEU:CG | 1.80 | 1.60 |
| 1:H:469:LEU:CD2 | 1:H:469:LEU:CG | 1.80 | 1.60 |
| 1:I:277:ILE:CG1 | 1:I:277:ILE:CD1 | 1.79 | 1.60 |
| 1:O:187:PRO:CG | 1:O:187:PRO:CD | 1.74 | 1.60 |
| 1:I:82:LYS:CD | 1:I:82:LYS:CE | 1.79 | 1.59 |
| 1:A:381:ILE:CB | 1:A:381:ILE:CG2 | 1.77 | 1.59 |
| 1:B:467:LYS:CD | 1:B:467:LYS:CG | 1.79 | 1.59 |
| 1:D:53:LYS:CB | 1:D:53:LYS:CG | 1.75 | 1.59 |
| 1:E:389:THR:CB | 1:E:389:THR:CG2 | 1.75 | 1.59 |
| 1:L:61:LEU:CG | 1:L:61:LEU:CD1 | 1.75 | 1.59 |
| 1:F:154:THR:CB | 1:F:154:THR:CG2 | 1.77 | 1.59 |
| 1:I:236:LYS:CB | 1:I:236:LYS:CG | 1.79 | 1.59 |
| 1:C:178:VAL:CG1 | 1:C:178:VAL:CB | 1.80 | 1.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:117:ILE:CB | 1:F:117:ILE:CG2 | 1.74 | 1.59 |
| 1:F:117:ILE:CG1 | 1:F:117:ILE:CD1 | 1.76 | 1.59 |
| 1:J:178:VAL:CB | 1:J:178:VAL:CG1 | 1.77 | 1.59 |
| 1:D:194:VAL:CB | 1:D:194:VAL:CG2 | 1.74 | 1.59 |
| 1:F:139:ALA:CA | 1:F:139:ALA:CB | 1.79 | 1.59 |
| 1:A:300:VAL:CG1 | 1:A:300:VAL:CB | 1.77 | 1.58 |
| 1:F:33:ILE:CG1 | 1:F:33:ILE:CD1 | 1.80 | 1.58 |
| 1:J:236:LYS:CG | 1:J:236:LYS:CD | 1.79 | 1.58 |
| 1:N:228:ILE:CG1 | 1:N:228:ILE:CD1 | 1.78 | 1.58 |
| 1:O:452:LYS:CE | 1:O:452:LYS:CD | 1.74 | 1.58 |
| 1:C:59:LYS:CD | 1:C:59:LYS:CE | 1.77 | 1.58 |
| 1:E:33:ILE:CG1 | 1:E:33:ILE:CD1 | 1.75 | 1.58 |
| 1:C:217:LYS:CD | 1:C:217:LYS:CE | 1.78 | 1.58 |
| 1:I:193:THR:CB | 1:I:193:THR:CG2 | 1.74 | 1.58 |
| 1:J:105:VAL:CB | 1:J:105:VAL:CG2 | 1.77 | 1.58 |
| 1:K:30:ARG:CG | 1:K:30:ARG:CD | 1.74 | 1.58 |
| 1:F:467:LYS:CD | 1:F:467:LYS:CE | 1.79 | 1.58 |
| 1:F:383:LEU:CD2 | 1:F:383:LEU:CG | 1.78 | 1.58 |
| 1:K:266:THR:CB | 1:K:266:THR:CG2 | 1.77 | 1.58 |
| 1:N:112:PRO:CD | 1:N:112:PRO:CG | 1.78 | 1.58 |
| 1:O:235:ILE:CG1 | 1:O:235:ILE:CD1 | 1.82 | 1.58 |
| 1:B:171:LYS:CG | 1:B:171:LYS:CD | 1.75 | 1.57 |
| 1:E:213:LEU:CD1 | 1:E:213:LEU:CG | 1.76 | 1.57 |
| 1:G:337:THR:CB | 1:G:337:THR:CG2 | 1.74 | 1.57 |
| 1:I:358:THR:CB | 1:I:358:THR:CG2 | 1.74 | 1.57 |
| 1:E:152:LYS:CD | 1:E:152:LYS:CE | 1.81 | 1.57 |
| 1:E:178:VAL:CB | 1:E:178:VAL:CG1 | 1.76 | 1.57 |
| 1:C:356:LYS:NZ | 1:C:356:LYS:CE | 1.68 | 1.57 |
| 1:G:98:LEU:CG | 1:G:98:LEU:CD1 | 1.78 | 1.57 |
| 1:N:28:VAL:CG1 | 1:N:28:VAL:CB | 1.75 | 1.57 |
| 1:C:353:THR:CB | 1:C:353:THR:CG2 | 1.77 | 1.57 |
| 1:N:338:ARG:CG | 1:N:338:ARG:CD | 1.75 | 1.57 |
| 1:A:178:VAL:CB | 1:A:178:VAL:CG2 | 1.78 | 1.57 |
| 1:F:365:ARG:CD | 1:F:365:ARG:CG | 1.83 | 1.57 |
| 1:H:59:LYS:CD | 1:H:59:LYS:CE | 1.76 | 1.57 |
| 1:H:266:THR:CB | 1:H:266:THR:CG2 | 1.74 | 1.57 |
| 1:J:88:THR:CB | 1:J:88:THR:CG2 | 1.80 | 1.57 |
| 1:B:442:LYS:NZ | 1:B:442:LYS:CE | 1.68 | 1.56 |
| 1:I:179:ALA:CB | 1:I:179:ALA:CA | 1.81 | 1.56 |
| 1:N:61:LEU:CD1 | 1:N:61:LEU:CG | 1.74 | 1.56 |
| 1:A:64:LYS:CB | 1:A:64:LYS:CG | 1.75 | 1.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:123:LEU:CD2 | 1:D:123:LEU:CG | 1.76 | 1.56 |
| 1:O:98:LEU:CG | 1:O:98:LEU:CD1 | 1.76 | 1.56 |
| 1:E:228:ILE:CG1 | 1:E:228:ILE:CD1 | 1.83 | 1.56 |
| 1:I:117:ILE:CG1 | 1:I:117:ILE:CD1 | 1.78 | 1.56 |
| 1:I:369:GLU:CB | 1:I:369:GLU:CG | 1.76 | 1.56 |
| 1:M:64:LYS:CG | 1:M:64:LYS:CB | 1.80 | 1.56 |
| 1:N:88:THR:CB | 1:N:88:THR:CG2 | 1.75 | 1.56 |
| 1:O:117:ILE:CD1 | 1:O:117:ILE:CG1 | 1.77 | 1.56 |
| 1:N:313:LEU:CD2 | 1:N:313:LEU:CG | 1.81 | 1.56 |
| 1:C:464:LEU:CG | 1:C:464:LEU:CD1 | 1.84 | 1.56 |
| 1:G:201:VAL:CB | 1:G:201:VAL:CG2 | 1.76 | 1.56 |
| 1:K:452:LYS:CD | 1:K:452:LYS:CE | 1.79 | 1.56 |
| 1:E:165:ILE:CD1 | 1:E:165:ILE:CG1 | 1.81 | 1.55 |
| 1:H:277:ILE:CG1 | 1:H:277:ILE:CD1 | 1.83 | 1.55 |
| 1:C:441:LEU:CD2 | 1:C:441:LEU:CG | 1.83 | 1.55 |
| 1:G:470:LEU:CG | 1:G:470:LEU:CD1 | 1.75 | 1.55 |
| 1:K:178:VAL:CG1 | 1:K:178:VAL:CB | 1.77 | 1.55 |
| 1:N:382:THR:CB | 1:N:382:THR:CG2 | 1.78 | 1.55 |
| 1:O:176:THR:CB | 1:O:176:THR:CG2 | 1.77 | 1.55 |
| 1:F:54:LYS:NZ | 1:F:54:LYS:CE | 1.68 | 1.55 |
| 1:L:361:LYS:NZ | 1:L:361:LYS:CE | 1.70 | 1.55 |
| 1:N:32:ASN:CG | 1:N:32:ASN:CB | 1.74 | 1.55 |
| 1:C:77:LEU:CD2 | 1:C:77:LEU:CG | 1.79 | 1.55 |
| 1:D:80:PRO:CG | 1:D:80:PRO:CD | 1.76 | 1.55 |
| 1:G:105:VAL:CB | 1:G:105:VAL:CG2 | 1.78 | 1.55 |
| 1:H:139:ALA:CB | 1:H:139:ALA:CA | 1.78 | 1.55 |
| 1:H:361:LYS:CG | 1:H:361:LYS:CB | 1.77 | 1.55 |
| 1:L:152:LYS:CD | 1:L:152:LYS:CE | 1.79 | 1.55 |
| 1:B:123:LEU:CG | 1:B:123:LEU:CD2 | 1.83 | 1.54 |
| 1:D:174:PRO:CB | 1:D:174:PRO:CG | 1.81 | 1.54 |
| 1:L:275:LEU:CD2 | 1:L:275:LEU:CG | 1.83 | 1.54 |
| 1:G:230:LYS:NZ | 1:G:230:LYS:CE | 1.68 | 1.54 |
| 1:J:147:ILE:CG1 | 1:J:147:ILE:CD1 | 1.85 | 1.54 |
| 1:M:32:ASN:CB | 1:M:32:ASN:CG | 1.76 | 1.54 |
| 1:D:176:THR:CA | 1:D:176:THR:CB | 1.78 | 1.54 |
| 1:K:165:ILE:CG1 | 1:K:165:ILE:CD1 | 1.83 | 1.54 |
| 1:N:123:LEU:CD2 | 1:N:123:LEU:CG | 1.82 | 1.54 |
| 1:K:159:ILE:CG1 | 1:K:159:ILE:CD1 | 1.76 | 1.54 |
| 1:K:162:LYS:CD | 1:K:162:LYS:CE | 1.79 | 1.54 |
| 1:M:178:VAL:CB | 1:M:178:VAL:CG1 | 1.77 | 1.54 |
| 1:O:217:LYS:NZ | 1:O:217:LYS:CE | 1.70 | 1.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:164:PRO:CG | 1:O:164:PRO:CD | 1.77 | 1.53 |
| 1:D:137:ALA:CA | 1:D:137:ALA:CB | 1.77 | 1.53 |
| 1:F:467:LYS:CD | 1:F:467:LYS:CG | 1.87 | 1.53 |
| 1:G:178:VAL:CB | 1:G:178:VAL:CG1 | 1.86 | 1.53 |
| 1:G:217:LYS:NZ | 1:G:217:LYS:CE | 1.68 | 1.53 |
| 1:L:152:LYS:CE | 1:L:152:LYS:NZ | 1.71 | 1.53 |
| 1:O:398:ILE:CD1 | 1:O:398:ILE:CG1 | 1.84 | 1.53 |
| 1:B:176:THR:CB | 1:B:176:THR:CG2 | 1.84 | 1.53 |
| 1:G:20:ALA:CA | 1:G:20:ALA:CB | 1.81 | 1.53 |
| 1:E:235:ILE:CG1 | 1:E:235:ILE:CD1 | 1.80 | 1.53 |
| 1:M:147:ILE:CG1 | 1:M:147:ILE:CD1 | 1.86 | 1.53 |
| 1:C:467:LYS:CG | 1:C:467:LYS:CD | 1.80 | 1.53 |
| 1:G:309:LYS:NZ | 1:G:309:LYS:CE | 1.69 | 1.52 |
| 1:L:117:ILE:CD1 | 1:L:117:ILE:CG1 | 1.84 | 1.52 |
| 1:M:144:ARG:CG | 1:M:144:ARG:CB | 1.83 | 1.52 |
| 1:A:162:LYS:NZ | 1:A:162:LYS:CE | 1.72 | 1.52 |
| 1:A:278:LYS:NZ | 1:A:278:LYS:CE | 1.70 | 1.52 |
| 1:E:117:ILE:CG1 | 1:E:117:ILE:CD1 | 1.83 | 1.52 |
| 1:G:442:LYS:NZ | 1:G:442:LYS:CE | 1.69 | 1.52 |
| 1:N:454:LYS:NZ | 1:N:454:LYS:CE | 1.67 | 1.52 |
| 1:E:177:GLN:CD | 1:E:177:GLN:CG | 1.78 | 1.52 |
| 1:M:323:ILE:CG1 | 1:M:323:ILE:CD1 | 1.80 | 1.52 |
| 1:A:454:LYS:NZ | 1:A:454:LYS:CE | 1.69 | 1.52 |
| 1:C:60:ILE:CD1 | 1:C:60:ILE:CG1 | 1.87 | 1.52 |
| 1:H:178:VAL:CG1 | 1:H:178:VAL:CB | 1.86 | 1.52 |
| 1:A:82:LYS:NZ | 1:A:82:LYS:CE | 1.68 | 1.51 |
| 1:D:361:LYS:CG | 1:D:361:LYS:CD | 1.86 | 1.51 |
| 1:L:228:ILE:CD1 | 1:L:228:ILE:CG1 | 1.88 | 1.51 |
| 1:D:356:LYS:NZ | 1:D:356:LYS:CE | 1.71 | 1.51 |
| 1:J:454:LYS:NZ | 1:J:454:LYS:CE | 1.71 | 1.51 |
| 1:A:64:LYS:CD | 1:A:64:LYS:CE | 1.85 | 1.51 |
| 1:A:443:LYS:NZ | 1:A:443:LYS:CE | 1.68 | 1.51 |
| 1:D:454:LYS:NZ | 1:D:454:LYS:CE | 1.71 | 1.51 |
| 1:O:230:LYS:NZ | 1:O:230:LYS:CE | 1.74 | 1.51 |
| 1:A:356:LYS:NZ | 1:A:356:LYS:CE | 1.73 | 1.50 |
| 1:D:178:VAL:CB | 1:D:178:VAL:CG2 | 1.87 | 1.50 |
| 1:H:32:ASN:CB | 1:H:32:ASN:CG | 1.77 | 1.50 |
| 1:J:74:ARG:CG | 1:J:74:ARG:CD | 1.85 | 1.50 |
| 1:J:96:GLN:CA | 1:J:96:GLN:C | 1.76 | 1.50 |
| 1:D:381:ILE:CG1 | 1:D:381:ILE:CD1 | 1.83 | 1.50 |
| 1:M:86:PRO:CA | 1:M:86:PRO:C | 1.77 | 1.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:165:ILE:CD1 | 1:B:165:ILE:CG1 | 1.85 | 1.50 |
| 1:G:467:LYS:NZ | 1:G:467:LYS:CE | 1.74 | 1.50 |
| 1:L:230:LYS:NZ | 1:L:230:LYS:CE | 1.67 | 1.50 |
| 1:D:152:LYS:NZ | 1:D:152:LYS:CE | 1.70 | 1.49 |
| 1:C:241:PRO:CG | 1:C:241:PRO:CB | 1.83 | 1.49 |
| 1:A:152:LYS:NZ | 1:A:152:LYS:CE | 1.70 | 1.49 |
| 1:D:181:GLN:CG | 1:D:181:GLN:CD | 1.79 | 1.49 |
| 1:O:442:LYS:NZ | 1:O:442:LYS:CE | 1.76 | 1.49 |
| 1:D:32:ASN:CB | 1:D:32:ASN:CG | 1.79 | 1.49 |
| 1:D:60:ILE:CG1 | 1:D:60:ILE:CD1 | 1.91 | 1.49 |
| 1:L:159:ILE:CG1 | 1:L:159:ILE:CD1 | 1.90 | 1.49 |
| 1:B:272:PRO:CB | 1:B:272:PRO:CG | 1.82 | 1.48 |
| 1:B:463:PRO:CB | 1:B:463:PRO:CG | 1.84 | 1.48 |
| 1:N:356:LYS:NZ | 1:N:356:LYS:CE | 1.73 | 1.48 |
| 1:C:54:LYS:NZ | 1:C:54:LYS:CE | 1.73 | 1.48 |
| 1:C:467:LYS:NZ | 1:C:467:LYS:CE | 1.73 | 1.48 |
| 1:H:54:LYS:NZ | 1:H:54:LYS:CE | 1.74 | 1.47 |
| 1:M:82:LYS:NZ | 1:M:82:LYS:CE | 1.77 | 1.47 |
| 1:E:236:LYS:NZ | 1:E:236:LYS:CE | 1.77 | 1.47 |
| 1:I:217:LYS:NZ | 1:I:217:LYS:CE | 1.73 | 1.47 |
| 1:I:361:LYS:NZ | 1:I:361:LYS:CE | 1.75 | 1.47 |
| 1:O:452:LYS:CE | 1:O:452:LYS:NZ | 1.76 | 1.47 |
| 1:N:255:MET:CE | 1:N:255:MET:SD | 2.02 | 1.47 |
| 1:B:225:CYS:SG | 1:B:225:CYS:CB | 2.03 | 1.47 |
| 1:C:440:PRO:CG | 1:C:440:PRO:CB | 1.75 | 1.46 |
| 1:D:63:PRO:CB | 1:D:63:PRO:CG | 1.82 | 1.46 |
| 1:H:301:THR:CB | 1:H:301:THR:CG2 | 1.94 | 1.46 |
| 1:L:165:ILE:CG1 | 1:L:165:ILE:CD1 | 1.90 | 1.46 |
| 1:G:241:PRO:CB | 1:G:241:PRO:CG | 1.81 | 1.46 |
| 1:A:64:LYS:CE | 1:A:64:LYS:NZ | 1.77 | 1.46 |
| 1:H:152:LYS:NZ | 1:H:152:LYS:CE | 1.72 | 1.46 |
| 1:I:241:PRO:CG | 1:I:241:PRO:CB | 1.79 | 1.46 |
| 1:K:272:PRO:CG | 1:K:272:PRO:CB | 1.76 | 1.45 |
| 1:M:356:LYS:NZ | 1:M:356:LYS:CE | 1.75 | 1.45 |
| 1:C:452:LYS:NZ | 1:C:452:LYS:CE | 1.78 | 1.45 |
| 1:H:59:LYS:CE | 1:H:59:LYS:NZ | 1.76 | 1.45 |
| 1:A:80:PRO:CG | 1:A:80:PRO:CB | 1.78 | 1.45 |
| 1:H:237:MET:SD | 1:H:237:MET:CG | 2.02 | 1.45 |
| 1:D:342:MET:CE | 1:D:342:MET:SD | 2.05 | 1.44 |
| 1:E:342:MET:CE | 1:E:342:MET:SD | 2.05 | 1.44 |
| 1:H:361:LYS:CG | 1:H:361:LYS:CD | 1.91 | 1.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:63:PRO:CB | 1:H:63:PRO:CG | 1.77 | 1.44 |
| 1:L:463:PRO:CB | 1:L:463:PRO:CG | 1.80 | 1.43 |
| 1:C:82:LYS:NZ | 1:C:82:LYS:CE | 1.78 | 1.43 |
| 1:M:63:PRO:CG | 1:M:63:PRO:CB | 1.78 | 1.43 |
| 1:F:175:CYS:SG | 1:F:175:CYS:CB | 2.05 | 1.43 |
| 1:L:440:PRO:CB | 1:L:440:PRO:CG | 1.74 | 1.43 |
| 1:J:388:MET:CE | 1:J:388:MET:SD | 2.05 | 1.42 |
| 1:F:59:LYS:NZ | 1:F:59:LYS:CE | 1.80 | 1.42 |
| 1:L:59:LYS:NZ | 1:L:59:LYS:CE | 1.81 | 1.41 |
| 1:N:63:PRO:CB | 1:N:63:PRO:CG | 1.75 | 1.40 |
| 1:M:230:LYS:NZ | 1:M:230:LYS:CE | 1.85 | 1.39 |
| 1:L:161:CYS:SG | 1:L:161:CYS:CB | 2.10 | 1.39 |
| 1:A:342:MET:SD | 1:A:342:MET:CE | 2.10 | 1.38 |
| 1:I:163:PRO:CG | 1:I:163:PRO:CB | 1.77 | 1.38 |
| 1:M:86:PRO:CG | 1:M:86:PRO:CB | 1.75 | 1.38 |
| 1:H:217:LYS:NZ | 1:H:217:LYS:CE | 1.88 | 1.36 |
| 1:C:51:PRO:CB | 1:C:51:PRO:CG | 1.92 | 1.36 |
| 1:G:51:PRO:CG | 1:G:51:PRO:CB | 1.89 | 1.35 |
| 1:L:272:PRO:CB | 1:L:272:PRO:CG | 1.96 | 1.35 |
| 1:O:241:PRO:CB | 1:O:241:PRO:CG | 1.78 | 1.34 |
| 1:E:63:PRO:CG | 1:E:63:PRO:CB | 1.75 | 1.34 |
| 1:I:356:LYS:NZ | 1:I:356:LYS:CE | 1.91 | 1.33 |
| 1:L:241:PRO:CB | 1:L:241:PRO:CG | 1.92 | 1.32 |
| 1:F:241:PRO:CG | 1:F:241:PRO:CB | 1.82 | 1.31 |
| 1:K:245:SER:OG | 1:K:245:SER:CB | 1.80 | 1.27 |
| 1:J:81:ASN:OD1 | 1:J:97:ARG:NH1 | 1.66 | 1.26 |
| 1:M:180:VAL:CG1 | 1:M:184:ASP:HB2 | 1.69 | 1.23 |
| 1:D:70:TYR:OH | 1:D:232:PRO:HD3 | 1.33 | 1.23 |
| 1:N:151:TYR:CD2 | 1:N:203:THR:HB | 1.76 | 1.20 |
| 1:C:345:CYS:SG | 1:D:216:ASN:HB2 | 1.82 | 1.19 |
| 1:L:180:VAL:CG1 | 1:L:184:ASP:HB2 | 1.72 | 1.19 |
| 1:G:345:CYS:SG | 1:H:216:ASN:HB2 | 1.82 | 1.17 |
| 1:C:180:VAL:HG12 | 1:C:184:ASP:HB2 | 1.22 | 1.17 |
| 1:O:70:TYR:OH | 1:O:232:PRO:HD3 | 1.41 | 1.17 |
| 1:O:46:GLY:HA3 | 1:O:65:VAL:HG23 | 1.17 | 1.16 |
| 1:F:167:GLU:HB2 | 1:F:190:LEU:HD11 | 1.24 | 1.16 |
| 1:J:242:TYR:CD2 | 1:J:394:MET:HG3 | 1.81 | 1.16 |
| 1:G:151:TYR:CD2 | 1:G:203:THR:HB | 1.78 | 1.16 |
| 1:D:98:LEU:HD13 | 1:D:378:LEU:HD11 | 1.19 | 1.16 |
| 1:F:151:TYR:CD2 | 1:F:203:THR:HB | 1.81 | 1.15 |
| 1:I:472:LEU:CD2 | 1:M:138:ASN:HD22 | 1.59 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:152:LYS:HB2 | 1:L:255:MET:HB2 | 1.30 | 1.14 |
| 1:J:180:VAL:CG1 | 1:J:184:ASP:HB2 | 1.77 | 1.14 |
| 1:G:180:VAL:HG12 | 1:G:184:ASP:HB2 | 1.25 | 1.14 |
| 1:A:34:TYR:CE2 | 1:A:377:GLN:HG3 | 1.81 | 1.13 |
| 1:D:34:TYR:CE2 | 1:D:377:GLN:HG3 | 1.83 | 1.13 |
| 1:O:152:LYS:HB2 | 1:O:255:MET:HB2 | 1.31 | 1.12 |
| 1:D:68:LEU:O | 1:D:201:VAL:HG22 | 1.49 | 1.12 |
| 1:G:463:PRO:HG2 | 1:G:464:LEU:H | 1.12 | 1.12 |
| 1:M:79:ASP:OD2 | 1:M:81:ASN:HB2 | 1.49 | 1.11 |
| 1:A:286:LEU:HD12 | 1:E:122:LEU:HD21 | 1.33 | 1.11 |
| 1:B:54:LYS:HE3 | 1:B:55:PRO:HD2 | 1.30 | 1.11 |
| 1:M:117:ILE:HG21 | 1:N:293:PRO:HD3 | 1.33 | 1.11 |
| 1:A:65:VAL:HA | 1:A:69:GLN:HE22 | 1.09 | 1.10 |
| 1:C:451:LEU:HD23 | 1:C:454:LYS:HG3 | 1.27 | 1.10 |
| 1:G:320:ASN:HD21 | 1:G:323:ILE:HB | 1.11 | 1.10 |
| 1:N:75:ILE:HD12 | 1:N:75:ILE:N | 1.55 | 1.10 |
| 1:D:112:PRO:HD3 | 1:E:231:TYR:CD2 | 1.84 | 1.10 |
| 1:G:74:ARG:HG3 | 1:G:330:PHE:CE2 | 1.87 | 1.10 |
| 1:K:216:ASN:HB2 | 1:O:345:CYS:SG | 1.92 | 1.10 |
| 1:A:255:MET:HG2 | 1:A:256:PHE:N | 1.33 | 1.09 |
| 1:F:78:PRO:HD3 | 1:F:452:LYS:HA | 1.32 | 1.09 |
| 1:L:71:ARG:HH11 | 1:L:71:ARG:HA | 1.15 | 1.09 |
| 1:A:345:CYS:SG | 1:B:216:ASN:HB2 | 1.93 | 1.09 |
| 1:G:74:ARG:HG3 | 1:G:330:PHE:HE2 | 1.16 | 1.09 |
| 1:G:122:LEU:HD11 | 1:H:286:LEU:HD11 | 1.33 | 1.09 |
| 1:M:34:TYR:CE2 | 1:M:377:GLN:HB2 | 1.86 | 1.09 |
| 1:A:180:VAL:HG12 | 1:A:184:ASP:HB2 | 1.26 | 1.09 |
| 1:E:98:LEU:HD13 | 1:E:378:LEU:HD11 | 1.21 | 1.09 |
| 1:K:345:CYS:SG | 1:L:216:ASN:HB2 | 1.91 | 1.09 |
| 1:G:180:VAL:CG1 | 1:G:184:ASP:HB2 | 1.83 | 1.09 |
| 1:N:344:LEU:HD23 | 1:N:344:LEU:N | 1.68 | 1.09 |
| 1:J:98:LEU:HD22 | 1:J:378:LEU:CD1 | 1.83 | 1.08 |
| 1:M:74:ARG:NH2 | 1:M:441:LEU:HD12 | 1.67 | 1.08 |
| 1:N:98:LEU:HD13 | 1:N:378:LEU:HD11 | 1.30 | 1.08 |
| 1:L:250:LEU:H | 1:L:250:LEU:HD12 | 1.04 | 1.08 |
| 1:B:78:PRO:HD3 | 1:B:452:LYS:HA | 1.34 | 1.08 |
| 1:N:217:LYS:HD3 | 1:O:274:ASP:O | 1.53 | 1.08 |
| 1:N:67:GLY:O | 1:N:68:LEU:HG | 1.54 | 1.08 |
| 1:E:149:MET:HE3 | 1:E:294:THR:HG22 | 1.16 | 1.07 |
| 1:B:344:LEU:HD12 | 1:C:186:PRO:HD2 | 1.33 | 1.07 |
| 1:I:123:LEU:HD23 | 1:I:147:ILE:HB | 1.37 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:167:GLU:HB2 | 1:I:190:LEU:HD11 | 1.34 | 1.07 |
| 1:J:180:VAL:HG12 | 1:J:184:ASP:HB2 | 1.27 | 1.07 |
| 1:A:54:LYS:HG3 | 1:A:55:PRO:HD2 | 1.35 | 1.07 |
| 1:A:286:LEU:CD1 | 1:E:122:LEU:HD11 | 1.84 | 1.07 |
| 1:N:78:PRO:HD3 | 1:N:452:LYS:HA | 1.34 | 1.07 |
| 1:L:166:GLY:CA | 1:L:195:ILE:HD11 | 1.84 | 1.06 |
| 1:N:151:TYR:OH | 1:N:221:PRO:HG2 | 1.55 | 1.06 |
| 1:N:345:CYS:SG | 1:O:216:ASN:HB2 | 1.95 | 1.06 |
| 1:K:152:LYS:HB2 | 1:K:255:MET:HB2 | 1.37 | 1.06 |
| 1:K:252:ARG:HD2 | 1:K:306:ILE:HD11 | 1.36 | 1.06 |
| 1:B:152:LYS:HB2 | 1:B:255:MET:HB2 | 1.37 | 1.06 |
| 1:J:98:LEU:CD2 | 1:J:378:LEU:HD11 | 1.85 | 1.06 |
| 1:H:345:CYS:SG | 1:I:216:ASN:HB2 | 1.96 | 1.05 |
| 1:E:176:THR:O | 1:E:177:GLN:HG3 | 1.56 | 1.05 |
| 1:A:139:ALA:HA | 1:A:143:ASN:HD21 | 1.13 | 1.05 |
| 1:D:54:LYS:HE3 | 1:D:55:PRO:HD2 | 1.37 | 1.05 |
| 1:E:101:ALA:HA | 1:E:322:GLY:O | 1.56 | 1.05 |
| 1:E:152:LYS:HB2 | 1:E:255:MET:HB2 | 1.32 | 1.05 |
| 1:L:166:GLY:N | 1:L:195:ILE:HD11 | 1.70 | 1.05 |
| 1:D:167:GLU:HB2 | 1:D:190:LEU:HD11 | 1.39 | 1.04 |
| 1:A:266:THR:OG1 | 1:E:361:LYS:HA | 1.55 | 1.04 |
| 1:M:180:VAL:HG13 | 1:M:184:ASP:HB2 | 1.38 | 1.04 |
| 1:O:46:GLY:HA3 | 1:O:65:VAL:CG2 | 1.87 | 1.04 |
| 1:J:255:MET:HG2 | 1:J:256:PHE:N | 1.72 | 1.04 |
| 1:L:123:LEU:HD23 | 1:L:147:ILE:HB | 1.35 | 1.04 |
| 1:L:344:LEU:HD11 | 1:M:185:CYS:SG | 1.98 | 1.04 |
| 1:B:46:GLY:HA3 | 1:B:65:VAL:HG23 | 1.36 | 1.03 |
| 1:E:472:LEU:HD23 | 1:J:138:ASN:HD22 | 0.92 | 1.03 |
| 1:B:23:SER:OG | 1:B:25:ASP:HB2 | 1.57 | 1.03 |
| 1:B:348:ILE:HG22 | 1:B:359:ASN:OD1 | 1.58 | 1.03 |
| 1:O:123:LEU:HD23 | 1:O:147:ILE:HB | 1.40 | 1.03 |
| 1:D:30:ARG:HH11 | 1:D:377:GLN:HE22 | 1.07 | 1.03 |
| 1:A:255:MET:CG | 1:A:256:PHE:N | 2.22 | 1.02 |
| 1:H:169:TRP:HB3 | 1:H:188:LEU:HD12 | 1.42 | 1.02 |
| 1:D:152:LYS:HB2 | 1:D:255:MET:HB2 | 1.40 | 1.02 |
| 1:M:115:VAL:H | 1:N:255:MET:HE1 | 1.17 | 1.02 |
| 1:N:348:ILE:HG22 | 1:N:359:ASN:OD1 | 1.59 | 1.02 |
| 1:A:286:LEU:HD11 | 1:E:122:LEU:HD11 | 1.02 | 1.02 |
| 1:K:443:LYS:H | 1:K:443:LYS:HD3 | 1.19 | 1.02 |
| 1:E:96:GLN:HB3 | 1:E:382:THR:HG22 | 1.39 | 1.01 |
| 1:K:67:GLY:O | 1:K:68:LEU:HG | 1.59 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:167:GLU:HB2 | 1:O:190:LEU:HD11 | 1.41 | 1.01 |
| 1:E:472:LEU:HD23 | 1:J:138:ASN:ND2 | 1.74 | 1.01 |
| 1:J:96:GLN:HA | 1:J:382:THR:HA | 1.36 | 1.01 |
| 1:D:176:THR:O | 1:D:177:GLN:HG3 | 1.61 | 1.01 |
| 1:H:70:TYR:OH | 1:H:232:PRO:HD3 | 1.60 | 1.01 |
| 1:F:149:MET:HE3 | 1:F:294:THR:HG22 | 1.37 | 1.01 |
| 1:N:66:SER:H | 1:N:69:GLN:NE2 | 1.58 | 1.01 |
| 1:H:30:ARG:HH11 | 1:H:377:GLN:HE22 | 1.07 | 1.00 |
| 1:L:166:GLY:HA3 | 1:L:195:ILE:HD11 | 1.43 | 1.00 |
| 1:M:344:LEU:N | 1:M:344:LEU:HD23 | 1.76 | 1.00 |
| 1:O:158:LEU:HB2 | 1:O:332:THR:OG1 | 1.61 | 1.00 |
| 1:C:74:ARG:HG3 | 1:C:330:PHE:CE2 | 1.96 | 1.00 |
| 1:K:180:VAL:CG1 | 1:K:184:ASP:HB2 | 1.92 | 1.00 |
| 1:M:361:LYS:HA | 1:N:266:THR:HG1 | 1.26 | 1.00 |
| 1:D:252:ARG:HD2 | 1:D:306:ILE:HD11 | 1.39 | 1.00 |
| 1:J:44:ALA:O | 1:J:45:VAL:HG23 | 1.61 | 1.00 |
| 1:N:152:LYS:HB2 | 1:N:255:MET:HB2 | 1.44 | 1.00 |
| 1:C:302:SER:O | 1:C:304:ALA:N | 1.93 | 1.00 |
| 1:H:259:HIS:C | 1:H:260:LEU:HD12 | 1.82 | 1.00 |
| 1:J:130:GLU:HB2 | 1:J:260:LEU:HD13 | 1.39 | 1.00 |
| 1:H:71:ARG:HA | 1:H:71:ARG:HH11 | 1.26 | 1.00 |
| 1:I:152:LYS:HB2 | 1:I:255:MET:HB2 | 1.43 | 1.00 |
| 1:A:75:ILE:HG23 | 1:A:451:LEU:HD12 | 1.44 | 0.99 |
| 1:F:71:ARG:HH11 | 1:F:71:ARG:HA | 1.21 | 0.99 |
| 1:G:361:LYS:HA | 1:H:266:THR:OG1 | 1.61 | 0.99 |
| 1:G:463:PRO:HG2 | 1:G:464:LEU:N | 1.77 | 0.99 |
| 1:H:68:LEU:HD22 | 1:H:203:THR:HG22 | 1.41 | 0.99 |
| 1:H:78:PRO:HD3 | 1:H:452:LYS:HA | 1.44 | 0.99 |
| 1:L:250:LEU:HD12 | 1:L:250:LEU:N | 1.72 | 0.99 |
| 1:A:71:ARG:HH11 | 1:A:71:ARG:HA | 1.25 | 0.99 |
| 1:E:472:LEU:CD2 | 1:J:138:ASN:HD22 | 1.75 | 0.99 |
| 1:G:242:TYR:CD2 | 1:G:394:MET:HG3 | 1.98 | 0.98 |
| 1:F:21:VAL:HB | 1:J:461:GLN:HE22 | 1.27 | 0.98 |
| 1:N:262:ASN:HD21 | 1:N:288:SER:HB3 | 1.26 | 0.98 |
| 1:D:71:ARG:HA | 1:D:71:ARG:HH11 | 1.27 | 0.98 |
| 1:G:302:SER:O | 1:G:304:ALA:N | 1.97 | 0.98 |
| 1:O:151:TYR:CD2 | 1:O:203:THR:HB | 1.98 | 0.98 |
| 1:D:255:MET:HG2 | 1:D:256:PHE:N | 1.78 | 0.98 |
| 1:G:54:LYS:HG3 | 1:G:55:PRO:HD2 | 1.45 | 0.98 |
| 1:E:71:ARG:HA | 1:E:71:ARG:HH11 | 1.26 | 0.98 |
| 1:N:71:ARG:HH11 | 1:N:71:ARG:HA | 1.28 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:255:MET:HG2 | 1:G:256:PHE:H | 1.27 | 0.98 |
| 1:N:52:ILE:HD12 | 1:N:52:ILE:N | 1.78 | 0.98 |
| 1:A:66:SER:H | 1:A:69:GLN:NE2 | 1.62 | 0.97 |
| 1:A:286:LEU:HD11 | 1:E:122:LEU:CD1 | 1.94 | 0.97 |
| 1:F:255:MET:HE1 | 1:J:115:VAL:H | 1.26 | 0.97 |
| 1:A:279:GLY:HA3 | 1:A:283:THR:O | 1.65 | 0.97 |
| 1:O:242:TYR:CE2 | 1:O:394:MET:HG3 | 1.99 | 0.97 |
| 1:N:167:GLU:HB2 | 1:N:190:LEU:HD11 | 1.46 | 0.97 |
| 1:E:99:VAL:HG11 | 1:E:323:ILE:HG22 | 1.46 | 0.97 |
| 1:K:54:LYS:HE3 | 1:K:55:PRO:HD2 | 1.44 | 0.97 |
| 1:M:74:ARG:HB2 | 1:M:330:PHE:HE2 | 1.30 | 0.97 |
| 1:A:65:VAL:HA | 1:A:69:GLN:NE2 | 1.77 | 0.97 |
| 1:A:122:LEU:HD11 | 1:B:286:LEU:HD11 | 1.47 | 0.97 |
| 1:L:34:TYR:CE2 | 1:L:377:GLN:HB2 | 2.00 | 0.97 |
| 1:N:68:LEU:O | 1:N:201:VAL:HG22 | 1.63 | 0.97 |
| 1:J:180:VAL:CG1 | 1:J:184:ASP:CB | 2.42 | 0.96 |
| 1:K:279:GLY:HA3 | 1:K:283:THR:O | 1.65 | 0.96 |
| 1:A:57:ASN:HD21 | 1:A:59:LYS:CB | 1.77 | 0.96 |
| 1:H:152:LYS:HB2 | 1:H:255:MET:HB2 | 1.48 | 0.96 |
| 1:F:70:TYR:OH | 1:F:232:PRO:HD3 | 1.63 | 0.96 |
| 1:N:262:ASN:ND2 | 1:N:288:SER:HB3 | 1.81 | 0.96 |
| 1:N:374:PHE:HB3 | 1:N:376:PHE:CE1 | 2.01 | 0.96 |
| 1:A:52:ILE:N | 1:A:52:ILE:HD12 | 1.78 | 0.96 |
| 1:N:92:ASN:ND2 | 1:N:95:THR:H | 1.61 | 0.96 |
| 1:C:190:LEU:HD12 | 1:C:191:ILE:H | 1.28 | 0.96 |
| 1:M:361:LYS:HA | 1:N:266:THR:OG1 | 1.64 | 0.96 |
| 1:I:166:GLY:CA | 1:I:195:ILE:HD11 | 1.94 | 0.95 |
| 1:I:472:LEU:HD23 | 1:M:138:ASN:HD22 | 1.28 | 0.95 |
| 1:A:367:GLY:O | 1:A:368:GLU:HG2 | 1.64 | 0.95 |
| 1:D:237:MET:O | 1:D:240:GLU:HB3 | 1.66 | 0.95 |
| 1:L:70:TYR:OH | 1:L:232:PRO:HD3 | 1.66 | 0.95 |
| 1:M:67:GLY:O | 1:M:68:LEU:HG | 1.67 | 0.95 |
| 1:B:345:CYS:SG | 1:C:216:ASN:HB2 | 2.04 | 0.95 |
| 1:A:135:TYR:HE2 | 1:A:287:ALA:HB2 | 1.31 | 0.95 |
| 1:H:99:VAL:HG11 | 1:H:323:ILE:HG22 | 1.48 | 0.95 |
| 1:I:180:VAL:HG12 | 1:I:184:ASP:HB2 | 1.48 | 0.95 |
| 1:M:345:CYS:SG | 1:N:216:ASN:HB2 | 2.05 | 0.95 |
| 1:A:180:VAL:CG1 | 1:A:184:ASP:HB2 | 1.95 | 0.95 |
| 1:G:180:VAL:CG1 | 1:G:184:ASP:CB | 2.44 | 0.95 |
| 1:I:75:ILE:CD1 | 1:I:329:LEU:O | 2.15 | 0.95 |
| 1:H:115:VAL:H | 1:I:255:MET:HE1 | 1.30 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:117:ILE:CG2 | 1:F:117:ILE:CA | 2.44 | 0.94 |
| 1:F:216:ASN:HB2 | 1:J:345:CYS:SG | 2.08 | 0.94 |
| 1:L:262:ASN:HD21 | 1:L:288:SER:HB3 | 1.27 | 0.94 |
| 1:M:98:LEU:HD13 | 1:M:378:LEU:HD21 | 1.48 | 0.94 |
| 1:F:97:ARG:HG2 | 1:F:383:LEU:HD11 | 1.49 | 0.94 |
| 1:O:180:VAL:CG1 | 1:O:184:ASP:HB2 | 1.95 | 0.94 |
| 1:E:123:LEU:HD23 | 1:E:147:ILE:HB | 1.46 | 0.94 |
| 1:O:246:LEU:HD23 | 1:O:246:LEU:H | 1.29 | 0.94 |
| 1:J:96:GLN:CA | 1:J:382:THR:HA | 1.97 | 0.94 |
| 1:I:152:LYS:CB | 1:I:255:MET:HB2 | 1.97 | 0.94 |
| 1:J:23:SER:OG | 1:J:25:ASP:HB2 | 1.66 | 0.94 |
| 1:A:242:TYR:CD2 | 1:A:394:MET:HG3 | 2.03 | 0.94 |
| 1:K:180:VAL:HG12 | 1:K:184:ASP:HB2 | 1.48 | 0.94 |
| 1:O:98:LEU:HD22 | 1:O:378:LEU:HD11 | 1.48 | 0.94 |
| 1:A:361:LYS:HA | 1:B:266:THR:OG1 | 1.67 | 0.94 |
| 1:I:67:GLY:O | 1:I:68:LEU:HG | 1.68 | 0.94 |
| 1:F:180:VAL:CG1 | 1:F:184:ASP:HB2 | 1.97 | 0.94 |
| 1:H:320:ASN:OD1 | 1:H:321:ASN:N | 2.01 | 0.94 |
| 1:J:96:GLN:HB3 | 1:J:382:THR:HG22 | 1.50 | 0.94 |
| 1:B:361:LYS:HA | 1:C:266:THR:OG1 | 1.67 | 0.93 |
| 1:F:101:ALA:HA | 1:F:322:GLY:O | 1.67 | 0.93 |
| 1:G:49:TYR:HE2 | 1:G:118:SER:HA | 1.32 | 0.93 |
| 1:K:202:ASP:OD2 | 1:O:112:PRO:HB2 | 1.68 | 0.93 |
| 1:N:358:THR:HA | 1:O:266:THR:CG2 | 1.98 | 0.93 |
| 1:G:167:GLU:HG2 | 1:G:231:TYR:O | 1.68 | 0.93 |
| 1:H:166:GLY:CA | 1:H:195:ILE:HD11 | 1.97 | 0.93 |
| 1:D:443:LYS:HD3 | 1:D:443:LYS:H | 1.33 | 0.93 |
| 1:G:74:ARG:CG | 1:G:330:PHE:HE2 | 1.82 | 0.93 |
| 1:N:122:LEU:HD11 | 1:O:286:LEU:HD11 | 1.51 | 0.93 |
| 1:N:361:LYS:HA | 1:O:266:THR:OG1 | 1.68 | 0.93 |
| 1:A:117:ILE:HG13 | 1:A:149:MET:O | 1.69 | 0.93 |
| 1:C:188:LEU:CD1 | 1:C:213:LEU:HD11 | 1.99 | 0.93 |
| 1:F:97:ARG:CG | 1:F:383:LEU:HD11 | 1.99 | 0.93 |
| 1:N:154:THR:H | 1:N:336:THR:HG21 | 1.33 | 0.93 |
| 1:M:185:CYS:SG | 1:M:186:PRO:HD2 | 2.08 | 0.93 |
| 1:F:23:SER:OG | 1:F:25:ASP:HB2 | 1.69 | 0.93 |
| 1:G:44:ALA:HB3 | 1:G:368:GLU:HB2 | 1.51 | 0.93 |
| 1:G:262:ASN:C | 1:G:262:ASN:HD22 | 1.69 | 0.93 |
| 1:H:49:TYR:HE2 | 1:H:118:SER:HA | 1.31 | 0.93 |
| 1:H:67:GLY:O | 1:H:68:LEU:HG | 1.69 | 0.93 |
| 1:I:75:ILE:HD13 | 1:I:329:LEU:O | 1.66 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:180:VAL:HG13 | 1:M:184:ASP:CB | 1.99 | 0.93 |
| 1:C:115:VAL:HG22 | 1:D:255:MET:SD | 2.09 | 0.92 |
| 1:C:180:VAL:CG1 | 1:C:184:ASP:HB2 | 1.99 | 0.92 |
| 1:H:176:THR:C | 1:H:177:GLN:HG3 | 1.90 | 0.92 |
| 1:C:361:LYS:HA | 1:D:266:THR:OG1 | 1.69 | 0.92 |
| 1:G:71:ARG:HH12 | 1:G:198:GLY:H | 1.10 | 0.92 |
| 1:O:65:VAL:HA | 1:O:69:GLN:HE22 | 1.33 | 0.92 |
| 1:K:162:LYS:CE | 1:K:162:LYS:CG | 2.47 | 0.92 |
| 1:M:71:ARG:HA | 1:M:71:ARG:HH11 | 1.32 | 0.92 |
| 1:N:180:VAL:HG13 | 1:N:184:ASP:HB2 | 1.49 | 0.92 |
| 1:A:262:ASN:HD21 | 1:A:288:SER:HB3 | 1.33 | 0.92 |
| 1:C:262:ASN:C | 1:C:262:ASN:HD22 | 1.67 | 0.92 |
| 1:J:242:TYR:CE2 | 1:J:394:MET:HG3 | 2.05 | 0.92 |
| 1:B:115:VAL:HG21 | 1:C:257:VAL:HG13 | 1.50 | 0.92 |
| 1:F:266:THR:OG1 | 1:J:361:LYS:HA | 1.67 | 0.92 |
| 1:K:259:HIS:C | 1:K:260:LEU:HD12 | 1.90 | 0.92 |
| 1:M:117:ILE:CG2 | 1:N:293:PRO:HD3 | 2.00 | 0.92 |
| 1:M:281:GLY:O | 1:M:284:ALA:N | 2.02 | 0.92 |
| 1:N:344:LEU:HD23 | 1:N:344:LEU:H | 1.32 | 0.92 |
| 1:F:443:LYS:H | 1:F:443:LYS:HD3 | 1.30 | 0.92 |
| 1:K:117:ILE:HG13 | 1:K:149:MET:O | 1.70 | 0.92 |
| 1:K:320:ASN:OD1 | 1:K:321:ASN:N | 2.03 | 0.92 |
| 1:N:79:ASP:OD2 | 1:N:81:ASN:HB2 | 1.68 | 0.92 |
| 1:B:344:LEU:HD11 | 1:C:185:CYS:SG | 2.10 | 0.92 |
| 1:N:66:SER:H | 1:N:69:GLN:HE21 | 1.05 | 0.92 |
| 1:N:126:LEU:HB3 | 1:N:262:ASN:HB3 | 1.52 | 0.92 |
| 1:J:260:LEU:N | 1:J:260:LEU:HD12 | 1.84 | 0.92 |
| 1:K:466:ARG:HD3 | 1:L:319:HIS:CE1 | 2.05 | 0.92 |
| 1:A:74:ARG:NH2 | 1:A:441:LEU:HD12 | 1.84 | 0.91 |
| 1:A:139:ALA:HB1 | 1:A:143:ASN:OD1 | 1.70 | 0.91 |
| 1:D:305:GLN:HE22 | 1:D:337:THR:HG21 | 1.36 | 0.91 |
| 1:H:451:LEU:HD23 | 1:H:454:LYS:HG3 | 1.51 | 0.91 |
| 1:J:71:ARG:HG2 | 1:J:71:ARG:NH1 | 1.84 | 0.91 |
| 1:J:123:LEU:HD23 | 1:J:147:ILE:HB | 1.51 | 0.91 |
| 1:M:98:LEU:CD1 | 1:M:98:LEU:CD2 | 2.47 | 0.91 |
| 1:B:28:VAL:HG22 | 1:B:381:ILE:HD11 | 1.52 | 0.91 |
| 1:H:74:ARG:HG3 | 1:H:330:PHE:CE2 | 2.06 | 0.91 |
| 1:H:75:ILE:HG23 | 1:H:451:LEU:HD12 | 1.51 | 0.91 |
| 1:J:71:ARG:HG2 | 1:J:71:ARG:HH11 | 1.36 | 0.91 |
| 1:C:385:ALA:O | 1:C:389:THR:HG23 | 1.71 | 0.91 |
| 1:O:178:VAL:O | 1:O:180:VAL:N | 2.03 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:79:ASP:OD2 | 1:A:81:ASN:HB2 | 1.69 | 0.91 |
| 1:B:71:ARG:HA | 1:B:71:ARG:HH11 | 1.35 | 0.91 |
| 1:F:344:LEU:HD12 | 1:G:186:PRO:HD2 | 1.52 | 0.91 |
| 1:H:30:ARG:HH11 | 1:H:377:GLN:NE2 | 1.68 | 0.91 |
| 1:K:123:LEU:HD23 | 1:K:147:ILE:HB | 1.52 | 0.91 |
| 1:F:246:LEU:HD23 | 1:F:246:LEU:H | 1.36 | 0.91 |
| 1:K:228:ILE:HD12 | 1:K:228:ILE:N | 1.86 | 0.91 |
| 1:K:361:LYS:HA | 1:L:266:THR:OG1 | 1.69 | 0.91 |
| 1:N:471:GLN:OE1 | 1:N:472:LEU:N | 2.03 | 0.91 |
| 1:K:246:LEU:O | 1:K:246:LEU:HD23 | 1.69 | 0.91 |
| 1:D:472:LEU:CD2 | 1:I:138:ASN:HD22 | 1.84 | 0.91 |
| 1:L:152:LYS:CB | 1:L:255:MET:HB2 | 2.00 | 0.91 |
| 1:O:180:VAL:HG13 | 1:O:184:ASP:HB2 | 1.53 | 0.91 |
| 1:B:49:TYR:HE2 | 1:B:118:SER:HA | 1.36 | 0.90 |
| 1:K:74:ARG:HG3 | 1:K:330:PHE:CE2 | 2.06 | 0.90 |
| 1:L:230:LYS:NZ | 1:L:230:LYS:CD | 2.34 | 0.90 |
| 1:N:154:THR:O | 1:N:336:THR:HG23 | 1.70 | 0.90 |
| 1:D:66:SER:H | 1:D:69:GLN:NE2 | 1.69 | 0.90 |
| 1:F:443:LYS:HD3 | 1:F:443:LYS:N | 1.87 | 0.90 |
| 1:L:122:LEU:HD11 | 1:M:286:LEU:HD11 | 1.53 | 0.90 |
| 1:O:101:ALA:HA | 1:O:322:GLY:O | 1.72 | 0.90 |
| 1:H:167:GLU:HB2 | 1:H:190:LEU:HD11 | 1.53 | 0.90 |
| 1:D:246:LEU:HD23 | 1:D:246:LEU:H | 1.37 | 0.90 |
| 1:H:112:PRO:HD3 | 1:I:231:TYR:CD2 | 2.06 | 0.90 |
| 1:H:260:LEU:HD12 | 1:H:260:LEU:N | 1.80 | 0.90 |
| 1:L:67:GLY:O | 1:L:68:LEU:HG | 1.70 | 0.90 |
| 1:C:167:GLU:HG2 | 1:C:231:TYR:O | 1.70 | 0.90 |
| 1:H:373:GLN:CB | 1:H:464:LEU:HD12 | 2.01 | 0.90 |
| 1:L:66:SER:H | 1:L:69:GLN:NE2 | 1.70 | 0.90 |
| 1:N:28:VAL:CG1 | 1:N:28:VAL:HB | 2.02 | 0.90 |
| 1:O:242:TYR:CD2 | 1:O:394:MET:HG3 | 2.08 | 0.89 |
| 1:A:164:PRO:HG3 | 1:A:332:THR:OG1 | 1.71 | 0.89 |
| 1:I:378:LEU:HD12 | 1:I:379:CYS:N | 1.86 | 0.89 |
| 1:D:344:LEU:HD13 | 1:E:213:LEU:CD1 | 2.02 | 0.89 |
| 1:C:279:GLY:HA3 | 1:C:283:THR:O | 1.72 | 0.89 |
| 1:F:52:ILE:HB | 1:F:62:VAL:HB | 1.53 | 0.89 |
| 1:J:54:LYS:HG3 | 1:J:55:PRO:HD2 | 1.53 | 0.89 |
| 1:O:65:VAL:HA | 1:O:69:GLN:NE2 | 1.85 | 0.89 |
| 1:G:120:HIS:NE2 | 1:G:218:SER:HB3 | 1.87 | 0.89 |
| 1:L:39:THR:HG23 | 1:L:372:LEU:HB2 | 1.54 | 0.89 |
| 1:C:345:CYS:HG | 1:D:216:ASN:HB2 | 1.38 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:159:ILE:HD12 | 1:G:248:PHE:HD2 | 1.34 | 0.89 |
| 1:H:361:LYS:HD3 | 1:I:268:GLY:HA2 | 1.52 | 0.89 |
| 1:C:82:LYS:HZ1 | 1:C:403:ASN:HD22 | 0.91 | 0.89 |
| 1:D:375:ILE:HG12 | 1:D:464:LEU:HD13 | 1.53 | 0.89 |
| 1:E:70:TYR:OH | 1:E:232:PRO:HD3 | 1.72 | 0.89 |
| 1:I:166:GLY:HA3 | 1:I:195:ILE:HD11 | 1.53 | 0.89 |
| 1:M:255:MET:HG2 | 1:M:256:PHE:N | 1.85 | 0.89 |
| 1:N:75:ILE:HD12 | 1:N:75:ILE:H | 1.32 | 0.89 |
| 1:A:126:LEU:HB3 | 1:A:262:ASN:HB3 | 1.55 | 0.89 |
| 1:H:367:GLY:O | 1:H:368:GLU:HG2 | 1.71 | 0.89 |
| 1:A:237:MET:O | 1:A:240:GLU:HB3 | 1.73 | 0.89 |
| 1:D:54:LYS:HB3 | 1:D:57:ASN:HB3 | 1.55 | 0.89 |
| 1:D:31:THR:HG23 | 1:D:378:LEU:O | 1.72 | 0.88 |
| 1:H:342:MET:HB2 | 1:I:208:MET:HE1 | 1.53 | 0.88 |
| 1:M:78:PRO:HD3 | 1:M:452:LYS:HA | 1.55 | 0.88 |
| 1:I:345:CYS:SG | 1:J:216:ASN:HB2 | 2.12 | 0.88 |
| 1:J:167:GLU:HB2 | 1:J:190:LEU:HD11 | 1.55 | 0.88 |
| 1:D:65:VAL:HA | 1:D:69:GLN:HE22 | 1.36 | 0.88 |
| 1:O:320:ASN:OD1 | 1:O:323:ILE:HG12 | 1.73 | 0.88 |
| 1:H:373:GLN:HB3 | 1:H:464:LEU:HD12 | 1.55 | 0.88 |
| 1:O:74:ARG:HG3 | 1:O:330:PHE:HE2 | 1.38 | 0.88 |
| 1:D:250:LEU:HD12 | 1:D:250:LEU:N | 1.88 | 0.88 |
| 1:G:361:LYS:HA | 1:H:266:THR:HG1 | 1.34 | 0.88 |
| 1:K:260:LEU:HD12 | 1:K:260:LEU:N | 1.84 | 0.88 |
| 1:A:286:LEU:CD1 | 1:E:122:LEU:HD21 | 2.04 | 0.88 |
| 1:C:300:VAL:HG23 | 1:C:300:VAL:O | 1.72 | 0.88 |
| 1:A:255:MET:HG2 | 1:A:256:PHE:H | 1.37 | 0.88 |
| 1:O:280:SER:N | 1:O:284:ALA:HB2 | 1.87 | 0.88 |
| 1:K:226:THR:HG21 | 1:L:275:LEU:HD22 | 1.54 | 0.88 |
| 1:N:344:LEU:N | 1:N:344:LEU:CD2 | 2.34 | 0.88 |
| 1:E:50:PHE:HB2 | 1:E:51:PRO:HD2 | 1.55 | 0.88 |
| 1:G:463:PRO:CA | 1:G:466:ARG:HH21 | 1.86 | 0.88 |
| 1:B:142:ASP:OD1 | 1:C:283:THR:OG1 | 1.91 | 0.88 |
| 1:C:250:LEU:N | 1:C:250:LEU:HD12 | 1.87 | 0.88 |
| 1:D:126:LEU:HB3 | 1:D:262:ASN:HB3 | 1.54 | 0.88 |
| 1:I:174:PRO:HG3 | 1:I:187:PRO:HG2 | 1.54 | 0.88 |
| 1:N:21:VAL:CG1 | 1:N:390:TYR:OH | 2.22 | 0.88 |
| 1:A:64:LYS:CG | 1:A:64:LYS:CA | 2.53 | 0.87 |
| 1:B:152:LYS:CB | 1:B:255:MET:HB2 | 2.04 | 0.87 |
| 1:B:344:LEU:CD1 | 1:C:186:PRO:HD2 | 2.03 | 0.87 |
| 1:O:228:ILE:N | 1:O:228:ILE:HD12 | 1.88 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:97:ARG:HG2 | 1:F:383:LEU:CD1 | 2.03 | 0.87 |
| 1:A:75:ILE:N | 1:A:75:ILE:HD12 | 1.88 | 0.87 |
| 1:B:163:PRO:HD3 | 1:B:330:PHE:HE1 | 1.39 | 0.87 |
| 1:D:472:LEU:HD23 | 1:I:138:ASN:HD22 | 1.39 | 0.87 |
| 1:F:260:LEU:HD12 | 1:F:260:LEU:N | 1.89 | 0.87 |
| 1:O:149:MET:CE | 1:O:294:THR:HG22 | 2.05 | 0.87 |
| 1:A:68:LEU:HD23 | 1:A:201:VAL:HG21 | 1.56 | 0.87 |
| 1:B:74:ARG:HG3 | 1:B:330:PHE:CE2 | 2.09 | 0.87 |
| 1:I:74:ARG:HG3 | 1:I:330:PHE:CE2 | 2.09 | 0.87 |
| 1:O:149:MET:HE3 | 1:O:294:THR:HG22 | 1.56 | 0.87 |
| 1:B:122:LEU:HD21 | 1:C:286:LEU:HD12 | 1.57 | 0.87 |
| 1:B:180:VAL:HG12 | 1:B:181:GLN:O | 1.74 | 0.87 |
| 1:C:35:TYR:CE2 | 1:C:457:ALA:HB2 | 2.10 | 0.87 |
| 1:I:180:VAL:CG1 | 1:I:184:ASP:HB2 | 2.05 | 0.87 |
| 1:K:41:ARG:HH22 | 1:L:192:ASN:HD21 | 1.19 | 0.87 |
| 1:K:344:LEU:HD12 | 1:L:186:PRO:HD2 | 1.56 | 0.87 |
| 1:C:255:MET:HG2 | 1:C:256:PHE:H | 1.38 | 0.87 |
| 1:L:255:MET:HG2 | 1:L:256:PHE:N | 1.86 | 0.87 |
| 1:N:52:ILE:N | 1:N:52:ILE:CD1 | 2.36 | 0.87 |
| 1:F:180:VAL:HG12 | 1:F:184:ASP:HB2 | 1.57 | 0.87 |
| 1:H:54:LYS:HZ2 | 1:H:55:PRO:HD2 | 1.39 | 0.87 |
| 1:A:61:LEU:HD12 | 1:A:61:LEU:O | 1.73 | 0.86 |
| 1:O:463:PRO:HB3 | 1:O:466:ARG:HH21 | 1.38 | 0.86 |
| 1:I:156:LEU:HG | 1:I:334:VAL:HB | 1.54 | 0.86 |
| 1:K:78:PRO:HD3 | 1:K:452:LYS:HA | 1.56 | 0.86 |
| 1:L:142:ASP:O | 1:M:283:THR:HG21 | 1.75 | 0.86 |
| 1:O:66:SER:H | 1:O:69:GLN:NE2 | 1.73 | 0.86 |
| 1:F:260:LEU:HD23 | 1:J:117:ILE:HD11 | 1.57 | 0.86 |
| 1:I:171:LYS:HA | 1:I:187:PRO:O | 1.74 | 0.86 |
| 1:L:262:ASN:ND2 | 1:L:288:SER:HB3 | 1.89 | 0.86 |
| 1:O:66:SER:O | 1:O:69:GLN:HG3 | 1.75 | 0.86 |
| 1:A:302:SER:HB2 | 1:B:253:GLU:H | 1.40 | 0.86 |
| 1:G:242:TYR:CE2 | 1:G:394:MET:HG3 | 2.10 | 0.86 |
| 1:B:82:LYS:CB | 1:B:82:LYS:CD | 2.53 | 0.86 |
| 1:F:217:LYS:HD3 | 1:G:274:ASP:O | 1.76 | 0.86 |
| 1:J:75:ILE:CG2 | 1:J:451:LEU:HD12 | 2.04 | 0.86 |
| 1:L:180:VAL:HG13 | 1:L:184:ASP:HB2 | 1.58 | 0.86 |
| 1:C:348:ILE:HG22 | 1:C:359:ASN:OD1 | 1.74 | 0.86 |
| 1:F:21:VAL:HG12 | 1:F:22:VAL:N | 1.88 | 0.86 |
| 1:K:443:LYS:HD3 | 1:K:443:LYS:N | 1.90 | 0.86 |
| 1:A:78:PRO:HD3 | 1:A:452:LYS:HA | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:154:THR:O | 1:F:336:THR:HG23 | 1.76 | 0.86 |
| 1:N:153:GLN:HE22 | 1:N:300:VAL:HA | 1.39 | 0.86 |
| 1:H:151:TYR:CD2 | 1:H:203:THR:HB | 2.10 | 0.86 |
| 1:I:34:TYR:CE2 | 1:I:377:GLN:HB2 | 2.11 | 0.86 |
| 1:K:345:CYS:SG | 1:L:216:ASN:CB | 2.63 | 0.86 |
| 1:A:66:SER:H | 1:A:69:GLN:HE21 | 1.24 | 0.86 |
| 1:J:207:ALA:HB1 | 1:J:229:CYS:O | 1.75 | 0.86 |
| 1:F:65:VAL:HA | 1:F:69:GLN:HE22 | 1.38 | 0.85 |
| 1:F:126:LEU:HB3 | 1:F:262:ASN:HB3 | 1.58 | 0.85 |
| 1:G:96:GLN:HB3 | 1:G:382:THR:HG22 | 1.58 | 0.85 |
| 1:N:156:LEU:HG | 1:N:334:VAL:HB | 1.58 | 0.85 |
| 1:H:121:PRO:O | 1:H:122:LEU:HD23 | 1.75 | 0.85 |
| 1:I:70:TYR:OH | 1:I:232:PRO:HD3 | 1.77 | 0.85 |
| 1:N:363:TYR:CD1 | 1:O:185:CYS:HB2 | 2.11 | 0.85 |
| 1:A:156:LEU:C | 1:A:156:LEU:HD12 | 1.97 | 0.85 |
| 1:F:254:GLN:HA | 1:J:300:VAL:O | 1.76 | 0.85 |
| 1:F:255:MET:SD | 1:J:114:GLY:HA2 | 2.17 | 0.85 |
| 1:J:50:PHE:HB2 | 1:J:51:PRO:HD2 | 1.58 | 0.85 |
| 1:O:443:LYS:HD3 | 1:O:443:LYS:H | 1.40 | 0.85 |
| 1:C:40:SER:O | 1:C:371:ASP:OD1 | 1.95 | 0.85 |
| 1:D:180:VAL:HG12 | 1:D:184:ASP:HB2 | 1.58 | 0.85 |
| 1:E:23:SER:OG | 1:E:25:ASP:HB2 | 1.75 | 0.85 |
| 1:E:151:TYR:CD2 | 1:E:203:THR:HB | 2.11 | 0.85 |
| 1:E:183:GLY:O | 1:E:185:CYS:N | 2.10 | 0.85 |
| 1:J:66:SER:H | 1:J:69:GLN:NE2 | 1.74 | 0.85 |
| 1:D:78:PRO:HD3 | 1:D:452:LYS:HA | 1.56 | 0.85 |
| 1:A:46:GLY:HA3 | 1:A:65:VAL:HG23 | 1.57 | 0.85 |
| 1:C:345:CYS:SG | 1:D:216:ASN:CB | 2.63 | 0.85 |
| 1:F:99:VAL:HG11 | 1:F:323:ILE:HG22 | 1.58 | 0.85 |
| 1:G:104:GLY:O | 1:G:374:PHE:HA | 1.75 | 0.85 |
| 1:C:142:ASP:OD2 | 1:C:144:ARG:HG3 | 1.76 | 0.85 |
| 1:L:74:ARG:HG3 | 1:L:330:PHE:CE2 | 2.11 | 0.85 |
| 1:F:253:GLU:H | 1:J:302:SER:HB2 | 1.41 | 0.84 |
| 1:G:320:ASN:ND2 | 1:G:323:ILE:HB | 1.91 | 0.84 |
| 1:O:74:ARG:HG3 | 1:O:330:PHE:CE2 | 2.12 | 0.84 |
| 1:B:46:GLY:HA3 | 1:B:65:VAL:CG2 | 2.07 | 0.84 |
| 1:F:345:CYS:SG | 1:G:216:ASN:HB2 | 2.17 | 0.84 |
| 1:G:344:LEU:HD13 | 1:H:213:LEU:HD12 | 1.57 | 0.84 |
| 1:J:246:LEU:H | 1:J:246:LEU:HD23 | 1.40 | 0.84 |
| 1:N:390:TYR:O | 1:N:392:HIS:N | 2.10 | 0.84 |
| 1:C:180:VAL:HG12 | 1:C:184:ASP:CB | 2.05 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:255:MET:HG2 | 1:G:256:PHE:N | 1.86 | 0.84 |
| 1:A:147:ILE:HA | 1:B:129:THR:O | 1.77 | 0.84 |
| 1:A:151:TYR:CD2 | 1:A:203:THR:HB | 2.12 | 0.84 |
| 1:A:176:THR:O | 1:A:177:GLN:HG3 | 1.77 | 0.84 |
| 1:C:166:GLY:CA | 1:C:195:ILE:HD11 | 2.06 | 0.84 |
| 1:D:358:THR:HA | 1:E:266:THR:CG2 | 2.07 | 0.84 |
| 1:K:156:LEU:HG | 1:K:334:VAL:HB | 1.57 | 0.84 |
| 1:M:117:ILE:HD11 | 1:N:260:LEU:HD23 | 1.59 | 0.84 |
| 1:D:52:ILE:N | 1:D:52:ILE:HD12 | 1.93 | 0.84 |
| 1:J:151:TYR:CD2 | 1:J:203:THR:HB | 2.12 | 0.84 |
| 1:L:172:GLY:O | 1:L:173:SER:O | 1.94 | 0.84 |
| 1:M:66:SER:H | 1:M:69:GLN:NE2 | 1.75 | 0.84 |
| 1:M:180:VAL:HG12 | 1:M:184:ASP:HB2 | 1.58 | 0.84 |
| 1:O:451:LEU:HD23 | 1:O:454:LYS:HG3 | 1.57 | 0.84 |
| 1:D:272:PRO:HD2 | 1:D:275:LEU:HD12 | 1.59 | 0.84 |
| 1:G:176:THR:O | 1:G:177:GLN:HG3 | 1.77 | 0.84 |
| 1:O:250:LEU:H | 1:O:250:LEU:HD12 | 1.43 | 0.84 |
| 1:B:344:LEU:HD12 | 1:C:186:PRO:CD | 2.06 | 0.84 |
| 1:G:112:PRO:HD3 | 1:H:231:TYR:CD2 | 2.12 | 0.84 |
| 1:H:171:LYS:HA | 1:H:187:PRO:O | 1.76 | 0.84 |
| 1:C:466:ARG:HD2 | 1:D:317:GLN:O | 1.77 | 0.84 |
| 1:F:389:THR:CG2 | 1:F:389:THR:HB | 2.04 | 0.84 |
| 1:G:188:LEU:CD1 | 1:G:213:LEU:HD11 | 2.07 | 0.84 |
| 1:N:154:THR:H | 1:N:336:THR:CG2 | 1.89 | 0.84 |
| 1:A:300:VAL:O | 1:B:254:GLN:HA | 1.76 | 0.84 |
| 1:D:380:LYS:CE | 1:D:380:LYS:CG | 2.56 | 0.84 |
| 1:C:250:LEU:HD12 | 1:C:250:LEU:H | 1.42 | 0.84 |
| 1:A:361:LYS:HA | 1:B:266:THR:HG1 | 1.42 | 0.83 |
| 1:B:152:LYS:HB2 | 1:B:255:MET:CB | 2.08 | 0.83 |
| 1:C:34:TYR:CE2 | 1:C:377:GLN:HB2 | 2.13 | 0.83 |
| 1:G:23:SER:OG | 1:G:25:ASP:HB2 | 1.78 | 0.83 |
| 1:K:167:GLU:HB2 | 1:K:190:LEU:HD11 | 1.60 | 0.83 |
| 1:M:113:LEU:HD22 | 1:N:253:GLU:HG3 | 1.60 | 0.83 |
| 1:N:248:PHE:CZ | 1:N:311:TYR:HB3 | 2.13 | 0.83 |
| 1:A:57:ASN:HD21 | 1:A:59:LYS:HB3 | 1.42 | 0.83 |
| 1:C:65:VAL:HA | 1:C:69:GLN:NE2 | 1.93 | 0.83 |
| 1:E:67:GLY:O | 1:E:68:LEU:HG | 1.78 | 0.83 |
| 1:K:443:LYS:H | 1:K:443:LYS:CD | 1.91 | 0.83 |
| 1:N:70:TYR:OH | 1:N:230:LYS:O | 1.96 | 0.83 |
| 1:F:75:ILE:CG2 | 1:F:451:LEU:HD12 | 2.07 | 0.83 |
| 1:N:21:VAL:HG13 | 1:N:390:TYR:OH | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:152:LYS:CB | 1:E:255:MET:HB2 | 2.07 | 0.83 |
| 1:F:154:THR:H | 1:F:336:THR:HG21 | 1.44 | 0.83 |
| 1:L:92:ASN:ND2 | 1:L:95:THR:OG1 | 2.10 | 0.83 |
| 1:M:228:ILE:N | 1:M:228:ILE:HD12 | 1.92 | 0.83 |
| 1:E:57:ASN:ND2 | 1:E:59:LYS:H | 1.76 | 0.83 |
| 1:E:156:LEU:HG | 1:E:334:VAL:HB | 1.58 | 0.83 |
| 1:J:152:LYS:HG3 | 1:J:152:LYS:O | 1.78 | 0.83 |
| 1:K:276:TYR:HA | 1:O:217:LYS:HG2 | 1.61 | 0.83 |
| 1:A:231:TYR:CD2 | 1:E:112:PRO:HD3 | 2.14 | 0.83 |
| 1:I:71:ARG:HH11 | 1:I:71:ARG:HA | 1.42 | 0.83 |
| 1:L:180:VAL:HG12 | 1:L:184:ASP:HB2 | 1.59 | 0.83 |
| 1:L:470:LEU:O | 1:L:470:LEU:HD23 | 1.78 | 0.83 |
| 1:O:36:HIS:CG | 1:O:462:PHE:CD1 | 2.67 | 0.83 |
| 1:O:78:PRO:HD3 | 1:O:452:LYS:HA | 1.58 | 0.83 |
| 1:O:98:LEU:CD1 | 1:O:98:LEU:HG | 2.06 | 0.83 |
| 1:B:122:LEU:HD21 | 1:C:286:LEU:CD1 | 2.09 | 0.83 |
| 1:E:46:GLY:HA3 | 1:E:65:VAL:HG23 | 1.59 | 0.83 |
| 1:F:75:ILE:HD12 | 1:F:75:ILE:N | 1.93 | 0.83 |
| 1:I:217:LYS:HD3 | 1:J:274:ASP:O | 1.76 | 0.83 |
| 1:K:189:GLU:O | 1:K:191:ILE:HG13 | 1.77 | 0.83 |
| 1:L:167:GLU:HB2 | 1:L:190:LEU:HD11 | 1.58 | 0.83 |
| 1:C:82:LYS:HZ1 | 1:C:403:ASN:ND2 | 1.74 | 0.83 |
| 1:E:459:LEU:HB3 | 1:E:465:GLY:HA3 | 1.58 | 0.83 |
| 1:G:71:ARG:HH12 | 1:G:198:GLY:N | 1.77 | 0.83 |
| 1:G:112:PRO:HB2 | 1:H:202:ASP:OD2 | 1.79 | 0.83 |
| 1:L:361:LYS:HA | 1:M:266:THR:OG1 | 1.78 | 0.83 |
| 1:M:180:VAL:CG1 | 1:M:184:ASP:CB | 2.53 | 0.83 |
| 1:A:171:LYS:HA | 1:A:187:PRO:O | 1.78 | 0.83 |
| 1:B:52:ILE:HD12 | 1:B:52:ILE:N | 1.92 | 0.83 |
| 1:C:188:LEU:HD11 | 1:C:213:LEU:HD11 | 1.58 | 0.83 |
| 1:G:70:TYR:OH | 1:G:232:PRO:HD3 | 1.79 | 0.83 |
| 1:I:152:LYS:HE2 | 1:I:202:ASP:HB3 | 1.59 | 0.83 |
| 1:L:166:GLY:N | 1:L:195:ILE:CD1 | 2.41 | 0.83 |
| 1:N:72:VAL:HG21 | 1:N:195:ILE:O | 1.79 | 0.83 |
| 1:O:152:LYS:HB2 | 1:O:255:MET:CB | 2.09 | 0.83 |
| 1:O:279:GLY:HA3 | 1:O:283:THR:O | 1.78 | 0.83 |
| 1:C:117:ILE:HD11 | 1:D:260:LEU:HD23 | 1.60 | 0.83 |
| 1:C:190:LEU:HD12 | 1:C:191:ILE:N | 1.94 | 0.83 |
| 1:F:123:LEU:HD23 | 1:F:147:ILE:HB | 1.61 | 0.83 |
| 1:G:71:ARG:NH1 | 1:G:198:GLY:H | 1.75 | 0.83 |
| 1:M:65:VAL:HA | 1:M:69:GLN:HE22 | 1.44 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:216:ASN:CG | 1:G:219:GLU:OE2 | 2.17 | 0.82 |
| 1:H:384:THR:HG23 | 1:H:387:VAL:HG21 | 1.60 | 0.82 |
| 1:J:178:VAL:O | 1:J:180:VAL:N | 2.12 | 0.82 |
| 1:C:71:ARG:HH11 | 1:C:71:ARG:HA | 1.43 | 0.82 |
| 1:D:79:ASP:OD2 | 1:D:81:ASN:HB2 | 1.78 | 0.82 |
| 1:I:174:PRO:HG3 | 1:I:187:PRO:CG | 2.09 | 0.82 |
| 1:K:378:LEU:C | 1:K:378:LEU:HD12 | 1.99 | 0.82 |
| 1:D:361:LYS:HA | 1:E:266:THR:OG1 | 1.79 | 0.82 |
| 1:E:43:LEU:HD12 | 1:E:369:GLU:HA | 1.58 | 0.82 |
| 1:F:49:TYR:HE2 | 1:F:118:SER:HA | 1.42 | 0.82 |
| 1:G:65:VAL:HA | 1:G:69:GLN:HE22 | 1.44 | 0.82 |
| 1:H:122:LEU:HD13 | 1:H:144:ARG:NH2 | 1.94 | 0.82 |
| 1:I:109:ARG:NH1 | 1:I:370:TYR:CE1 | 2.47 | 0.82 |
| 1:O:272:PRO:HD2 | 1:O:275:LEU:HD11 | 1.61 | 0.82 |
| 1:A:92:ASN:ND2 | 1:A:95:THR:H | 1.76 | 0.82 |
| 1:A:159:ILE:HD12 | 1:A:248:PHE:HD2 | 1.45 | 0.82 |
| 1:F:30:ARG:HH11 | 1:F:377:GLN:HE22 | 1.27 | 0.82 |
| 1:F:176:THR:O | 1:F:177:GLN:HG3 | 1.78 | 0.82 |
| 1:B:52:ILE:HB | 1:B:62:VAL:HB | 1.59 | 0.82 |
| 1:D:101:ALA:HA | 1:D:322:GLY:O | 1.77 | 0.82 |
| 1:H:99:VAL:HG11 | 1:H:323:ILE:CG2 | 2.09 | 0.82 |
| 1:L:242:TYR:CE2 | 1:L:394:MET:HG3 | 2.14 | 0.82 |
| 1:M:75:ILE:HB | 1:M:329:LEU:HB3 | 1.62 | 0.82 |
| 1:A:139:ALA:CA | 1:A:143:ASN:HD21 | 1.92 | 0.82 |
| 1:I:82:LYS:CE | 1:I:82:LYS:CG | 2.57 | 0.82 |
| 1:K:192:ASN:HD21 | 1:O:41:ARG:HH22 | 1.24 | 0.82 |
| 1:N:338:ARG:CD | 1:N:338:ARG:CB | 2.58 | 0.82 |
| 1:F:95:THR:O | 1:F:383:LEU:N | 2.11 | 0.82 |
| 1:O:92:ASN:ND2 | 1:O:95:THR:H | 1.77 | 0.82 |
| 1:O:123:LEU:CD2 | 1:O:147:ILE:HB | 2.10 | 0.82 |
| 1:E:98:LEU:HD22 | 1:E:379:CYS:O | 1.80 | 0.82 |
| 1:F:451:LEU:HD23 | 1:F:454:LYS:HG3 | 1.59 | 0.82 |
| 1:M:451:LEU:HD23 | 1:M:454:LYS:HG3 | 1.61 | 0.82 |
| 1:N:97:ARG:HA | 1:N:97:ARG:HH11 | 1.44 | 0.82 |
| 1:C:82:LYS:NZ | 1:C:403:ASN:HD22 | 1.78 | 0.82 |
| 1:L:71:ARG:HA | 1:L:71:ARG:NH1 | 1.95 | 0.82 |
| 1:L:237:MET:O | 1:L:240:GLU:HB3 | 1.80 | 0.82 |
| 1:A:375:ILE:HG12 | 1:A:464:LEU:HD13 | 1.61 | 0.81 |
| 1:C:180:VAL:CG1 | 1:C:184:ASP:CB | 2.57 | 0.81 |
| 1:M:115:VAL:H | 1:N:255:MET:CE | 1.92 | 0.81 |
| 1:M:298:SER:OG | 1:M:299:MET:N | 2.12 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:122:LEU:HD13 | 1:B:144:ARG:NH2 | 1.95 | 0.81 |
| 1:F:72:VAL:HG21 | 1:F:195:ILE:O | 1.78 | 0.81 |
| 1:F:156:LEU:HG | 1:F:334:VAL:HB | 1.62 | 0.81 |
| 1:H:24:THR:CG2 | 1:H:320:ASN:HA | 2.10 | 0.81 |
| 1:K:242:TYR:CD2 | 1:K:394:MET:HG3 | 2.15 | 0.81 |
| 1:M:262:ASN:C | 1:M:262:ASN:HD22 | 1.82 | 0.81 |
| 1:C:126:LEU:HB3 | 1:C:262:ASN:HB3 | 1.59 | 0.81 |
| 1:C:298:SER:OG | 1:C:299:MET:N | 2.12 | 0.81 |
| 1:D:152:LYS:NZ | 1:D:253:GLU:OE1 | 2.13 | 0.81 |
| 1:G:54:LYS:HB2 | 1:G:57:ASN:HD22 | 1.44 | 0.81 |
| 1:I:156:LEU:HD12 | 1:I:156:LEU:O | 1.79 | 0.81 |
| 1:J:180:VAL:HG13 | 1:J:184:ASP:CB | 2.09 | 0.81 |
| 1:K:171:LYS:HA | 1:K:187:PRO:O | 1.80 | 0.81 |
| 1:L:344:LEU:HD12 | 1:M:186:PRO:HG2 | 1.61 | 0.81 |
| 1:B:96:GLN:HB3 | 1:B:382:THR:HG22 | 1.61 | 0.81 |
| 1:F:361:LYS:HA | 1:G:266:THR:OG1 | 1.80 | 0.81 |
| 1:H:156:LEU:HD11 | 1:H:334:VAL:HG23 | 1.63 | 0.81 |
| 1:H:391:ILE:HB | 1:H:399:LEU:HD21 | 1.62 | 0.81 |
| 1:N:34:TYR:CE2 | 1:N:377:GLN:HB2 | 2.14 | 0.81 |
| 1:O:170:GLY:HA2 | 1:O:213:LEU:HD21 | 1.62 | 0.81 |
| 1:C:375:ILE:HG12 | 1:C:464:LEU:HD13 | 1.62 | 0.81 |
| 1:G:123:LEU:HD23 | 1:G:147:ILE:HB | 1.60 | 0.81 |
| 1:H:70:TYR:OH | 1:H:230:LYS:O | 1.97 | 0.81 |
| 1:A:97:ARG:HH11 | 1:A:97:ARG:HA | 1.46 | 0.81 |
| 1:G:470:LEU:CD1 | 1:G:470:LEU:CB | 2.59 | 0.81 |
| 1:I:75:ILE:CG2 | 1:I:451:LEU:HD12 | 2.09 | 0.81 |
| 1:K:159:ILE:HD12 | 1:K:248:PHE:HD2 | 1.45 | 0.81 |
| 1:L:154:THR:O | 1:L:336:THR:HG23 | 1.80 | 0.81 |
| 1:M:167:GLU:HG2 | 1:M:231:TYR:O | 1.81 | 0.81 |
| 1:D:302:SER:HB2 | 1:E:253:GLU:H | 1.43 | 0.81 |
| 1:B:172:GLY:O | 1:B:173:SER:C | 2.17 | 0.81 |
| 1:K:122:LEU:HD13 | 1:K:144:ARG:NH2 | 1.95 | 0.81 |
| 1:M:237:MET:O | 1:M:240:GLU:HB3 | 1.81 | 0.81 |
| 1:D:30:ARG:HH11 | 1:D:377:GLN:NE2 | 1.78 | 0.81 |
| 1:I:57:ASN:ND2 | 1:I:59:LYS:H | 1.79 | 0.81 |
| 1:K:151:TYR:CD2 | 1:K:203:THR:HB | 2.16 | 0.81 |
| 1:M:156:LEU:C | 1:M:156:LEU:HD12 | 2.01 | 0.81 |
| 1:N:65:VAL:HA | 1:N:69:GLN:HE22 | 1.46 | 0.81 |
| 1:N:67:GLY:C | 1:N:68:LEU:HG | 1.94 | 0.81 |
| 1:A:52:ILE:N | 1:A:52:ILE:CD1 | 2.43 | 0.81 |
| 1:G:262:ASN:HD22 | 1:G:263:ARG:N | 1.79 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:70:TYR:OH | 1:K:232:PRO:HD3 | 1.81 | 0.81 |
| 1:C:74:ARG:HG3 | 1:C:330:PHE:HE2 | 1.45 | 0.80 |
| 1:D:471:GLN:O | 1:D:472:LEU:OXT | 1.98 | 0.80 |
| 1:F:52:ILE:HD12 | 1:F:52:ILE:N | 1.95 | 0.80 |
| 1:H:101:ALA:HA | 1:H:322:GLY:O | 1.80 | 0.80 |
| 1:I:358:THR:HG22 | 1:J:266:THR:HG22 | 1.62 | 0.80 |
| 1:L:344:LEU:HD12 | 1:M:186:PRO:HD2 | 1.63 | 0.80 |
| 1:A:262:ASN:ND2 | 1:A:288:SER:HB3 | 1.94 | 0.80 |
| 1:D:64:LYS:CG | 1:D:64:LYS:CA | 2.59 | 0.80 |
| 1:G:152:LYS:HB2 | 1:G:255:MET:HB2 | 1.63 | 0.80 |
| 1:J:99:VAL:HG11 | 1:J:323:ILE:HG23 | 1.63 | 0.80 |
| 1:D:34:TYR:CE2 | 1:D:377:GLN:CG | 2.64 | 0.80 |
| 1:E:96:GLN:HB3 | 1:E:382:THR:CG2 | 2.11 | 0.80 |
| 1:F:96:GLN:HA | 1:F:383:LEU:HD12 | 1.63 | 0.80 |
| 1:M:64:LYS:CG | 1:M:64:LYS:CA | 2.58 | 0.80 |
| 1:G:49:TYR:CE2 | 1:G:118:SER:HA | 2.17 | 0.80 |
| 1:H:280:SER:O | 1:H:280:SER:OG | 1.99 | 0.80 |
| 1:L:241:PRO:HG2 | 1:L:242:TYR:H | 1.45 | 0.80 |
| 1:A:101:ALA:HA | 1:A:322:GLY:O | 1.81 | 0.80 |
| 1:H:360:PHE:O | 1:I:266:THR:OG1 | 2.00 | 0.80 |
| 1:L:344:LEU:N | 1:L:344:LEU:HD23 | 1.96 | 0.80 |
| 1:M:344:LEU:HD23 | 1:M:344:LEU:H | 1.43 | 0.80 |
| 1:A:74:ARG:CZ | 1:A:441:LEU:HD12 | 2.11 | 0.80 |
| 1:A:461:GLN:HE22 | 1:B:21:VAL:HB | 1.46 | 0.80 |
| 1:C:441:LEU:CD2 | 1:C:441:LEU:HG | 2.07 | 0.80 |
| 1:F:246:LEU:H | 1:F:246:LEU:CD2 | 1.93 | 0.80 |
| 1:I:367:GLY:O | 1:I:368:GLU:HG2 | 1.81 | 0.80 |
| 1:N:313:LEU:CD2 | 1:N:313:LEU:CD1 | 2.59 | 0.80 |
| 1:N:361:LYS:HA | 1:O:266:THR:HG1 | 1.44 | 0.80 |
| 1:O:230:LYS:NZ | 1:O:230:LYS:CD | 2.44 | 0.80 |
| 1:A:180:VAL:CG1 | 1:A:184:ASP:CB | 2.60 | 0.80 |
| 1:D:71:ARG:HH11 | 1:D:71:ARG:CA | 1.94 | 0.80 |
| 1:J:163:PRO:HD3 | 1:J:330:PHE:HE1 | 1.47 | 0.80 |
| 1:L:361:LYS:NZ | 1:L:361:LYS:CD | 2.45 | 0.80 |
| 1:M:52:ILE:HD12 | 1:M:52:ILE:N | 1.94 | 0.80 |
| 1:N:112:PRO:HD3 | 1:O:231:TYR:CD2 | 2.16 | 0.80 |
| 1:O:452:LYS:CE | 1:O:452:LYS:CG | 2.59 | 0.80 |
| 1:B:96:GLN:HB3 | 1:B:382:THR:CG2 | 2.11 | 0.80 |
| 1:K:323:ILE:HD13 | 1:K:323:ILE:N | 1.97 | 0.80 |
| 1:O:261:PHE:HB3 | 1:O:292:PHE:CE2 | 2.17 | 0.80 |
| 1:A:299:MET:HA | 1:B:256:PHE:HB3 | 1.61 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:65:VAL:HA | 1:E:69:GLN:NE2 | 1.97 | 0.80 |
| 1:F:78:PRO:CD | 1:F:452:LYS:HA | 2.12 | 0.80 |
| 1:F:363:TYR:CD1 | 1:G:185:CYS:HB2 | 2.17 | 0.80 |
| 1:M:463:PRO:HA | 1:M:466:ARG:HE | 1.47 | 0.80 |
| 1:D:70:TYR:HH | 1:D:232:PRO:HD3 | 1.46 | 0.80 |
| 1:E:395:ASN:O | 1:E:398:ILE:HG12 | 1.81 | 0.80 |
| 1:F:365:ARG:HD3 | 1:F:365:ARG:HA | 1.64 | 0.80 |
| 1:H:180:VAL:CG1 | 1:H:184:ASP:HB2 | 2.12 | 0.80 |
| 1:G:30:ARG:HH11 | 1:G:377:GLN:NE2 | 1.80 | 0.79 |
| 1:G:72:VAL:HG22 | 1:G:332:THR:CG2 | 2.12 | 0.79 |
| 1:G:113:LEU:HD22 | 1:H:253:GLU:HG3 | 1.62 | 0.79 |
| 1:G:399:LEU:O | 1:G:402:TRP:HB2 | 1.81 | 0.79 |
| 1:J:79:ASP:OD2 | 1:J:81:ASN:HB2 | 1.82 | 0.79 |
| 1:J:375:ILE:HG12 | 1:J:464:LEU:HD13 | 1.63 | 0.79 |
| 1:M:74:ARG:HB2 | 1:M:330:PHE:CE2 | 2.16 | 0.79 |
| 1:N:252:ARG:HD2 | 1:N:306:ILE:HD11 | 1.63 | 0.79 |
| 1:B:77:LEU:HD22 | 1:B:455:PHE:CZ | 2.17 | 0.79 |
| 1:B:451:LEU:O | 1:B:454:LYS:HB2 | 1.82 | 0.79 |
| 1:G:466:ARG:HD2 | 1:H:317:GLN:O | 1.80 | 0.79 |
| 1:M:130:GLU:HB2 | 1:M:260:LEU:HD13 | 1.65 | 0.79 |
| 1:M:255:MET:HG2 | 1:M:256:PHE:H | 1.46 | 0.79 |
| 1:K:373:GLN:HB3 | 1:K:464:LEU:HD12 | 1.63 | 0.79 |
| 1:F:30:ARG:HH11 | 1:F:377:GLN:NE2 | 1.81 | 0.79 |
| 1:F:252:ARG:HD2 | 1:F:306:ILE:HD11 | 1.64 | 0.79 |
| 1:N:320:ASN:OD1 | 1:N:321:ASN:N | 2.16 | 0.79 |
| 1:B:72:VAL:HG22 | 1:B:332:THR:HG23 | 1.65 | 0.79 |
| 1:B:172:GLY:O | 1:B:173:SER:O | 2.00 | 0.79 |
| 1:C:112:PRO:HB2 | 1:D:202:ASP:OD2 | 1.82 | 0.79 |
| 1:D:242:TYR:CE2 | 1:D:394:MET:HB2 | 2.17 | 0.79 |
| 1:E:30:ARG:HH11 | 1:E:377:GLN:NE2 | 1.81 | 0.79 |
| 1:G:461:GLN:HE22 | 1:H:21:VAL:HB | 1.48 | 0.79 |
| 1:J:54:LYS:HG2 | 1:J:56:ASN:OD1 | 1.83 | 0.79 |
| 1:K:142:ASP:O | 1:L:283:THR:HG21 | 1.82 | 0.79 |
| 1:M:323:ILE:HD13 | 1:M:323:ILE:N | 1.97 | 0.79 |
| 1:O:442:LYS:NZ | 1:O:442:LYS:HG2 | 1.97 | 0.79 |
| 1:A:117:ILE:HD12 | 1:B:293:PRO:HB3 | 1.65 | 0.79 |
| 1:D:23:SER:OG | 1:D:25:ASP:HB2 | 1.83 | 0.79 |
| 1:J:95:THR:O | 1:J:383:LEU:N | 2.11 | 0.79 |
| 1:C:344:LEU:HD13 | 1:D:213:LEU:HD12 | 1.65 | 0.79 |
| 1:E:160:GLY:HA3 | 1:E:245:SER:O | 1.83 | 0.79 |
| 1:G:120:HIS:HE2 | 1:G:218:SER:HB3 | 1.46 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:323:ILE:HG21 | 1:K:325:TRP:CH2 | 2.18 | 0.79 |
| 1:M:381:ILE:HG22 | 1:M:381:ILE:O | 1.83 | 0.79 |
| 1:O:280:SER:CA | 1:O:284:ALA:HB2 | 2.12 | 0.79 |
| 1:C:162:LYS:C | 1:C:330:PHE:HD1 | 1.85 | 0.79 |
| 1:G:54:LYS:HA | 1:G:54:LYS:NZ | 1.98 | 0.79 |
| 1:B:463:PRO:HB3 | 1:B:466:ARG:HH21 | 1.47 | 0.79 |
| 1:F:57:ASN:ND2 | 1:F:59:LYS:H | 1.81 | 0.79 |
| 1:G:78:PRO:HD3 | 1:G:452:LYS:HA | 1.64 | 0.79 |
| 1:D:72:VAL:HG22 | 1:D:332:THR:HG23 | 1.66 | 0.78 |
| 1:K:52:ILE:HD12 | 1:K:52:ILE:N | 1.98 | 0.78 |
| 1:A:162:LYS:NZ | 1:A:162:LYS:CD | 2.45 | 0.78 |
| 1:F:97:ARG:HA | 1:F:97:ARG:HH11 | 1.45 | 0.78 |
| 1:I:228:ILE:HD12 | 1:I:228:ILE:N | 1.96 | 0.78 |
| 1:J:96:GLN:HA | 1:J:382:THR:CA | 2.14 | 0.78 |
| 1:M:152:LYS:HB2 | 1:M:255:MET:HB2 | 1.64 | 0.78 |
| 1:B:117:ILE:HD11 | 1:C:260:LEU:HD23 | 1.65 | 0.78 |
| 1:B:123:LEU:CD2 | 1:B:123:LEU:HG | 2.10 | 0.78 |
| 1:C:255:MET:HG2 | 1:C:256:PHE:N | 1.98 | 0.78 |
| 1:D:176:THR:O | 1:D:177:GLN:CG | 2.31 | 0.78 |
| 1:D:300:VAL:O | 1:D:300:VAL:HG23 | 1.81 | 0.78 |
| 1:F:65:VAL:HA | 1:F:69:GLN:NE2 | 1.97 | 0.78 |
| 1:H:30:ARG:NH1 | 1:H:377:GLN:HE22 | 1.80 | 0.78 |
| 1:K:117:ILE:HD12 | 1:L:293:PRO:HB3 | 1.64 | 0.78 |
| 1:K:41:ARG:HH22 | 1:L:192:ASN:ND2 | 1.81 | 0.78 |
| 1:A:207:ALA:HB1 | 1:A:229:CYS:O | 1.82 | 0.78 |
| 1:E:257:VAL:HG12 | 1:E:293:PRO:HB2 | 1.62 | 0.78 |
| 1:F:97:ARG:HA | 1:F:97:ARG:NH1 | 1.98 | 0.78 |
| 1:I:348:ILE:HG22 | 1:I:359:ASN:OD1 | 1.84 | 0.78 |
| 1:L:120:HIS:HA | 1:L:222:LEU:HD13 | 1.65 | 0.78 |
| 1:M:323:ILE:CD1 | 1:M:323:ILE:CA | 2.61 | 0.78 |
| 1:B:101:ALA:HA | 1:B:322:GLY:O | 1.84 | 0.78 |
| 1:F:363:TYR:CG | 1:G:185:CYS:HB2 | 2.19 | 0.78 |
| 1:G:345:CYS:SG | 1:H:216:ASN:CB | 2.68 | 0.78 |
| 1:I:68:LEU:HD23 | 1:I:201:VAL:HG21 | 1.66 | 0.78 |
| 1:I:323:ILE:HD13 | 1:I:323:ILE:N | 1.99 | 0.78 |
| 1:J:236:LYS:CD | 1:J:236:LYS:CB | 2.61 | 0.78 |
| 1:K:300:VAL:O | 1:L:254:GLN:HA | 1.82 | 0.78 |
| 1:L:348:ILE:HG22 | 1:L:359:ASN:OD1 | 1.83 | 0.78 |
| 1:N:152:LYS:NZ | 1:N:253:GLU:OE1 | 2.17 | 0.78 |
| 1:D:117:ILE:HD11 | 1:E:260:LEU:HD23 | 1.65 | 0.78 |
| 1:F:255:MET:SD | 1:J:114:GLY:CA | 2.72 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:34:TYR:HE2 | 1:L:377:GLN:HB2 | 1.44 | 0.78 |
| 1:L:54:LYS:HG3 | 1:L:55:PRO:HD2 | 1.65 | 0.78 |
| 1:O:237:MET:HB3 | 1:O:246:LEU:HD22 | 1.64 | 0.78 |
| 1:C:151:TYR:CD2 | 1:C:203:THR:HB | 2.19 | 0.78 |
| 1:D:66:SER:OG | 1:D:67:GLY:N | 2.15 | 0.78 |
| 1:E:193:THR:HG23 | 1:E:230:LYS:HD2 | 1.63 | 0.78 |
| 1:H:277:ILE:CD1 | 1:H:277:ILE:CB | 2.61 | 0.78 |
| 1:H:469:LEU:CD2 | 1:H:469:LEU:CB | 2.61 | 0.78 |
| 1:I:193:THR:CG2 | 1:I:193:THR:CA | 2.62 | 0.78 |
| 1:N:66:SER:N | 1:N:69:GLN:HE21 | 1.80 | 0.78 |
| 1:C:356:LYS:NZ | 1:C:356:LYS:CD | 2.45 | 0.78 |
| 1:D:60:ILE:O | 1:D:60:ILE:HG13 | 1.84 | 0.78 |
| 1:D:395:ASN:HB3 | 1:D:398:ILE:HG12 | 1.66 | 0.78 |
| 1:E:250:LEU:N | 1:E:250:LEU:HD12 | 1.98 | 0.78 |
| 1:G:156:LEU:HG | 1:G:334:VAL:HB | 1.63 | 0.78 |
| 1:G:201:VAL:CG2 | 1:G:201:VAL:CG1 | 2.61 | 0.78 |
| 1:K:180:VAL:CG1 | 1:K:184:ASP:CB | 2.62 | 0.78 |
| 1:K:373:GLN:CB | 1:K:464:LEU:HD12 | 2.13 | 0.78 |
| 1:M:300:VAL:HG23 | 1:M:300:VAL:O | 1.83 | 0.78 |
| 1:N:75:ILE:N | 1:N:75:ILE:CD1 | 2.37 | 0.78 |
| 1:J:66:SER:H | 1:J:69:GLN:HE21 | 1.30 | 0.78 |
| 1:J:67:GLY:O | 1:J:68:LEU:HG | 1.84 | 0.78 |
| 1:L:39:THR:O | 1:L:39:THR:OG1 | 1.92 | 0.78 |
| 1:O:49:TYR:HE2 | 1:O:118:SER:HA | 1.47 | 0.78 |
| 1:O:54:LYS:HG3 | 1:O:55:PRO:HD2 | 1.64 | 0.78 |
| 1:E:250:LEU:HD12 | 1:E:250:LEU:H | 1.47 | 0.77 |
| 1:F:176:THR:CG2 | 1:F:176:THR:CA | 2.62 | 0.77 |
| 1:H:122:LEU:HD11 | 1:I:286:LEU:HD11 | 1.66 | 0.77 |
| 1:J:399:LEU:HD23 | 1:J:402:TRP:CE3 | 2.19 | 0.77 |
| 1:B:57:ASN:HD21 | 1:B:59:LYS:HB3 | 1.48 | 0.77 |
| 1:B:171:LYS:HA | 1:B:187:PRO:O | 1.83 | 0.77 |
| 1:C:156:LEU:HG | 1:C:334:VAL:HB | 1.66 | 0.77 |
| 1:D:54:LYS:CB | 1:D:57:ASN:HB3 | 2.15 | 0.77 |
| 1:K:65:VAL:HA | 1:K:69:GLN:HE22 | 1.49 | 0.77 |
| 1:K:375:ILE:CG1 | 1:K:464:LEU:HD22 | 2.15 | 0.77 |
| 1:M:262:ASN:HD22 | 1:M:263:ARG:N | 1.82 | 0.77 |
| 1:H:30:ARG:NH1 | 1:H:377:GLN:NE2 | 2.32 | 0.77 |
| 1:H:49:TYR:HA | 1:H:223:ASP:HB3 | 1.65 | 0.77 |
| 1:N:162:LYS:HB3 | 1:N:163:PRO:HD2 | 1.64 | 0.77 |
| 1:B:28:VAL:HG22 | 1:B:381:ILE:CD1 | 2.14 | 0.77 |
| 1:B:51:PRO:C | 1:B:52:ILE:HD12 | 2.04 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:158:LEU:HD22 | 1:C:249:TYR:HB2 | 1.67 | 0.77 |
| 1:F:365:ARG:CD | 1:F:365:ARG:HA | 2.13 | 0.77 |
| 1:I:78:PRO:HD3 | 1:I:452:LYS:HA | 1.64 | 0.77 |
| 1:K:54:LYS:HG3 | 1:K:55:PRO:HD2 | 1.67 | 0.77 |
| 1:K:122:LEU:HD21 | 1:L:286:LEU:HD12 | 1.67 | 0.77 |
| 1:B:210:PHE:O | 1:B:214:GLN:HB2 | 1.84 | 0.77 |
| 1:E:246:LEU:HD23 | 1:E:246:LEU:H | 1.48 | 0.77 |
| 1:F:24:THR:HG23 | 1:F:320:ASN:HA | 1.66 | 0.77 |
| 1:K:68:LEU:HD23 | 1:K:201:VAL:HG21 | 1.64 | 0.77 |
| 1:K:363:TYR:CG | 1:L:185:CYS:HB2 | 2.20 | 0.77 |
| 1:N:34:TYR:HE2 | 1:N:377:GLN:HB2 | 1.49 | 0.77 |
| 1:N:451:LEU:HD23 | 1:N:454:LYS:HG3 | 1.66 | 0.77 |
| 1:B:374:PHE:O | 1:B:375:ILE:HD13 | 1.83 | 0.77 |
| 1:F:139:ALA:O | 1:F:140:GLY:O | 2.03 | 0.77 |
| 1:G:105:VAL:CG2 | 1:G:105:VAL:HB | 2.11 | 0.77 |
| 1:H:380:LYS:CD | 1:H:380:LYS:NZ | 2.47 | 0.77 |
| 1:N:101:ALA:HA | 1:N:322:GLY:O | 1.84 | 0.77 |
| 1:J:156:LEU:C | 1:J:156:LEU:HD12 | 2.04 | 0.77 |
| 1:M:74:ARG:CZ | 1:M:441:LEU:HD12 | 2.15 | 0.77 |
| 1:N:344:LEU:H | 1:N:344:LEU:CD2 | 1.97 | 0.77 |
| 1:E:382:THR:O | 1:E:387:VAL:HG11 | 1.85 | 0.77 |
| 1:G:98:LEU:CD1 | 1:G:98:LEU:HG | 2.10 | 0.77 |
| 1:L:471:GLN:O | 1:L:472:LEU:OXT | 2.03 | 0.77 |
| 1:N:98:LEU:HD13 | 1:N:378:LEU:CD1 | 2.11 | 0.77 |
| 1:O:459:LEU:HD23 | 1:O:459:LEU:N | 1.99 | 0.77 |
| 1:A:66:SER:N | 1:A:69:GLN:HE21 | 1.83 | 0.77 |
| 1:F:154:THR:H | 1:F:336:THR:CG2 | 1.97 | 0.77 |
| 1:M:98:LEU:HD13 | 1:M:378:LEU:HD11 | 1.67 | 0.77 |
| 1:M:180:VAL:HG12 | 1:M:181:GLN:O | 1.84 | 0.77 |
| 1:N:99:VAL:HG11 | 1:N:323:ILE:HG22 | 1.67 | 0.77 |
| 1:N:395:ASN:HB3 | 1:N:398:ILE:HG12 | 1.65 | 0.77 |
| 1:A:139:ALA:HA | 1:A:143:ASN:ND2 | 1.97 | 0.77 |
| 1:B:180:VAL:HG13 | 1:B:184:ASP:HB2 | 1.66 | 0.77 |
| 1:C:170:GLY:HA2 | 1:C:213:LEU:HD21 | 1.67 | 0.77 |
| 1:F:78:PRO:HD3 | 1:F:452:LYS:CA | 2.14 | 0.77 |
| 1:H:219:GLU:O | 1:H:220:VAL:HG13 | 1.84 | 0.77 |
| 1:I:358:THR:CG2 | 1:I:358:THR:CA | 2.62 | 0.77 |
| 1:J:391:ILE:HG21 | 1:J:402:TRP:CZ3 | 2.20 | 0.77 |
| 1:O:69:GLN:HA | 1:O:199:ASP:O | 1.85 | 0.77 |
| 1:C:35:TYR:CZ | 1:C:457:ALA:HB2 | 2.19 | 0.76 |
| 1:D:154:THR:H | 1:D:336:THR:HG21 | 1.49 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:23:SER:HG | 1:E:25:ASP:HB2 | 1.48 | 0.76 |
| 1:G:451:LEU:HD23 | 1:G:454:LYS:HG3 | 1.67 | 0.76 |
| 1:H:361:LYS:HA | 1:I:266:THR:OG1 | 1.84 | 0.76 |
| 1:J:246:LEU:H | 1:J:246:LEU:CD2 | 1.96 | 0.76 |
| 1:L:260:LEU:HD12 | 1:L:260:LEU:N | 2.00 | 0.76 |
| 1:C:54:LYS:HZ3 | 1:C:54:LYS:HA | 1.51 | 0.76 |
| 1:F:185:CYS:SG | 1:F:186:PRO:HD2 | 2.25 | 0.76 |
| 1:I:166:GLY:N | 1:I:195:ILE:HD11 | 1.98 | 0.76 |
| 1:M:302:SER:O | 1:M:304:ALA:N | 2.18 | 0.76 |
| 1:B:122:LEU:HD11 | 1:C:286:LEU:HD11 | 1.67 | 0.76 |
| 1:B:395:ASN:O | 1:B:398:ILE:HG12 | 1.85 | 0.76 |
| 1:F:344:LEU:HD11 | 1:G:185:CYS:SG | 2.26 | 0.76 |
| 1:J:144:ARG:C | 1:J:145:GLU:HG2 | 2.05 | 0.76 |
| 1:K:71:ARG:HH11 | 1:K:71:ARG:HA | 1.50 | 0.76 |
| 1:M:123:LEU:HD23 | 1:M:147:ILE:HB | 1.66 | 0.76 |
| 1:N:151:TYR:CG | 1:N:203:THR:HB | 2.19 | 0.76 |
| 1:A:266:THR:HG1 | 1:E:361:LYS:HA | 1.47 | 0.76 |
| 1:F:79:ASP:OD2 | 1:F:81:ASN:HB2 | 1.85 | 0.76 |
| 1:G:375:ILE:HG12 | 1:G:464:LEU:HD13 | 1.67 | 0.76 |
| 1:J:242:TYR:CE2 | 1:J:394:MET:HB2 | 2.21 | 0.76 |
| 1:N:338:ARG:CG | 1:N:338:ARG:NE | 2.48 | 0.76 |
| 1:O:54:LYS:HG2 | 1:O:56:ASN:OD1 | 1.86 | 0.76 |
| 1:E:237:MET:O | 1:E:240:GLU:HB3 | 1.86 | 0.76 |
| 1:H:117:ILE:HD12 | 1:I:293:PRO:HB3 | 1.66 | 0.76 |
| 1:K:105:VAL:CG1 | 1:K:106:GLU:N | 2.47 | 0.76 |
| 1:L:385:ALA:O | 1:L:389:THR:HG23 | 1.85 | 0.76 |
| 1:M:142:ASP:OD2 | 1:M:144:ARG:HG3 | 1.86 | 0.76 |
| 1:F:126:LEU:CB | 1:F:262:ASN:HB3 | 2.15 | 0.76 |
| 1:I:305:GLN:C | 1:I:306:ILE:HD13 | 2.06 | 0.76 |
| 1:K:378:LEU:HD12 | 1:K:379:CYS:N | 2.00 | 0.76 |
| 1:N:200:MET:O | 1:N:229:CYS:HA | 1.86 | 0.76 |
| 1:O:300:VAL:HG11 | 1:O:337:THR:HA | 1.68 | 0.76 |
| 1:A:344:LEU:HD13 | 1:B:213:LEU:HD12 | 1.65 | 0.76 |
| 1:D:348:ILE:HG22 | 1:D:359:ASN:OD1 | 1.86 | 0.76 |
| 1:F:107:VAL:HG23 | 1:F:311:TYR:HE1 | 1.50 | 0.76 |
| 1:G:166:GLY:CA | 1:G:195:ILE:HD11 | 2.16 | 0.76 |
| 1:K:65:VAL:HA | 1:K:69:GLN:NE2 | 2.01 | 0.76 |
| 1:N:54:LYS:HB3 | 1:N:57:ASN:HD22 | 1.51 | 0.76 |
| 1:B:97:ARG:HG3 | 1:B:383:LEU:HD13 | 1.66 | 0.76 |
| 1:D:120:HIS:NE2 | 1:D:218:SER:HB3 | 2.00 | 0.76 |
| 1:E:75:ILE:HD13 | 1:E:331:VAL:HG23 | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:323:ILE:HD13 | 1:A:323:ILE:N | 2.01 | 0.76 |
| 1:E:367:GLY:O | 1:E:368:GLU:HG2 | 1.85 | 0.76 |
| 1:F:231:TYR:CD2 | 1:J:112:PRO:HD3 | 2.21 | 0.76 |
| 1:I:255:MET:HG2 | 1:I:256:PHE:H | 1.51 | 0.76 |
| 1:J:180:VAL:CG2 | 1:J:180:VAL:HB | 2.13 | 0.76 |
| 1:K:153:GLN:NE2 | 1:K:300:VAL:HG12 | 2.00 | 0.76 |
| 1:L:228:ILE:N | 1:L:228:ILE:HD12 | 2.01 | 0.76 |
| 1:C:60:ILE:HG21 | 1:C:60:ILE:HD13 | 1.67 | 0.76 |
| 1:H:209:ASP:O | 1:H:213:LEU:HD23 | 1.86 | 0.76 |
| 1:H:220:VAL:O | 1:H:221:PRO:O | 2.04 | 0.76 |
| 1:A:66:SER:N | 1:A:69:GLN:NE2 | 2.33 | 0.75 |
| 1:A:162:LYS:C | 1:A:330:PHE:HD1 | 1.89 | 0.75 |
| 1:C:71:ARG:HH12 | 1:C:198:GLY:H | 1.32 | 0.75 |
| 1:C:78:PRO:HD2 | 1:C:455:PHE:CE1 | 2.21 | 0.75 |
| 1:F:457:ALA:O | 1:F:459:LEU:HD23 | 1.86 | 0.75 |
| 1:G:188:LEU:HD11 | 1:G:213:LEU:HD11 | 1.67 | 0.75 |
| 1:G:391:ILE:CG2 | 1:G:398:ILE:HG21 | 2.16 | 0.75 |
| 1:J:399:LEU:HD23 | 1:J:402:TRP:HE3 | 1.50 | 0.75 |
| 1:C:142:ASP:O | 1:D:283:THR:HG21 | 1.86 | 0.75 |
| 1:E:65:VAL:HA | 1:E:69:GLN:HE22 | 1.50 | 0.75 |
| 1:G:171:LYS:HA | 1:G:187:PRO:O | 1.84 | 0.75 |
| 1:H:154:THR:O | 1:H:336:THR:HG23 | 1.86 | 0.75 |
| 1:I:74:ARG:HG3 | 1:I:330:PHE:HE2 | 1.50 | 0.75 |
| 1:I:174:PRO:CG | 1:I:187:PRO:HG2 | 2.16 | 0.75 |
| 1:I:472:LEU:HD23 | 1:M:138:ASN:ND2 | 2.02 | 0.75 |
| 1:J:52:ILE:HB | 1:J:62:VAL:HB | 1.69 | 0.75 |
| 1:K:141:VAL:HG13 | 1:O:357:ASN:H | 1.49 | 0.75 |
| 1:N:115:VAL:H | 1:O:255:MET:HE1 | 1.51 | 0.75 |
| 1:F:255:MET:CE | 1:J:115:VAL:H | 2.00 | 0.75 |
| 1:G:246:LEU:HD12 | 1:G:249:TYR:HB3 | 1.68 | 0.75 |
| 1:I:160:GLY:HA3 | 1:I:245:SER:O | 1.87 | 0.75 |
| 1:L:395:ASN:O | 1:L:398:ILE:HG12 | 1.86 | 0.75 |
| 1:M:471:GLN:OE1 | 1:M:472:LEU:N | 2.18 | 0.75 |
| 1:B:165:ILE:CD1 | 1:B:165:ILE:CB | 2.63 | 0.75 |
| 1:C:60:ILE:HG13 | 1:C:60:ILE:O | 1.84 | 0.75 |
| 1:C:395:ASN:O | 1:C:398:ILE:HG12 | 1.85 | 0.75 |
| 1:F:113:LEU:HD22 | 1:G:253:GLU:HG3 | 1.67 | 0.75 |
| 1:H:28:VAL:HG12 | 1:H:29:ALA:N | 2.00 | 0.75 |
| 1:K:21:VAL:HG13 | 1:K:390:TYR:OH | 1.87 | 0.75 |
| 1:O:250:LEU:HD12 | 1:O:250:LEU:N | 1.99 | 0.75 |
| 1:D:115:VAL:CG1 | 1:D:115:VAL:CA | 2.62 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:363:TYR:CD2 | 1:I:185:CYS:HB2 | 2.21 | 0.75 |
| 1:J:171:LYS:HA | 1:J:187:PRO:O | 1.86 | 0.75 |
| 1:J:262:ASN:C | 1:J:262:ASN:HD22 | 1.90 | 0.75 |
| 1:K:213:LEU:CD1 | 1:O:344:LEU:HD13 | 2.17 | 0.75 |
| 1:M:112:PRO:HB2 | 1:N:202:ASP:OD2 | 1.86 | 0.75 |
| 1:B:142:ASP:O | 1:C:283:THR:HG21 | 1.87 | 0.75 |
| 1:B:214:GLN:OE1 | 1:B:219:GLU:HB2 | 1.87 | 0.75 |
| 1:E:341:ASN:HB3 | 1:E:366:HIS:HB2 | 1.67 | 0.75 |
| 1:F:237:MET:O | 1:F:240:GLU:HB3 | 1.86 | 0.75 |
| 1:G:463:PRO:CB | 1:G:466:ARG:HH21 | 1.99 | 0.75 |
| 1:H:300:VAL:HG23 | 1:H:300:VAL:O | 1.85 | 0.75 |
| 1:J:375:ILE:CG1 | 1:J:464:LEU:HD13 | 2.16 | 0.75 |
| 1:N:61:LEU:HD12 | 1:N:61:LEU:O | 1.86 | 0.75 |
| 1:A:363:TYR:CD2 | 1:B:185:CYS:HB2 | 2.22 | 0.75 |
| 1:C:152:LYS:HB2 | 1:C:255:MET:HB2 | 1.69 | 0.75 |
| 1:D:122:LEU:HD11 | 1:E:286:LEU:HD11 | 1.68 | 0.75 |
| 1:D:345:CYS:SG | 1:E:216:ASN:HB2 | 2.27 | 0.75 |
| 1:H:49:TYR:CE2 | 1:H:118:SER:HA | 2.19 | 0.75 |
| 1:J:237:MET:O | 1:J:240:GLU:HB3 | 1.87 | 0.75 |
| 1:K:156:LEU:C | 1:K:156:LEU:HD12 | 2.07 | 0.75 |
| 1:B:78:PRO:CD | 1:B:452:LYS:HA | 2.17 | 0.75 |
| 1:F:117:ILE:CB | 1:F:117:ILE:CD1 | 2.64 | 0.75 |
| 1:H:363:TYR:CG | 1:I:185:CYS:HB2 | 2.21 | 0.75 |
| 1:L:172:GLY:O | 1:L:173:SER:C | 2.24 | 0.75 |
| 1:A:242:TYR:CE2 | 1:A:394:MET:HG3 | 2.21 | 0.75 |
| 1:D:34:TYR:HE2 | 1:D:377:GLN:HG3 | 1.52 | 0.75 |
| 1:D:250:LEU:HD12 | 1:D:250:LEU:H | 1.49 | 0.75 |
| 1:E:246:LEU:HD23 | 1:E:246:LEU:N | 1.99 | 0.75 |
| 1:K:112:PRO:HD3 | 1:L:231:TYR:CD2 | 2.22 | 0.75 |
| 1:L:70:TYR:HE1 | 1:L:201:VAL:HA | 1.51 | 0.75 |
| 1:N:164:PRO:HG3 | 1:N:332:THR:HG21 | 1.69 | 0.75 |
| 1:O:104:GLY:O | 1:O:374:PHE:HA | 1.87 | 0.75 |
| 1:O:343:SER:HB3 | 1:O:364:LEU:HD23 | 1.69 | 0.75 |
| 1:B:66:SER:H | 1:B:69:GLN:NE2 | 1.85 | 0.74 |
| 1:C:77:LEU:HD22 | 1:C:455:PHE:CZ | 2.22 | 0.74 |
| 1:D:246:LEU:H | 1:D:246:LEU:CD2 | 2.00 | 0.74 |
| 1:H:125:LYS:NZ | 1:I:132:ALA:O | 2.19 | 0.74 |
| 1:I:472:LEU:CD2 | 1:M:138:ASN:ND2 | 2.45 | 0.74 |
| 1:K:383:LEU:HD23 | 1:K:388:MET:HE2 | 1.69 | 0.74 |
| 1:M:344:LEU:N | 1:M:344:LEU:CD2 | 2.49 | 0.74 |
| 1:N:78:PRO:HD3 | 1:N:452:LYS:CA | 2.17 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:112:PRO:HD3 | 1:B:231:TYR:CD2 | 2.22 | 0.74 |
| 1:D:71:ARG:HA | 1:D:71:ARG:NH1 | 2.01 | 0.74 |
| 1:I:169:TRP:HB3 | 1:I:188:LEU:HD12 | 1.68 | 0.74 |
| 1:J:156:LEU:HG | 1:J:334:VAL:HB | 1.67 | 0.74 |
| 1:N:385:ALA:O | 1:N:389:THR:HG23 | 1.86 | 0.74 |
| 1:J:180:VAL:HG13 | 1:J:184:ASP:HB3 | 1.69 | 0.74 |
| 1:K:344:LEU:HB3 | 1:L:213:LEU:HD12 | 1.67 | 0.74 |
| 1:O:223:ASP:OD1 | 1:O:224:ILE:HG12 | 1.88 | 0.74 |
| 1:B:98:LEU:HD13 | 1:B:378:LEU:HD11 | 1.68 | 0.74 |
| 1:B:262:ASN:ND2 | 1:B:288:SER:HB3 | 2.02 | 0.74 |
| 1:C:33:ILE:HB | 1:C:378:LEU:HB3 | 1.68 | 0.74 |
| 1:F:209:ASP:O | 1:F:213:LEU:HD23 | 1.86 | 0.74 |
| 1:F:348:ILE:HG22 | 1:F:359:ASN:OD1 | 1.86 | 0.74 |
| 1:I:217:LYS:NZ | 1:I:217:LYS:CD | 2.49 | 0.74 |
| 1:J:463:PRO:HA | 1:J:466:ARG:HE | 1.52 | 0.74 |
| 1:N:390:TYR:C | 1:N:392:HIS:H | 1.91 | 0.74 |
| 1:O:385:ALA:O | 1:O:389:THR:HG23 | 1.88 | 0.74 |
| 1:B:463:PRO:HG2 | 1:B:464:LEU:N | 2.02 | 0.74 |
| 1:C:172:GLY:O | 1:C:173:SER:C | 2.26 | 0.74 |
| 1:F:168:HIS:HB2 | 1:F:208:MET:HA | 1.68 | 0.74 |
| 1:I:21:VAL:HG12 | 1:I:390:TYR:OH | 1.88 | 0.74 |
| 1:J:170:GLY:HA2 | 1:J:213:LEU:HD21 | 1.68 | 0.74 |
| 1:K:66:SER:H | 1:K:69:GLN:NE2 | 1.86 | 0.74 |
| 1:M:75:ILE:CG2 | 1:M:451:LEU:HD12 | 2.17 | 0.74 |
| 1:B:361:LYS:HA | 1:C:266:THR:HG1 | 1.52 | 0.74 |
| 1:E:50:PHE:HB2 | 1:E:51:PRO:CD | 2.18 | 0.74 |
| 1:E:71:ARG:HH11 | 1:E:71:ARG:CA | 2.00 | 0.74 |
| 1:F:110:GLY:O | 1:F:111:GLN:NE2 | 2.20 | 0.74 |
| 1:H:166:GLY:HA3 | 1:H:195:ILE:HD11 | 1.68 | 0.74 |
| 1:I:305:GLN:O | 1:I:306:ILE:HD13 | 1.88 | 0.74 |
| 1:J:71:ARG:HH11 | 1:J:71:ARG:HA | 1.51 | 0.74 |
| 1:J:74:ARG:HD2 | 1:J:330:PHE:CE2 | 2.23 | 0.74 |
| 1:K:348:ILE:HG22 | 1:K:359:ASN:OD1 | 1.87 | 0.74 |
| 1:K:367:GLY:O | 1:K:368:GLU:HG2 | 1.88 | 0.74 |
| 1:M:151:TYR:CD2 | 1:M:203:THR:HB | 2.23 | 0.74 |
| 1:M:395:ASN:HB3 | 1:M:398:ILE:HG12 | 1.69 | 0.74 |
| 1:C:464:LEU:CD1 | 1:C:464:LEU:HG | 2.09 | 0.74 |
| 1:F:372:LEU:HB3 | 1:F:374:PHE:HE1 | 1.52 | 0.74 |
| 1:L:24:THR:HG21 | 1:L:323:ILE:HG13 | 1.70 | 0.74 |
| 1:M:144:ARG:CB | 1:M:144:ARG:CD | 2.66 | 0.74 |
| 1:N:358:THR:HA | 1:O:266:THR:HG22 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:302:SER:O | 1:O:304:ALA:N | 2.20 | 0.74 |
| 1:D:112:PRO:HD3 | 1:E:231:TYR:CG | 2.22 | 0.74 |
| 1:E:49:TYR:O | 1:E:64:LYS:HE2 | 1.87 | 0.74 |
| 1:J:75:ILE:HB | 1:J:329:LEU:CB | 2.17 | 0.74 |
| 1:J:107:VAL:HG23 | 1:J:311:TYR:HE1 | 1.52 | 0.74 |
| 1:K:31:THR:HG23 | 1:K:378:LEU:O | 1.86 | 0.74 |
| 1:L:66:SER:O | 1:L:69:GLN:HG3 | 1.88 | 0.74 |
| 1:A:246:LEU:HD23 | 1:A:246:LEU:H | 1.53 | 0.74 |
| 1:B:183:GLY:O | 1:B:185:CYS:N | 2.21 | 0.74 |
| 1:F:68:LEU:O | 1:F:201:VAL:HG13 | 1.87 | 0.74 |
| 1:G:92:ASN:HD21 | 1:G:94:ASP:HB2 | 1.52 | 0.74 |
| 1:H:117:ILE:HD11 | 1:I:260:LEU:HB3 | 1.70 | 0.74 |
| 1:H:126:LEU:HB3 | 1:H:262:ASN:HB3 | 1.70 | 0.74 |
| 1:I:344:LEU:HD12 | 1:J:186:PRO:HD2 | 1.68 | 0.74 |
| 1:K:213:LEU:HD12 | 1:O:344:LEU:HD13 | 1.68 | 0.74 |
| 1:K:248:PHE:CZ | 1:K:311:TYR:HB3 | 2.22 | 0.74 |
| 1:K:286:LEU:HD11 | 1:O:122:LEU:HD11 | 1.68 | 0.74 |
| 1:O:81:ASN:O | 1:O:82:LYS:HG3 | 1.88 | 0.74 |
| 1:A:23:SER:OG | 1:A:25:ASP:HB2 | 1.87 | 0.73 |
| 1:B:78:PRO:HD3 | 1:B:452:LYS:CA | 2.16 | 0.73 |
| 1:B:142:ASP:OD2 | 1:B:144:ARG:HG3 | 1.88 | 0.73 |
| 1:B:472:LEU:HD23 | 1:G:138:ASN:HD22 | 1.53 | 0.73 |
| 1:C:214:GLN:OE1 | 1:C:219:GLU:HB2 | 1.87 | 0.73 |
| 1:D:154:THR:O | 1:D:336:THR:HG23 | 1.86 | 0.73 |
| 1:F:21:VAL:HB | 1:J:461:GLN:NE2 | 2.01 | 0.73 |
| 1:F:49:TYR:CE2 | 1:F:118:SER:HA | 2.23 | 0.73 |
| 1:F:75:ILE:HB | 1:F:329:LEU:HB3 | 1.69 | 0.73 |
| 1:G:159:ILE:HD12 | 1:G:248:PHE:CD2 | 2.22 | 0.73 |
| 1:I:150:ASP:OD1 | 1:I:296:SER:HA | 1.88 | 0.73 |
| 1:L:189:GLU:O | 1:L:191:ILE:HG13 | 1.88 | 0.73 |
| 1:F:250:LEU:HD12 | 1:F:250:LEU:N | 2.03 | 0.73 |
| 1:G:71:ARG:HB3 | 1:G:73:PHE:CE1 | 2.23 | 0.73 |
| 1:H:149:MET:HE3 | 1:H:294:THR:HG22 | 1.68 | 0.73 |
| 1:I:461:GLN:HE22 | 1:J:21:VAL:HB | 1.51 | 0.73 |
| 1:N:345:CYS:SG | 1:O:216:ASN:CB | 2.76 | 0.73 |
| 1:B:220:VAL:O | 1:B:221:PRO:C | 2.22 | 0.73 |
| 1:C:242:TYR:CE2 | 1:C:394:MET:HB2 | 2.23 | 0.73 |
| 1:C:353:THR:CG2 | 1:C:353:THR:HB | 2.14 | 0.73 |
| 1:H:130:GLU:HB2 | 1:H:260:LEU:HD13 | 1.70 | 0.73 |
| 1:I:23:SER:OG | 1:I:25:ASP:HB2 | 1.88 | 0.73 |
| 1:O:171:LYS:HA | 1:O:187:PRO:O | 1.89 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:30:ARG:HH11 | 1:C:377:GLN:NE2 | 1.85 | 0.73 |
| 1:D:99:VAL:HG11 | 1:D:323:ILE:HG22 | 1.69 | 0.73 |
| 1:E:213:LEU:CD1 | 1:E:213:LEU:CB | 2.66 | 0.73 |
| 1:F:92:ASN:ND2 | 1:F:95:THR:OG1 | 2.18 | 0.73 |
| 1:F:271:VAL:HG12 | 1:F:276:TYR:HE2 | 1.52 | 0.73 |
| 1:G:170:GLY:HA2 | 1:G:213:LEU:HD21 | 1.69 | 0.73 |
| 1:C:166:GLY:HA3 | 1:C:195:ILE:HD11 | 1.68 | 0.73 |
| 1:C:262:ASN:HD22 | 1:C:263:ARG:N | 1.86 | 0.73 |
| 1:D:65:VAL:HA | 1:D:69:GLN:NE2 | 2.03 | 0.73 |
| 1:E:200:MET:O | 1:E:229:CYS:HA | 1.88 | 0.73 |
| 1:G:316:ALA:HB3 | 1:G:321:ASN:OD1 | 1.87 | 0.73 |
| 1:J:122:LEU:HD13 | 1:J:144:ARG:NH2 | 2.04 | 0.73 |
| 1:K:74:ARG:HG3 | 1:K:330:PHE:HE2 | 1.54 | 0.73 |
| 1:M:34:TYR:CD2 | 1:M:377:GLN:HB2 | 2.21 | 0.73 |
| 1:N:153:GLN:NE2 | 1:N:300:VAL:HA | 2.04 | 0.73 |
| 1:N:223:ASP:OD1 | 1:N:224:ILE:HG23 | 1.87 | 0.73 |
| 1:O:272:PRO:HD2 | 1:O:275:LEU:CD1 | 2.18 | 0.73 |
| 1:O:443:LYS:HD3 | 1:O:443:LYS:N | 2.02 | 0.73 |
| 1:B:344:LEU:N | 1:B:344:LEU:HD23 | 2.04 | 0.73 |
| 1:G:34:TYR:CE2 | 1:G:377:GLN:HB2 | 2.23 | 0.73 |
| 1:H:96:GLN:HB3 | 1:H:382:THR:HG22 | 1.70 | 0.73 |
| 1:H:247:PHE:HD1 | 1:H:248:PHE:H | 1.35 | 0.73 |
| 1:I:49:TYR:HE2 | 1:I:118:SER:HA | 1.53 | 0.73 |
| 1:K:147:ILE:HA | 1:L:129:THR:O | 1.88 | 0.73 |
| 1:M:96:GLN:HB3 | 1:M:382:THR:HG22 | 1.70 | 0.73 |
| 1:M:463:PRO:HB3 | 1:M:466:ARG:HH21 | 1.54 | 0.73 |
| 1:N:96:GLN:NE2 | 1:N:382:THR:HG22 | 2.03 | 0.73 |
| 1:N:374:PHE:CB | 1:N:376:PHE:CE1 | 2.71 | 0.73 |
| 1:A:97:ARG:HA | 1:A:97:ARG:NH1 | 2.04 | 0.73 |
| 1:C:34:TYR:HE2 | 1:C:377:GLN:HB2 | 1.52 | 0.73 |
| 1:C:79:ASP:OD2 | 1:C:81:ASN:HB2 | 1.88 | 0.73 |
| 1:D:248:PHE:CZ | 1:D:311:TYR:HB3 | 2.22 | 0.73 |
| 1:D:320:ASN:OD1 | 1:D:321:ASN:N | 2.22 | 0.73 |
| 1:E:272:PRO:HD2 | 1:E:275:LEU:CD1 | 2.18 | 0.73 |
| 1:J:151:TYR:CG | 1:J:203:THR:HB | 2.23 | 0.73 |
| 1:D:30:ARG:NH1 | 1:D:377:GLN:HE22 | 1.82 | 0.73 |
| 1:D:162:LYS:C | 1:D:330:PHE:HD1 | 1.91 | 0.73 |
| 1:E:57:ASN:HD21 | 1:E:59:LYS:H | 1.34 | 0.73 |
| 1:L:156:LEU:HG | 1:L:334:VAL:HB | 1.70 | 0.73 |
| 1:A:112:PRO:HB2 | 1:B:202:ASP:OD2 | 1.88 | 0.73 |
| 1:B:165:ILE:O | 1:B:165:ILE:HG22 | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:71:ARG:HH11 | 1:F:71:ARG:CA | 2.01 | 0.73 |
| 1:I:159:ILE:HD12 | 1:I:248:PHE:HD2 | 1.53 | 0.73 |
| 1:I:463:PRO:CA | 1:I:466:ARG:HH21 | 2.01 | 0.73 |
| 1:M:257:VAL:HG12 | 1:M:293:PRO:HB2 | 1.71 | 0.73 |
| 1:A:156:LEU:HG | 1:A:334:VAL:HB | 1.71 | 0.73 |
| 1:B:52:ILE:N | 1:B:52:ILE:CD1 | 2.51 | 0.73 |
| 1:C:188:LEU:HD13 | 1:C:213:LEU:HD11 | 1.70 | 0.73 |
| 1:G:274:ASP:OD1 | 1:G:274:ASP:N | 2.22 | 0.73 |
| 1:K:395:ASN:O | 1:K:398:ILE:HG12 | 1.88 | 0.73 |
| 1:O:142:ASP:OD2 | 1:O:144:ARG:HG3 | 1.88 | 0.73 |
| 1:A:471:GLN:OE1 | 1:A:472:LEU:N | 2.22 | 0.72 |
| 1:E:180:VAL:CG1 | 1:E:184:ASP:HB2 | 2.19 | 0.72 |
| 1:F:202:ASP:OD2 | 1:J:112:PRO:HB2 | 1.89 | 0.72 |
| 1:G:69:GLN:HA | 1:G:199:ASP:O | 1.89 | 0.72 |
| 1:K:154:THR:O | 1:K:336:THR:HG23 | 1.89 | 0.72 |
| 1:K:459:LEU:HB3 | 1:K:465:GLY:HA3 | 1.71 | 0.72 |
| 1:M:200:MET:O | 1:M:229:CYS:HA | 1.88 | 0.72 |
| 1:N:75:ILE:HG23 | 1:N:451:LEU:HD12 | 1.71 | 0.72 |
| 1:B:121:PRO:HD3 | 1:B:222:LEU:HD22 | 1.71 | 0.72 |
| 1:B:237:MET:O | 1:B:240:GLU:HB3 | 1.89 | 0.72 |
| 1:C:60:ILE:CD1 | 1:C:60:ILE:CB | 2.67 | 0.72 |
| 1:F:115:VAL:HG21 | 1:G:257:VAL:HG13 | 1.70 | 0.72 |
| 1:I:151:TYR:CG | 1:I:203:THR:HB | 2.25 | 0.72 |
| 1:J:96:GLN:HA | 1:J:381:ILE:O | 1.88 | 0.72 |
| 1:M:462:PHE:O | 1:M:466:ARG:HG3 | 1.89 | 0.72 |
| 1:O:66:SER:N | 1:O:69:GLN:NE2 | 2.36 | 0.72 |
| 1:A:54:LYS:HG3 | 1:A:55:PRO:CD | 2.17 | 0.72 |
| 1:B:21:VAL:HG12 | 1:B:22:VAL:N | 2.04 | 0.72 |
| 1:G:151:TYR:CD2 | 1:G:203:THR:CB | 2.66 | 0.72 |
| 1:H:201:VAL:HG23 | 1:H:202:ASP:O | 1.89 | 0.72 |
| 1:H:372:LEU:HB3 | 1:H:374:PHE:CE1 | 2.24 | 0.72 |
| 1:J:101:ALA:O | 1:J:376:PHE:HA | 1.89 | 0.72 |
| 1:F:24:THR:HA | 1:F:27:TYR:CE2 | 2.24 | 0.72 |
| 1:G:54:LYS:HA | 1:G:54:LYS:HZ3 | 1.54 | 0.72 |
| 1:H:42:LEU:HD12 | 1:H:73:PHE:HE2 | 1.53 | 0.72 |
| 1:A:115:VAL:H | 1:B:255:MET:CE | 2.02 | 0.72 |
| 1:B:113:LEU:HD22 | 1:C:253:GLU:HG3 | 1.71 | 0.72 |
| 1:B:344:LEU:CD1 | 1:C:185:CYS:SG | 2.77 | 0.72 |
| 1:E:250:LEU:HD22 | 1:E:306:ILE:HG23 | 1.69 | 0.72 |
| 1:F:256:PHE:HB3 | 1:J:299:MET:HA | 1.71 | 0.72 |
| 1:H:23:SER:OG | 1:H:25:ASP:HB2 | 1.88 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:54:LYS:HZ3 | 1:H:54:LYS:HA | 1.54 | 0.72 |
| 1:H:152:LYS:CB | 1:H:255:MET:HB2 | 2.18 | 0.72 |
| 1:I:75:ILE:N | 1:I:75:ILE:HD12 | 2.03 | 0.72 |
| 1:B:208:MET:SD | 1:B:210:PHE:HE2 | 2.13 | 0.72 |
| 1:E:171:LYS:HA | 1:E:187:PRO:O | 1.88 | 0.72 |
| 1:I:61:LEU:CD1 | 1:I:61:LEU:HG | 2.11 | 0.72 |
| 1:I:369:GLU:CG | 1:I:369:GLU:CA | 2.66 | 0.72 |
| 1:N:78:PRO:CD | 1:N:452:LYS:HA | 2.16 | 0.72 |
| 1:O:71:ARG:HA | 1:O:71:ARG:HH11 | 1.53 | 0.72 |
| 1:C:72:VAL:HG23 | 1:C:197:ASP:HA | 1.69 | 0.72 |
| 1:C:167:GLU:HB2 | 1:C:190:LEU:HD11 | 1.70 | 0.72 |
| 1:F:152:LYS:HB2 | 1:F:255:MET:HB2 | 1.71 | 0.72 |
| 1:I:117:ILE:HG13 | 1:I:149:MET:O | 1.89 | 0.72 |
| 1:N:29:ALA:O | 1:N:379:CYS:HB3 | 1.89 | 0.72 |
| 1:A:67:GLY:O | 1:A:68:LEU:HG | 1.89 | 0.72 |
| 1:B:49:TYR:CE2 | 1:B:118:SER:HA | 2.21 | 0.72 |
| 1:E:157:CYS:HB2 | 1:E:307:PHE:HE2 | 1.55 | 0.72 |
| 1:H:274:ASP:OD1 | 1:H:274:ASP:N | 2.23 | 0.72 |
| 1:H:465:GLY:O | 1:H:467:LYS:N | 2.22 | 0.72 |
| 1:I:75:ILE:HD12 | 1:I:329:LEU:O | 1.89 | 0.72 |
| 1:A:152:LYS:HB2 | 1:A:255:MET:HB2 | 1.72 | 0.72 |
| 1:F:117:ILE:CG2 | 1:F:117:ILE:N | 2.52 | 0.72 |
| 1:G:248:PHE:HE2 | 1:G:311:TYR:CD1 | 2.07 | 0.72 |
| 1:H:220:VAL:O | 1:H:221:PRO:C | 2.25 | 0.72 |
| 1:H:372:LEU:HB3 | 1:H:374:PHE:HE1 | 1.55 | 0.72 |
| 1:I:200:MET:O | 1:I:229:CYS:HA | 1.90 | 0.72 |
| 1:L:57:ASN:ND2 | 1:L:59:LYS:H | 1.87 | 0.72 |
| 1:O:152:LYS:CB | 1:O:255:MET:HB2 | 2.15 | 0.72 |
| 1:D:151:TYR:CD2 | 1:D:203:THR:HB | 2.25 | 0.72 |
| 1:F:142:ASP:O | 1:G:283:THR:HG21 | 1.90 | 0.72 |
| 1:F:375:ILE:HG12 | 1:F:464:LEU:HD13 | 1.72 | 0.72 |
| 1:I:122:LEU:HD11 | 1:J:286:LEU:HD11 | 1.70 | 0.72 |
| 1:H:74:ARG:HG3 | 1:H:330:PHE:HE2 | 1.55 | 0.71 |
| 1:H:166:GLY:H | 1:H:195:ILE:HG13 | 1.54 | 0.71 |
| 1:J:54:LYS:HG3 | 1:J:55:PRO:CD | 2.20 | 0.71 |
| 1:L:344:LEU:CD1 | 1:M:185:CYS:SG | 2.76 | 0.71 |
| 1:M:98:LEU:CD1 | 1:M:378:LEU:HD21 | 2.20 | 0.71 |
| 1:N:142:ASP:OD2 | 1:N:144:ARG:HG3 | 1.90 | 0.71 |
| 1:G:49:TYR:HA | 1:G:223:ASP:HB3 | 1.71 | 0.71 |
| 1:J:472:LEU:CD2 | 1:N:138:ASN:HD22 | 2.02 | 0.71 |
| 1:K:230:LYS:CD | 1:K:230:LYS:CB | 2.67 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:464:LEU:O | 1:L:464:LEU:HD23 | 1.90 | 0.71 |
| 1:O:463:PRO:HB3 | 1:O:466:ARG:NH2 | 2.04 | 0.71 |
| 1:B:70:TYR:OH | 1:B:230:LYS:O | 2.06 | 0.71 |
| 1:B:121:PRO:HG3 | 1:C:289:SER:OG | 1.90 | 0.71 |
| 1:C:464:LEU:CD1 | 1:C:464:LEU:CD2 | 2.68 | 0.71 |
| 1:D:33:ILE:HB | 1:D:378:LEU:HB3 | 1.71 | 0.71 |
| 1:D:188:LEU:CD1 | 1:D:213:LEU:HD11 | 2.18 | 0.71 |
| 1:E:300:VAL:HG11 | 1:E:337:THR:HA | 1.70 | 0.71 |
| 1:F:440:PRO:HA | 1:F:443:LYS:HZ1 | 1.53 | 0.71 |
| 1:G:104:GLY:HA3 | 1:G:375:ILE:HB | 1.71 | 0.71 |
| 1:G:463:PRO:HB3 | 1:G:466:ARG:HH21 | 1.55 | 0.71 |
| 1:L:66:SER:H | 1:L:69:GLN:HE21 | 1.38 | 0.71 |
| 1:N:72:VAL:HG22 | 1:N:332:THR:HG23 | 1.71 | 0.71 |
| 1:N:92:ASN:HD21 | 1:N:95:THR:H | 1.36 | 0.71 |
| 1:N:109:ARG:NH1 | 1:N:370:TYR:CE1 | 2.58 | 0.71 |
| 1:D:281:GLY:O | 1:D:284:ALA:N | 2.20 | 0.71 |
| 1:G:80:PRO:HG2 | 1:G:98:LEU:O | 1.90 | 0.71 |
| 1:J:99:VAL:HG11 | 1:J:323:ILE:CG2 | 2.20 | 0.71 |
| 1:L:66:SER:N | 1:L:69:GLN:NE2 | 2.39 | 0.71 |
| 1:N:459:LEU:HB3 | 1:N:465:GLY:HA3 | 1.73 | 0.71 |
| 1:A:34:TYR:HE2 | 1:A:377:GLN:HG3 | 1.52 | 0.71 |
| 1:B:33:ILE:HG23 | 1:B:33:ILE:HD12 | 1.72 | 0.71 |
| 1:E:451:LEU:HD23 | 1:E:454:LYS:HG3 | 1.72 | 0.71 |
| 1:H:160:GLY:HA3 | 1:H:245:SER:O | 1.90 | 0.71 |
| 1:J:236:LYS:CG | 1:J:236:LYS:CE | 2.67 | 0.71 |
| 1:J:255:MET:HG2 | 1:J:256:PHE:H | 1.54 | 0.71 |
| 1:L:152:LYS:NZ | 1:L:253:GLU:OE1 | 2.24 | 0.71 |
| 1:M:166:GLY:CA | 1:M:195:ILE:HD11 | 2.20 | 0.71 |
| 1:N:57:ASN:ND2 | 1:N:59:LYS:H | 1.89 | 0.71 |
| 1:N:262:ASN:HD21 | 1:N:288:SER:CB | 2.01 | 0.71 |
| 1:C:281:GLY:O | 1:C:284:ALA:HB3 | 1.90 | 0.71 |
| 1:E:33:ILE:CD1 | 1:E:33:ILE:CB | 2.68 | 0.71 |
| 1:E:323:ILE:CG2 | 1:E:323:ILE:CA | 2.65 | 0.71 |
| 1:F:213:LEU:HD12 | 1:J:344:LEU:HD13 | 1.72 | 0.71 |
| 1:A:113:LEU:HB2 | 1:B:253:GLU:OE1 | 1.90 | 0.71 |
| 1:C:24:THR:CG2 | 1:C:320:ASN:HA | 2.20 | 0.71 |
| 1:C:471:GLN:O | 1:C:472:LEU:OXT | 2.09 | 0.71 |
| 1:D:160:GLY:HA3 | 1:D:245:SER:O | 1.89 | 0.71 |
| 1:E:220:VAL:O | 1:E:221:PRO:O | 2.08 | 0.71 |
| 1:E:348:ILE:HG22 | 1:E:359:ASN:OD1 | 1.89 | 0.71 |
| 1:F:280:SER:CA | 1:F:284:ALA:HB2 | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:75:ILE:HB | 1:H:329:LEU:HB3 | 1.73 | 0.71 |
| 1:K:42:LEU:HD12 | 1:K:73:PHE:HE2 | 1.54 | 0.71 |
| 1:K:126:LEU:HB3 | 1:K:262:ASN:HB3 | 1.72 | 0.71 |
| 1:L:30:ARG:HH11 | 1:L:377:GLN:NE2 | 1.88 | 0.71 |
| 1:D:272:PRO:HD2 | 1:D:275:LEU:CD1 | 2.21 | 0.71 |
| 1:D:457:ALA:O | 1:D:459:LEU:HD23 | 1.90 | 0.71 |
| 1:F:21:VAL:CG1 | 1:F:22:VAL:N | 2.53 | 0.71 |
| 1:G:348:ILE:HG22 | 1:G:359:ASN:OD1 | 1.90 | 0.71 |
| 1:I:101:ALA:HA | 1:I:322:GLY:O | 1.91 | 0.71 |
| 1:I:398:ILE:HG22 | 1:I:402:TRP:CZ3 | 2.25 | 0.71 |
| 1:K:190:LEU:HD12 | 1:K:191:ILE:H | 1.55 | 0.71 |
| 1:N:180:VAL:CG1 | 1:N:184:ASP:HB2 | 2.20 | 0.71 |
| 1:O:74:ARG:CG | 1:O:330:PHE:HE2 | 2.04 | 0.71 |
| 1:C:246:LEU:HD23 | 1:C:246:LEU:H | 1.56 | 0.71 |
| 1:H:465:GLY:O | 1:H:466:ARG:C | 2.29 | 0.71 |
| 1:J:78:PRO:HD2 | 1:J:455:PHE:CE1 | 2.25 | 0.71 |
| 1:K:167:GLU:HG2 | 1:K:231:TYR:O | 1.91 | 0.71 |
| 1:M:31:THR:HG23 | 1:M:379:CYS:HA | 1.72 | 0.71 |
| 1:C:163:PRO:HD3 | 1:C:330:PHE:HE1 | 1.55 | 0.71 |
| 1:D:99:VAL:HG11 | 1:D:323:ILE:CG2 | 2.20 | 0.71 |
| 1:E:75:ILE:HG23 | 1:E:451:LEU:HD12 | 1.71 | 0.71 |
| 1:F:188:LEU:HD11 | 1:F:213:LEU:HD11 | 1.73 | 0.71 |
| 1:G:391:ILE:HB | 1:G:399:LEU:HD21 | 1.72 | 0.71 |
| 1:J:345:CYS:HB2 | 1:J:362:GLU:OE2 | 1.91 | 0.71 |
| 1:K:365:ARG:NH2 | 1:L:269:GLU:OE1 | 2.24 | 0.71 |
| 1:L:27:TYR:HH | 1:L:390:TYR:HE2 | 1.39 | 0.71 |
| 1:L:92:ASN:O | 1:L:94:ASP:N | 2.23 | 0.71 |
| 1:N:242:TYR:CE2 | 1:N:394:MET:HB2 | 2.26 | 0.71 |
| 1:O:235:ILE:HG23 | 1:O:235:ILE:HD12 | 1.73 | 0.71 |
| 1:O:331:VAL:CG1 | 1:O:331:VAL:CG2 | 2.68 | 0.71 |
| 1:B:70:TYR:OH | 1:B:232:PRO:HD3 | 1.91 | 0.70 |
| 1:D:115:VAL:CG1 | 1:D:115:VAL:HB | 2.14 | 0.70 |
| 1:I:246:LEU:HD23 | 1:I:246:LEU:H | 1.54 | 0.70 |
| 1:N:92:ASN:ND2 | 1:N:95:THR:OG1 | 2.24 | 0.70 |
| 1:N:95:THR:CG2 | 1:N:95:THR:CA | 2.67 | 0.70 |
| 1:N:151:TYR:CD2 | 1:N:203:THR:CB | 2.67 | 0.70 |
| 1:A:178:VAL:CG2 | 1:A:178:VAL:HB | 2.14 | 0.70 |
| 1:B:33:ILE:CD1 | 1:B:33:ILE:CB | 2.68 | 0.70 |
| 1:B:262:ASN:HD21 | 1:B:288:SER:HB3 | 1.54 | 0.70 |
| 1:C:299:MET:HA | 1:D:256:PHE:HB3 | 1.73 | 0.70 |
| 1:F:74:ARG:NH2 | 1:F:441:LEU:HD12 | 2.06 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:372:LEU:HB3 | 1:G:374:PHE:CE1 | 2.25 | 0.70 |
| 1:K:266:THR:HG22 | 1:O:358:THR:HG22 | 1.72 | 0.70 |
| 1:M:156:LEU:HG | 1:M:334:VAL:HB | 1.74 | 0.70 |
| 1:N:149:MET:CE | 1:N:205:PHE:CE1 | 2.74 | 0.70 |
| 1:C:60:ILE:CG1 | 1:C:60:ILE:O | 2.38 | 0.70 |
| 1:D:325:TRP:HB3 | 1:D:398:ILE:HD11 | 1.72 | 0.70 |
| 1:E:75:ILE:HB | 1:E:329:LEU:HB3 | 1.72 | 0.70 |
| 1:K:464:LEU:HD23 | 1:K:464:LEU:O | 1.91 | 0.70 |
| 1:M:147:ILE:HG22 | 1:M:148:SER:H | 1.55 | 0.70 |
| 1:M:307:PHE:O | 1:M:308:ASN:HB2 | 1.89 | 0.70 |
| 1:A:149:MET:HA | 1:B:260:LEU:HD21 | 1.74 | 0.70 |
| 1:A:159:ILE:HD12 | 1:A:248:PHE:CD2 | 2.26 | 0.70 |
| 1:B:74:ARG:HG3 | 1:B:330:PHE:HE2 | 1.55 | 0.70 |
| 1:D:148:SER:OG | 1:E:129:THR:HB | 1.92 | 0.70 |
| 1:H:344:LEU:HD13 | 1:I:213:LEU:CD1 | 2.20 | 0.70 |
| 1:L:78:PRO:HD3 | 1:L:452:LYS:HA | 1.74 | 0.70 |
| 1:L:344:LEU:HD12 | 1:M:186:PRO:CG | 2.21 | 0.70 |
| 1:M:323:ILE:CD1 | 1:M:323:ILE:CB | 2.68 | 0.70 |
| 1:N:219:GLU:O | 1:N:263:ARG:NH2 | 2.18 | 0.70 |
| 1:O:46:GLY:CA | 1:O:65:VAL:CG2 | 2.66 | 0.70 |
| 1:O:235:ILE:CD1 | 1:O:235:ILE:CB | 2.68 | 0.70 |
| 1:A:325:TRP:HB3 | 1:A:398:ILE:HD12 | 1.71 | 0.70 |
| 1:E:272:PRO:HD2 | 1:E:275:LEU:HD11 | 1.71 | 0.70 |
| 1:F:117:ILE:HG22 | 1:F:117:ILE:H | 1.55 | 0.70 |
| 1:G:237:MET:O | 1:G:240:GLU:HB3 | 1.90 | 0.70 |
| 1:K:144:ARG:HD3 | 1:O:355:TYR:CD1 | 2.27 | 0.70 |
| 1:A:54:LYS:CG | 1:A:55:PRO:HD2 | 2.19 | 0.70 |
| 1:A:99:VAL:HG11 | 1:A:323:ILE:HG23 | 1.73 | 0.70 |
| 1:C:65:VAL:HA | 1:C:69:GLN:HE22 | 1.56 | 0.70 |
| 1:C:463:PRO:HB3 | 1:C:466:ARG:HH21 | 1.56 | 0.70 |
| 1:D:53:LYS:CB | 1:D:53:LYS:CD | 2.70 | 0.70 |
| 1:D:180:VAL:CG1 | 1:D:184:ASP:HB2 | 2.21 | 0.70 |
| 1:G:152:LYS:O | 1:G:152:LYS:HG3 | 1.91 | 0.70 |
| 1:H:260:LEU:N | 1:H:260:LEU:CD1 | 2.53 | 0.70 |
| 1:J:101:ALA:HA | 1:J:322:GLY:O | 1.90 | 0.70 |
| 1:N:348:ILE:HD12 | 1:O:182:PRO:O | 1.91 | 0.70 |
| 1:O:24:THR:CG2 | 1:O:320:ASN:HA | 2.20 | 0.70 |
| 1:O:246:LEU:H | 1:O:246:LEU:CD2 | 2.03 | 0.70 |
| 1:A:65:VAL:CA | 1:A:69:GLN:NE2 | 2.55 | 0.70 |
| 1:A:466:ARG:HD2 | 1:B:317:GLN:O | 1.92 | 0.70 |
| 1:C:343:SER:HB3 | 1:C:364:LEU:HD23 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:70:TYR:OH | 1:D:232:PRO:CD | 2.28 | 0.70 |
| 1:D:117:ILE:HG13 | 1:D:149:MET:O | 1.91 | 0.70 |
| 1:D:210:PHE:CE1 | 1:D:224:ILE:HB | 2.27 | 0.70 |
| 1:E:30:ARG:HH11 | 1:E:377:GLN:HE22 | 1.37 | 0.70 |
| 1:F:458:ASP:OD2 | 1:F:458:ASP:N | 2.25 | 0.70 |
| 1:J:71:ARG:HH11 | 1:J:71:ARG:CG | 2.03 | 0.70 |
| 1:M:74:ARG:HD3 | 1:M:448:GLU:OE1 | 1.92 | 0.70 |
| 1:D:74:ARG:HG3 | 1:D:330:PHE:CE2 | 2.27 | 0.70 |
| 1:D:443:LYS:HD3 | 1:D:443:LYS:N | 2.05 | 0.70 |
| 1:G:101:ALA:HA | 1:G:322:GLY:O | 1.92 | 0.70 |
| 1:G:463:PRO:HA | 1:G:466:ARG:HE | 1.56 | 0.70 |
| 1:H:112:PRO:HB3 | 1:I:231:TYR:CD1 | 2.27 | 0.70 |
| 1:J:105:VAL:CG2 | 1:J:105:VAL:HB | 2.13 | 0.70 |
| 1:J:178:VAL:CG1 | 1:J:178:VAL:CA | 2.70 | 0.70 |
| 1:K:162:LYS:CE | 1:K:162:LYS:HG2 | 2.21 | 0.70 |
| 1:N:74:ARG:NH2 | 1:N:441:LEU:HD12 | 2.07 | 0.70 |
| 1:N:121:PRO:HG3 | 1:O:289:SER:HB2 | 1.74 | 0.70 |
| 1:O:320:ASN:HD21 | 1:O:323:ILE:HB | 1.57 | 0.70 |
| 1:A:178:VAL:O | 1:A:180:VAL:N | 2.22 | 0.70 |
| 1:C:60:ILE:CD1 | 1:C:60:ILE:HG21 | 2.22 | 0.70 |
| 1:F:320:ASN:OD1 | 1:F:321:ASN:N | 2.24 | 0.70 |
| 1:F:443:LYS:N | 1:F:443:LYS:CD | 2.55 | 0.70 |
| 1:H:180:VAL:HG13 | 1:H:184:ASP:HB2 | 1.74 | 0.70 |
| 1:K:344:LEU:HD11 | 1:L:185:CYS:SG | 2.32 | 0.70 |
| 1:L:364:LEU:HD11 | 1:M:290:ASN:HA | 1.71 | 0.70 |
| 1:F:34:TYR:HE2 | 1:F:377:GLN:HB2 | 1.56 | 0.70 |
| 1:H:344:LEU:HB3 | 1:I:213:LEU:HD12 | 1.74 | 0.70 |
| 1:I:74:ARG:CG | 1:I:330:PHE:HE2 | 2.05 | 0.70 |
| 1:K:361:LYS:HA | 1:L:266:THR:HG1 | 1.54 | 0.70 |
| 1:L:66:SER:N | 1:L:69:GLN:HE21 | 1.90 | 0.70 |
| 1:N:149:MET:HE1 | 1:N:205:PHE:CE1 | 2.26 | 0.70 |
| 1:O:463:PRO:CB | 1:O:466:ARG:HH21 | 2.05 | 0.70 |
| 1:B:154:THR:O | 1:B:336:THR:HG23 | 1.92 | 0.69 |
| 1:E:188:LEU:HD11 | 1:E:213:LEU:HD11 | 1.73 | 0.69 |
| 1:E:470:LEU:HD23 | 1:E:470:LEU:O | 1.92 | 0.69 |
| 1:G:196:GLN:O | 1:G:199:ASP:OD2 | 2.09 | 0.69 |
| 1:H:176:THR:C | 1:H:177:GLN:CG | 2.61 | 0.69 |
| 1:M:77:LEU:HD22 | 1:M:455:PHE:HZ | 1.56 | 0.69 |
| 1:N:21:VAL:HG12 | 1:N:390:TYR:OH | 1.90 | 0.69 |
| 1:N:365:ARG:CG | 1:N:365:ARG:HH11 | 2.05 | 0.69 |
| 1:C:167:GLU:CG | 1:C:231:TYR:O | 2.39 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:154:THR:H | 1:D:336:THR:CG2 | 2.05 | 0.69 |
| 1:E:193:THR:CG2 | 1:E:230:LYS:HD2 | 2.20 | 0.69 |
| 1:F:443:LYS:H | 1:F:443:LYS:CD | 1.97 | 0.69 |
| 1:I:241:PRO:HG2 | 1:I:242:TYR:H | 1.58 | 0.69 |
| 1:I:361:LYS:NZ | 1:I:361:LYS:CD | 2.54 | 0.69 |
| 1:J:75:ILE:HB | 1:J:329:LEU:HB3 | 1.75 | 0.69 |
| 1:J:75:ILE:HG23 | 1:J:451:LEU:HD12 | 1.74 | 0.69 |
| 1:O:273:ASP:OD2 | 1:O:273:ASP:N | 2.24 | 0.69 |
| 1:C:307:PHE:O | 1:C:308:ASN:HB2 | 1.93 | 0.69 |
| 1:E:152:LYS:NZ | 1:E:253:GLU:OE1 | 2.25 | 0.69 |
| 1:H:188:LEU:CD1 | 1:H:213:LEU:HD11 | 2.22 | 0.69 |
| 1:K:190:LEU:HD12 | 1:K:191:ILE:N | 2.07 | 0.69 |
| 1:O:34:TYR:CE2 | 1:O:377:GLN:HB2 | 2.28 | 0.69 |
| 1:O:459:LEU:HB3 | 1:O:465:GLY:HA3 | 1.74 | 0.69 |
| 1:B:375:ILE:HG21 | 1:B:468:PHE:CD2 | 2.27 | 0.69 |
| 1:F:66:SER:O | 1:F:69:GLN:HG3 | 1.93 | 0.69 |
| 1:F:129:THR:O | 1:J:147:ILE:HA | 1.92 | 0.69 |
| 1:F:151:TYR:CG | 1:F:203:THR:HB | 2.26 | 0.69 |
| 1:G:320:ASN:HD21 | 1:G:323:ILE:CB | 1.98 | 0.69 |
| 1:G:457:ALA:O | 1:G:459:LEU:HD23 | 1.93 | 0.69 |
| 1:G:463:PRO:CG | 1:G:464:LEU:N | 2.55 | 0.69 |
| 1:J:81:ASN:CG | 1:J:97:ARG:NH1 | 2.45 | 0.69 |
| 1:A:178:VAL:CG1 | 1:A:178:VAL:CA | 2.69 | 0.69 |
| 1:A:286:LEU:HD12 | 1:E:122:LEU:CD2 | 2.18 | 0.69 |
| 1:F:34:TYR:CE2 | 1:F:377:GLN:HB2 | 2.27 | 0.69 |
| 1:F:95:THR:O | 1:F:383:LEU:HB2 | 1.92 | 0.69 |
| 1:G:49:TYR:O | 1:G:223:ASP:HA | 1.92 | 0.69 |
| 1:H:399:LEU:HA | 1:H:402:TRP:HE3 | 1.57 | 0.69 |
| 1:J:300:VAL:CG1 | 1:J:300:VAL:CG2 | 2.69 | 0.69 |
| 1:K:227:SER:C | 1:K:228:ILE:HD12 | 2.13 | 0.69 |
| 1:N:65:VAL:HA | 1:N:69:GLN:NE2 | 2.07 | 0.69 |
| 1:O:66:SER:N | 1:O:69:GLN:HE21 | 1.91 | 0.69 |
| 1:O:75:ILE:CG2 | 1:O:451:LEU:HD12 | 2.22 | 0.69 |
| 1:D:141:VAL:HG12 | 1:D:142:ASP:N | 1.96 | 0.69 |
| 1:H:21:VAL:HG13 | 1:H:390:TYR:OH | 1.93 | 0.69 |
| 1:I:152:LYS:HG3 | 1:I:152:LYS:O | 1.93 | 0.69 |
| 1:N:164:PRO:HG3 | 1:N:332:THR:CG2 | 2.23 | 0.69 |
| 1:N:344:LEU:CD1 | 1:O:185:CYS:SG | 2.80 | 0.69 |
| 1:C:363:TYR:CE2 | 1:D:269:GLU:HG3 | 2.28 | 0.69 |
| 1:G:66:SER:H | 1:G:69:GLN:NE2 | 1.90 | 0.69 |
| 1:H:451:LEU:HA | 1:H:454:LYS:HG3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:272:PRO:HD2 | 1:I:275:LEU:HD12 | 1.75 | 0.69 |
| 1:J:34:TYR:CE2 | 1:J:377:GLN:HB2 | 2.27 | 0.69 |
| 1:J:49:TYR:HE2 | 1:J:118:SER:HA | 1.58 | 0.69 |
| 1:K:79:ASP:OD2 | 1:K:81:ASN:HB2 | 1.93 | 0.69 |
| 1:N:345:CYS:HA | 1:N:361:LYS:O | 1.93 | 0.69 |
| 1:A:180:VAL:HG12 | 1:A:184:ASP:CB | 2.13 | 0.69 |
| 1:B:463:PRO:HG2 | 1:B:464:LEU:H | 1.56 | 0.69 |
| 1:C:69:GLN:HA | 1:C:199:ASP:O | 1.91 | 0.69 |
| 1:D:34:TYR:HE2 | 1:D:377:GLN:CG | 2.04 | 0.69 |
| 1:D:188:LEU:HD11 | 1:D:213:LEU:HD11 | 1.74 | 0.69 |
| 1:E:151:TYR:OH | 1:E:221:PRO:HB2 | 1.93 | 0.69 |
| 1:E:152:LYS:CE | 1:E:152:LYS:CG | 2.67 | 0.69 |
| 1:H:345:CYS:SG | 1:I:216:ASN:CB | 2.79 | 0.69 |
| 1:J:451:LEU:HD23 | 1:J:454:LYS:HG3 | 1.75 | 0.69 |
| 1:K:105:VAL:HG12 | 1:K:106:GLU:N | 2.01 | 0.69 |
| 1:K:344:LEU:CD1 | 1:L:186:PRO:HD2 | 2.23 | 0.69 |
| 1:L:242:TYR:CD2 | 1:L:394:MET:HG3 | 2.27 | 0.69 |
| 1:M:67:GLY:C | 1:M:68:LEU:HG | 2.07 | 0.69 |
| 1:M:80:PRO:HD3 | 1:M:100:TRP:CD1 | 2.27 | 0.69 |
| 1:O:166:GLY:HA3 | 1:O:195:ILE:HD11 | 1.74 | 0.69 |
| 1:A:52:ILE:HB | 1:A:62:VAL:HB | 1.75 | 0.69 |
| 1:A:440:PRO:O | 1:A:443:LYS:NZ | 2.26 | 0.69 |
| 1:B:65:VAL:HA | 1:B:69:GLN:HE22 | 1.57 | 0.69 |
| 1:B:139:ALA:O | 1:B:140:GLY:O | 2.11 | 0.69 |
| 1:C:237:MET:O | 1:C:240:GLU:HB3 | 1.93 | 0.69 |
| 1:E:116:GLY:N | 1:E:339:SER:OG | 2.26 | 0.69 |
| 1:F:181:GLN:HE22 | 1:J:348:ILE:HD11 | 1.58 | 0.69 |
| 1:F:395:ASN:O | 1:F:398:ILE:HG12 | 1.93 | 0.69 |
| 1:J:78:PRO:HD3 | 1:J:452:LYS:HA | 1.74 | 0.69 |
| 1:J:81:ASN:CG | 1:J:97:ARG:HH11 | 1.92 | 0.69 |
| 1:K:81:ASN:ND2 | 1:K:402:TRP:CD1 | 2.61 | 0.69 |
| 1:K:182:PRO:O | 1:O:348:ILE:HD12 | 1.92 | 0.69 |
| 1:M:357:ASN:H | 1:N:141:VAL:HG13 | 1.56 | 0.69 |
| 1:O:205:PHE:CD1 | 1:O:220:VAL:HG12 | 2.28 | 0.69 |
| 1:C:262:ASN:C | 1:C:262:ASN:ND2 | 2.41 | 0.69 |
| 1:G:250:LEU:HD12 | 1:G:250:LEU:N | 2.08 | 0.69 |
| 1:H:54:LYS:O | 1:H:57:ASN:O | 2.11 | 0.69 |
| 1:K:143:ASN:O | 1:K:144:ARG:O | 2.10 | 0.69 |
| 1:M:150:ASP:CG | 1:N:257:VAL:HG21 | 2.12 | 0.69 |
| 1:N:162:LYS:C | 1:N:330:PHE:HD1 | 1.95 | 0.69 |
| 1:B:468:PHE:CD1 | 1:B:468:PHE:O | 2.46 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:23:SER:OG | 1:C:25:ASP:HB2 | 1.93 | 0.68 |
| 1:C:217:LYS:CE | 1:C:217:LYS:CG | 2.72 | 0.68 |
| 1:D:82:LYS:NZ | 1:D:403:ASN:HD22 | 1.92 | 0.68 |
| 1:E:180:VAL:HG12 | 1:E:184:ASP:HB2 | 1.75 | 0.68 |
| 1:E:312:TRP:CH2 | 1:E:468:PHE:HB2 | 2.28 | 0.68 |
| 1:F:348:ILE:HD11 | 1:G:181:GLN:HE22 | 1.58 | 0.68 |
| 1:F:372:LEU:HB3 | 1:F:374:PHE:CE1 | 2.27 | 0.68 |
| 1:G:24:THR:HG23 | 1:G:320:ASN:HA | 1.73 | 0.68 |
| 1:H:279:GLY:HA3 | 1:H:283:THR:O | 1.91 | 0.68 |
| 1:H:451:LEU:O | 1:H:454:LYS:HB2 | 1.93 | 0.68 |
| 1:L:52:ILE:HB | 1:L:62:VAL:HB | 1.75 | 0.68 |
| 1:L:378:LEU:HD12 | 1:L:379:CYS:H | 1.57 | 0.68 |
| 1:B:30:ARG:HH11 | 1:B:377:GLN:NE2 | 1.91 | 0.68 |
| 1:D:37:ALA:HB1 | 1:D:451:LEU:HD13 | 1.75 | 0.68 |
| 1:D:120:HIS:HE2 | 1:D:218:SER:HB3 | 1.57 | 0.68 |
| 1:E:66:SER:H | 1:E:69:GLN:NE2 | 1.91 | 0.68 |
| 1:J:54:LYS:HA | 1:J:54:LYS:NZ | 2.08 | 0.68 |
| 1:K:452:LYS:CG | 1:K:452:LYS:CE | 2.71 | 0.68 |
| 1:M:162:LYS:C | 1:M:330:PHE:HD1 | 1.95 | 0.68 |
| 1:N:120:HIS:HA | 1:N:222:LEU:HD13 | 1.76 | 0.68 |
| 1:E:49:TYR:HE2 | 1:E:118:SER:HA | 1.58 | 0.68 |
| 1:F:66:SER:H | 1:F:69:GLN:NE2 | 1.92 | 0.68 |
| 1:F:442:LYS:HB3 | 1:F:443:LYS:HD3 | 1.75 | 0.68 |
| 1:G:237:MET:HB3 | 1:G:246:LEU:HD22 | 1.75 | 0.68 |
| 1:H:247:PHE:HD1 | 1:H:248:PHE:N | 1.92 | 0.68 |
| 1:I:30:ARG:HH11 | 1:I:377:GLN:NE2 | 1.90 | 0.68 |
| 1:I:66:SER:O | 1:I:69:GLN:HG3 | 1.93 | 0.68 |
| 1:L:464:LEU:C | 1:L:464:LEU:CD2 | 2.62 | 0.68 |
| 1:M:115:VAL:HG22 | 1:N:255:MET:SD | 2.34 | 0.68 |
| 1:M:250:LEU:N | 1:M:250:LEU:HD12 | 2.06 | 0.68 |
| 1:O:163:PRO:N | 1:O:330:PHE:HD1 | 1.91 | 0.68 |
| 1:B:107:VAL:O | 1:B:107:VAL:HG12 | 1.94 | 0.68 |
| 1:B:461:GLN:HE22 | 1:C:21:VAL:HB | 1.56 | 0.68 |
| 1:D:262:ASN:ND2 | 1:D:288:SER:HB3 | 2.08 | 0.68 |
| 1:D:465:GLY:O | 1:D:468:PHE:N | 2.26 | 0.68 |
| 1:F:383:LEU:CD2 | 1:F:383:LEU:CD1 | 2.70 | 0.68 |
| 1:J:98:LEU:HD22 | 1:J:378:LEU:HD11 | 0.89 | 0.68 |
| 1:K:242:TYR:CE2 | 1:K:394:MET:HG3 | 2.29 | 0.68 |
| 1:L:149:MET:HE3 | 1:L:294:THR:HG22 | 1.74 | 0.68 |
| 1:N:276:TYR:C | 1:N:277:ILE:HG12 | 2.14 | 0.68 |
| 1:B:45:VAL:C | 1:B:65:VAL:HG21 | 2.14 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:252:ARG:HD2 | 1:B:306:ILE:HD11 | 1.74 | 0.68 |
| 1:D:66:SER:H | 1:D:69:GLN:HE21 | 1.39 | 0.68 |
| 1:G:316:ALA:CB | 1:G:321:ASN:OD1 | 2.41 | 0.68 |
| 1:N:262:ASN:HD22 | 1:N:263:ARG:N | 1.91 | 0.68 |
| 1:A:21:VAL:HG12 | 1:A:22:VAL:N | 2.07 | 0.68 |
| 1:F:57:ASN:HD21 | 1:F:59:LYS:CB | 2.06 | 0.68 |
| 1:F:75:ILE:HG23 | 1:F:451:LEU:HD12 | 1.76 | 0.68 |
| 1:F:115:VAL:CG2 | 1:G:257:VAL:HG13 | 2.23 | 0.68 |
| 1:F:353:THR:CG2 | 1:F:353:THR:HB | 2.12 | 0.68 |
| 1:J:74:ARG:CD | 1:J:74:ARG:CB | 2.71 | 0.68 |
| 1:K:185:CYS:SG | 1:O:344:LEU:HD11 | 2.33 | 0.68 |
| 1:O:29:ALA:HB3 | 1:O:380:LYS:HG3 | 1.73 | 0.68 |
| 1:O:77:LEU:HD22 | 1:O:455:PHE:HZ | 1.59 | 0.68 |
| 1:A:97:ARG:HG3 | 1:A:383:LEU:HD11 | 1.74 | 0.68 |
| 1:B:151:TYR:CD2 | 1:B:203:THR:HB | 2.29 | 0.68 |
| 1:B:463:PRO:HA | 1:B:466:ARG:HE | 1.58 | 0.68 |
| 1:C:151:TYR:OH | 1:C:221:PRO:HB2 | 1.94 | 0.68 |
| 1:E:46:GLY:HA3 | 1:E:65:VAL:CG2 | 2.22 | 0.68 |
| 1:E:302:SER:O | 1:E:304:ALA:N | 2.27 | 0.68 |
| 1:J:65:VAL:HA | 1:J:69:GLN:HE22 | 1.59 | 0.68 |
| 1:K:202:ASP:OD2 | 1:O:112:PRO:CB | 2.41 | 0.68 |
| 1:L:74:ARG:HG3 | 1:L:330:PHE:HE2 | 1.56 | 0.68 |
| 1:L:117:ILE:HD11 | 1:M:260:LEU:HB3 | 1.74 | 0.68 |
| 1:N:49:TYR:HE2 | 1:N:118:SER:HA | 1.58 | 0.68 |
| 1:O:116:GLY:N | 1:O:339:SER:OG | 2.23 | 0.68 |
| 1:O:120:HIS:NE2 | 1:O:218:SER:HB3 | 2.09 | 0.68 |
| 1:A:122:LEU:HD11 | 1:B:286:LEU:CD1 | 2.23 | 0.68 |
| 1:B:305:GLN:HE22 | 1:B:337:THR:HG21 | 1.58 | 0.68 |
| 1:D:246:LEU:CD2 | 1:D:246:LEU:N | 2.57 | 0.68 |
| 1:G:152:LYS:CB | 1:G:255:MET:HB2 | 2.24 | 0.68 |
| 1:I:96:GLN:HB3 | 1:I:382:THR:HG22 | 1.73 | 0.68 |
| 1:J:196:GLN:O | 1:J:199:ASP:OD2 | 2.11 | 0.68 |
| 1:K:96:GLN:HA | 1:K:381:ILE:O | 1.94 | 0.68 |
| 1:K:219:GLU:O | 1:K:220:VAL:HG13 | 1.94 | 0.68 |
| 1:L:24:THR:HG23 | 1:L:320:ASN:HA | 1.76 | 0.68 |
| 1:B:57:ASN:HD21 | 1:B:59:LYS:CB | 2.07 | 0.68 |
| 1:B:163:PRO:HD3 | 1:B:330:PHE:CE1 | 2.25 | 0.68 |
| 1:E:271:VAL:HG13 | 1:E:275:LEU:HD12 | 1.76 | 0.68 |
| 1:G:337:THR:CG2 | 1:G:337:THR:CA | 2.67 | 0.68 |
| 1:I:78:PRO:HD2 | 1:I:455:PHE:CE1 | 2.29 | 0.68 |
| 1:J:83:PHE:HB3 | 1:J:85:PHE:CE1 | 2.28 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:152:LYS:O | 1:J:152:LYS:CG | 2.42 | 0.68 |
| 1:K:237:MET:O | 1:K:240:GLU:HB3 | 1.94 | 0.68 |
| 1:N:293:PRO:O | 1:N:293:PRO:HG2 | 1.93 | 0.68 |
| 1:A:68:LEU:O | 1:A:201:VAL:HG22 | 1.94 | 0.68 |
| 1:H:54:LYS:NZ | 1:H:55:PRO:HD2 | 2.08 | 0.68 |
| 1:M:441:LEU:CD2 | 1:M:441:LEU:HG | 2.12 | 0.68 |
| 1:B:160:GLY:HA3 | 1:B:245:SER:O | 1.93 | 0.67 |
| 1:E:219:GLU:O | 1:E:263:ARG:NH2 | 2.20 | 0.67 |
| 1:G:71:ARG:HA | 1:G:71:ARG:HH11 | 1.58 | 0.67 |
| 1:L:159:ILE:HG22 | 1:L:247:PHE:HE1 | 1.57 | 0.67 |
| 1:L:363:TYR:CD2 | 1:M:185:CYS:HB2 | 2.29 | 0.67 |
| 1:M:52:ILE:N | 1:M:52:ILE:CD1 | 2.57 | 0.67 |
| 1:C:54:LYS:NZ | 1:C:54:LYS:HA | 2.09 | 0.67 |
| 1:C:70:TYR:HE1 | 1:C:201:VAL:HA | 1.59 | 0.67 |
| 1:D:113:LEU:HD22 | 1:E:253:GLU:HG3 | 1.76 | 0.67 |
| 1:D:120:HIS:HA | 1:D:222:LEU:HD13 | 1.77 | 0.67 |
| 1:E:98:LEU:CD1 | 1:E:378:LEU:HD11 | 2.12 | 0.67 |
| 1:E:117:ILE:CD1 | 1:E:117:ILE:CB | 2.73 | 0.67 |
| 1:G:262:ASN:C | 1:G:262:ASN:ND2 | 2.46 | 0.67 |
| 1:H:373:GLN:HB2 | 1:H:464:LEU:HD12 | 1.74 | 0.67 |
| 1:I:75:ILE:CG2 | 1:I:451:LEU:CD1 | 2.72 | 0.67 |
| 1:L:110:GLY:C | 1:L:111:GLN:HG2 | 2.14 | 0.67 |
| 1:M:348:ILE:HD12 | 1:N:182:PRO:O | 1.94 | 0.67 |
| 1:N:46:GLY:HA3 | 1:N:63:PRO:O | 1.94 | 0.67 |
| 1:A:36:HIS:ND1 | 1:A:37:ALA:N | 2.42 | 0.67 |
| 1:A:54:LYS:HA | 1:A:54:LYS:HZ2 | 1.59 | 0.67 |
| 1:A:70:TYR:OH | 1:A:232:PRO:HD3 | 1.94 | 0.67 |
| 1:A:223:ASP:OD1 | 1:A:224:ILE:N | 2.28 | 0.67 |
| 1:F:60:ILE:HG13 | 1:F:60:ILE:O | 1.93 | 0.67 |
| 1:F:92:ASN:O | 1:F:94:ASP:N | 2.27 | 0.67 |
| 1:G:112:PRO:HD3 | 1:H:231:TYR:CG | 2.29 | 0.67 |
| 1:G:358:THR:HA | 1:H:266:THR:CG2 | 2.24 | 0.67 |
| 1:H:152:LYS:NZ | 1:H:152:LYS:CD | 2.57 | 0.67 |
| 1:I:177:GLN:O | 1:I:178:VAL:C | 2.30 | 0.67 |
| 1:J:242:TYR:CE2 | 1:J:394:MET:CG | 2.77 | 0.67 |
| 1:L:98:LEU:HD13 | 1:L:378:LEU:HD11 | 1.75 | 0.67 |
| 1:M:395:ASN:O | 1:M:398:ILE:HG12 | 1.95 | 0.67 |
| 1:N:115:VAL:HG22 | 1:O:255:MET:SD | 2.34 | 0.67 |
| 1:N:356:LYS:NZ | 1:N:356:LYS:CD | 2.57 | 0.67 |
| 1:A:213:LEU:HD12 | 1:E:344:LEU:HD13 | 1.75 | 0.67 |
| 1:G:129:THR:HG21 | 1:G:291:TYR:HD2 | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:262:ASN:HD21 | 1:H:288:SER:CB | 2.07 | 0.67 |
| 1:I:36:HIS:ND1 | 1:I:37:ALA:N | 2.42 | 0.67 |
| 1:I:123:LEU:CD2 | 1:I:147:ILE:HB | 2.22 | 0.67 |
| 1:M:204:GLY:HA3 | 1:M:295:PRO:HG3 | 1.75 | 0.67 |
| 1:N:24:THR:CG2 | 1:N:320:ASN:HA | 2.24 | 0.67 |
| 1:O:246:LEU:HD23 | 1:O:246:LEU:N | 2.03 | 0.67 |
| 1:A:216:ASN:HB2 | 1:E:345:CYS:SG | 2.34 | 0.67 |
| 1:A:280:SER:N | 1:A:284:ALA:HB2 | 2.10 | 0.67 |
| 1:A:300:VAL:O | 1:A:300:VAL:HG23 | 1.94 | 0.67 |
| 1:C:323:ILE:HG21 | 1:C:325:TRP:CZ2 | 2.30 | 0.67 |
| 1:C:451:LEU:HD23 | 1:C:454:LYS:CG | 2.14 | 0.67 |
| 1:C:463:PRO:HA | 1:C:466:ARG:HE | 1.59 | 0.67 |
| 1:D:97:ARG:HH11 | 1:D:97:ARG:HA | 1.59 | 0.67 |
| 1:D:255:MET:HG2 | 1:D:256:PHE:H | 1.57 | 0.67 |
| 1:H:54:LYS:NZ | 1:H:54:LYS:HA | 2.09 | 0.67 |
| 1:K:363:TYR:CD1 | 1:L:185:CYS:HB2 | 2.30 | 0.67 |
| 1:L:180:VAL:CG1 | 1:L:184:ASP:CB | 2.64 | 0.67 |
| 1:M:188:LEU:HD11 | 1:M:213:LEU:HD11 | 1.76 | 0.67 |
| 1:O:139:ALA:O | 1:O:140:GLY:O | 2.13 | 0.67 |
| 1:C:54:LYS:HZ2 | 1:C:55:PRO:HD2 | 1.58 | 0.67 |
| 1:G:180:VAL:CG1 | 1:G:184:ASP:HB3 | 2.22 | 0.67 |
| 1:H:54:LYS:HG2 | 1:H:57:ASN:HB3 | 1.75 | 0.67 |
| 1:H:68:LEU:HD23 | 1:H:201:VAL:CG2 | 2.24 | 0.67 |
| 1:I:67:GLY:C | 1:I:68:LEU:HG | 2.11 | 0.67 |
| 1:I:369:GLU:OE1 | 1:J:190:LEU:HD21 | 1.95 | 0.67 |
| 1:L:247:PHE:HD1 | 1:L:248:PHE:H | 1.41 | 0.67 |
| 1:M:163:PRO:HD3 | 1:M:330:PHE:HE1 | 1.60 | 0.67 |
| 1:A:57:ASN:ND2 | 1:A:59:LYS:H | 1.93 | 0.67 |
| 1:A:135:TYR:CE2 | 1:A:287:ALA:HB2 | 2.21 | 0.67 |
| 1:B:472:LEU:CD2 | 1:G:138:ASN:HD22 | 2.07 | 0.67 |
| 1:C:220:VAL:O | 1:C:221:PRO:O | 2.13 | 0.67 |
| 1:G:163:PRO:N | 1:G:330:PHE:HD1 | 1.93 | 0.67 |
| 1:G:219:GLU:HB3 | 1:G:263:ARG:CZ | 2.24 | 0.67 |
| 1:J:162:LYS:C | 1:J:330:PHE:HD1 | 1.97 | 0.67 |
| 1:L:249:TYR:CG | 1:L:249:TYR:O | 2.47 | 0.67 |
| 1:B:82:LYS:CG | 1:B:82:LYS:CA | 2.69 | 0.67 |
| 1:C:464:LEU:CD2 | 1:C:464:LEU:C | 2.62 | 0.67 |
| 1:D:121:PRO:HG2 | 1:E:289:SER:HB2 | 1.77 | 0.67 |
| 1:F:467:LYS:CE | 1:F:467:LYS:CG | 2.72 | 0.67 |
| 1:I:30:ARG:HH11 | 1:I:377:GLN:HE22 | 1.40 | 0.67 |
| 1:I:34:TYR:HE2 | 1:I:377:GLN:HB2 | 1.58 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:302:SER:O | 1:I:304:ALA:N | 2.28 | 0.67 |
| 1:K:142:ASP:OD1 | 1:L:283:THR:OG1 | 2.11 | 0.67 |
| 1:N:122:LEU:O | 1:N:218:SER:HB2 | 1.95 | 0.67 |
| 1:N:178:VAL:O | 1:N:180:VAL:N | 2.25 | 0.67 |
| 1:A:92:ASN:HD21 | 1:A:94:ASP:HB2 | 1.59 | 0.67 |
| 1:B:103:VAL:HG23 | 1:B:104:GLY:N | 2.09 | 0.67 |
| 1:E:78:PRO:HB3 | 1:E:452:LYS:HG2 | 1.77 | 0.67 |
| 1:E:391:ILE:HG21 | 1:E:402:TRP:CZ3 | 2.30 | 0.67 |
| 1:F:21:VAL:HG13 | 1:F:390:TYR:OH | 1.95 | 0.67 |
| 1:I:120:HIS:HA | 1:I:222:LEU:HD13 | 1.77 | 0.67 |
| 1:M:462:PHE:HB3 | 1:M:463:PRO:HD2 | 1.75 | 0.67 |
| 1:N:142:ASP:O | 1:O:283:THR:HG21 | 1.95 | 0.67 |
| 1:N:219:GLU:C | 1:N:220:VAL:HG13 | 2.16 | 0.67 |
| 1:N:255:MET:HG2 | 1:N:256:PHE:N | 2.10 | 0.67 |
| 1:O:450:ASN:HD21 | 1:O:452:LYS:HD2 | 1.59 | 0.67 |
| 1:A:30:ARG:HH11 | 1:A:377:GLN:NE2 | 1.91 | 0.67 |
| 1:D:123:LEU:CD2 | 1:D:123:LEU:CD1 | 2.70 | 0.67 |
| 1:E:220:VAL:O | 1:E:221:PRO:C | 2.32 | 0.67 |
| 1:F:246:LEU:CD2 | 1:F:246:LEU:N | 2.57 | 0.67 |
| 1:H:112:PRO:HB3 | 1:I:231:TYR:CG | 2.30 | 0.67 |
| 1:K:41:ARG:NH2 | 1:L:192:ASN:HD21 | 1.90 | 0.67 |
| 1:K:42:LEU:CD1 | 1:K:73:PHE:HE2 | 2.07 | 0.67 |
| 1:K:97:ARG:HA | 1:K:97:ARG:HH11 | 1.59 | 0.67 |
| 1:L:139:ALA:HB1 | 1:L:143:ASN:OD1 | 1.95 | 0.67 |
| 1:L:149:MET:HE2 | 1:L:205:PHE:CE1 | 2.30 | 0.67 |
| 1:M:57:ASN:ND2 | 1:M:59:LYS:H | 1.94 | 0.67 |
| 1:M:151:TYR:OH | 1:M:221:PRO:HB2 | 1.94 | 0.67 |
| 1:N:363:TYR:CG | 1:O:185:CYS:HB2 | 2.30 | 0.67 |
| 1:A:257:VAL:HG12 | 1:A:293:PRO:HB2 | 1.76 | 0.66 |
| 1:B:77:LEU:HD22 | 1:B:455:PHE:CE1 | 2.29 | 0.66 |
| 1:C:178:VAL:CG1 | 1:C:178:VAL:HB | 2.16 | 0.66 |
| 1:D:52:ILE:N | 1:D:52:ILE:CD1 | 2.57 | 0.66 |
| 1:E:152:LYS:HE2 | 1:E:202:ASP:HB3 | 1.77 | 0.66 |
| 1:H:24:THR:HG21 | 1:H:320:ASN:HA | 1.76 | 0.66 |
| 1:I:70:TYR:HE1 | 1:I:201:VAL:HA | 1.59 | 0.66 |
| 1:J:96:GLN:HB3 | 1:J:382:THR:CG2 | 2.24 | 0.66 |
| 1:J:462:PHE:HB3 | 1:J:463:PRO:HD2 | 1.75 | 0.66 |
| 1:K:180:VAL:HG13 | 1:K:184:ASP:CB | 2.25 | 0.66 |
| 1:L:194:VAL:HG21 | 1:L:444:TYR:CE2 | 2.29 | 0.66 |
| 1:N:375:ILE:HG12 | 1:N:464:LEU:HD13 | 1.77 | 0.66 |
| 1:O:30:ARG:HH11 | 1:O:377:GLN:NE2 | 1.93 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:122:LEU:HD13 | 1:A:144:ARG:NH2 | 2.09 | 0.66 |
| 1:C:77:LEU:HD22 | 1:C:455:PHE:HZ | 1.61 | 0.66 |
| 1:C:113:LEU:HD12 | 1:C:113:LEU:N | 2.08 | 0.66 |
| 1:C:192:ASN:C | 1:C:193:THR:HG22 | 2.15 | 0.66 |
| 1:F:109:ARG:NH1 | 1:F:370:TYR:CE1 | 2.63 | 0.66 |
| 1:G:280:SER:N | 1:G:284:ALA:HB2 | 2.10 | 0.66 |
| 1:G:450:ASN:HD21 | 1:G:452:LYS:HD2 | 1.60 | 0.66 |
| 1:H:308:ASN:HD22 | 1:I:251:ARG:HH22 | 1.42 | 0.66 |
| 1:I:111:GLN:HG2 | 1:I:369:GLU:CB | 2.26 | 0.66 |
| 1:J:320:ASN:HD21 | 1:J:323:ILE:HB | 1.60 | 0.66 |
| 1:K:159:ILE:HD12 | 1:K:248:PHE:CD2 | 2.30 | 0.66 |
| 1:L:375:ILE:HG21 | 1:L:468:PHE:CD2 | 2.31 | 0.66 |
| 1:M:344:LEU:HD11 | 1:N:188:LEU:HD21 | 1.77 | 0.66 |
| 1:M:375:ILE:HG12 | 1:M:464:LEU:HD13 | 1.76 | 0.66 |
| 1:N:68:LEU:HB3 | 1:N:201:VAL:CG2 | 2.25 | 0.66 |
| 1:O:166:GLY:CA | 1:O:195:ILE:HD11 | 2.24 | 0.66 |
| 1:O:367:GLY:O | 1:O:368:GLU:HG2 | 1.94 | 0.66 |
| 1:D:21:VAL:CG1 | 1:D:390:TYR:OH | 2.43 | 0.66 |
| 1:F:114:GLY:HA3 | 1:F:340:THR:OG1 | 1.95 | 0.66 |
| 1:H:178:VAL:CG1 | 1:H:178:VAL:CA | 2.71 | 0.66 |
| 1:J:70:TYR:OH | 1:J:232:PRO:HD3 | 1.96 | 0.66 |
| 1:L:241:PRO:CG | 1:L:242:TYR:H | 2.07 | 0.66 |
| 1:O:77:LEU:HD22 | 1:O:455:PHE:CZ | 2.31 | 0.66 |
| 1:A:46:GLY:HA3 | 1:A:63:PRO:O | 1.96 | 0.66 |
| 1:A:237:MET:HB3 | 1:A:246:LEU:CD2 | 2.25 | 0.66 |
| 1:C:109:ARG:N | 1:C:308:ASN:OD1 | 2.28 | 0.66 |
| 1:F:98:LEU:HD13 | 1:F:378:LEU:HD11 | 1.76 | 0.66 |
| 1:G:463:PRO:N | 1:G:466:ARG:HH21 | 1.92 | 0.66 |
| 1:H:36:HIS:ND1 | 1:H:37:ALA:N | 2.43 | 0.66 |
| 1:L:344:LEU:HD12 | 1:M:186:PRO:CD | 2.24 | 0.66 |
| 1:N:391:ILE:O | 1:N:391:ILE:HG22 | 1.96 | 0.66 |
| 1:O:81:ASN:OD1 | 1:O:97:ARG:NH1 | 2.28 | 0.66 |
| 1:B:345:CYS:SG | 1:C:216:ASN:CB | 2.82 | 0.66 |
| 1:C:205:PHE:CD1 | 1:C:220:VAL:HG12 | 2.30 | 0.66 |
| 1:D:252:ARG:CD | 1:D:306:ILE:HD11 | 2.20 | 0.66 |
| 1:G:42:LEU:HD13 | 1:G:447:TRP:CE2 | 2.30 | 0.66 |
| 1:K:67:GLY:C | 1:K:68:LEU:HG | 2.16 | 0.66 |
| 1:K:299:MET:HA | 1:L:256:PHE:HB3 | 1.76 | 0.66 |
| 1:L:151:TYR:OH | 1:L:221:PRO:HB2 | 1.96 | 0.66 |
| 1:M:77:LEU:HD22 | 1:M:455:PHE:CZ | 2.31 | 0.66 |
| 1:M:237:MET:HB3 | 1:M:246:LEU:CD2 | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:97:ARG:HH11 | 1:A:97:ARG:CA | 2.07 | 0.66 |
| 1:A:300:VAL:CG1 | 1:A:300:VAL:CG2 | 2.70 | 0.66 |
| 1:B:363:TYR:CD1 | 1:C:185:CYS:HB2 | 2.31 | 0.66 |
| 1:C:374:PHE:N | 1:C:374:PHE:CD1 | 2.63 | 0.66 |
| 1:H:68:LEU:HD23 | 1:H:201:VAL:HG21 | 1.77 | 0.66 |
| 1:N:149:MET:HE1 | 1:N:205:PHE:HE1 | 1.61 | 0.66 |
| 1:A:75:ILE:HB | 1:A:329:LEU:CB | 2.25 | 0.66 |
| 1:B:72:VAL:HG13 | 1:B:332:THR:HG23 | 1.76 | 0.66 |
| 1:B:320:ASN:OD1 | 1:B:321:ASN:N | 2.29 | 0.66 |
| 1:B:325:TRP:NE1 | 1:B:394:MET:HE3 | 2.10 | 0.66 |
| 1:C:178:VAL:CG1 | 1:C:178:VAL:CA | 2.73 | 0.66 |
| 1:H:464:LEU:HD23 | 1:H:464:LEU:O | 1.95 | 0.66 |
| 1:I:208:MET:CG | 1:I:210:PHE:CE2 | 2.79 | 0.66 |
| 1:K:228:ILE:N | 1:K:228:ILE:CD1 | 2.58 | 0.66 |
| 1:L:355:TYR:CD1 | 1:M:144:ARG:HD3 | 2.30 | 0.66 |
| 1:M:137:ALA:CB | 1:M:137:ALA:C | 2.61 | 0.66 |
| 1:O:54:LYS:HG2 | 1:O:57:ASN:HB3 | 1.77 | 0.66 |
| 1:D:400:GLU:O | 1:D:402:TRP:N | 2.28 | 0.66 |
| 1:G:358:THR:HA | 1:H:266:THR:HG23 | 1.77 | 0.66 |
| 1:H:33:ILE:HB | 1:H:378:LEU:HB3 | 1.78 | 0.66 |
| 1:H:115:VAL:H | 1:I:255:MET:CE | 2.07 | 0.66 |
| 1:I:363:TYR:CD1 | 1:J:185:CYS:HB2 | 2.30 | 0.66 |
| 1:A:213:LEU:CD1 | 1:E:344:LEU:HD13 | 2.26 | 0.66 |
| 1:D:440:PRO:HA | 1:D:443:LYS:NZ | 2.10 | 0.66 |
| 1:F:145:GLU:OE1 | 1:G:134:ALA:CA | 2.44 | 0.66 |
| 1:G:147:ILE:HA | 1:H:129:THR:O | 1.96 | 0.66 |
| 1:I:70:TYR:CD2 | 1:I:195:ILE:HG21 | 2.31 | 0.66 |
| 1:I:152:LYS:HB3 | 1:I:255:MET:HB2 | 1.77 | 0.66 |
| 1:I:277:ILE:CD1 | 1:I:277:ILE:CB | 2.74 | 0.66 |
| 1:I:320:ASN:OD1 | 1:I:322:GLY:N | 2.23 | 0.66 |
| 1:K:219:GLU:HB3 | 1:K:263:ARG:CZ | 2.25 | 0.66 |
| 1:L:77:LEU:HD22 | 1:L:455:PHE:HZ | 1.61 | 0.66 |
| 1:M:54:LYS:HB3 | 1:M:57:ASN:HD22 | 1.60 | 0.66 |
| 1:M:86:PRO:C | 1:M:86:PRO:HA | 2.06 | 0.66 |
| 1:M:466:ARG:HD2 | 1:N:317:GLN:O | 1.96 | 0.66 |
| 1:N:246:LEU:O | 1:N:246:LEU:HD23 | 1.95 | 0.66 |
| 1:A:302:SER:O | 1:A:304:ALA:N | 2.29 | 0.66 |
| 1:J:444:TYR:HB3 | 1:J:446:PHE:CZ | 2.31 | 0.66 |
| 1:K:122:LEU:HD11 | 1:L:286:LEU:HD11 | 1.77 | 0.66 |
| 1:K:162:LYS:C | 1:K:330:PHE:HD1 | 1.98 | 0.66 |
| 1:G:188:LEU:HD13 | 1:G:213:LEU:HD11 | 1.75 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:188:LEU:HD11 | 1:J:213:LEU:HD11 | 1.77 | 0.65 |
| 1:K:383:LEU:HD23 | 1:K:388:MET:CE | 2.26 | 0.65 |
| 1:L:115:VAL:HG22 | 1:M:255:MET:SD | 2.37 | 0.65 |
| 1:M:147:ILE:CD1 | 1:M:147:ILE:CB | 2.74 | 0.65 |
| 1:M:255:MET:CG | 1:M:256:PHE:N | 2.58 | 0.65 |
| 1:N:344:LEU:HD12 | 1:O:185:CYS:SG | 2.35 | 0.65 |
| 1:B:123:LEU:HD23 | 1:B:147:ILE:HB | 1.77 | 0.65 |
| 1:B:361:LYS:HD2 | 1:C:183:GLY:HA3 | 1.77 | 0.65 |
| 1:F:71:ARG:HA | 1:F:71:ARG:NH1 | 2.03 | 0.65 |
| 1:F:459:LEU:HB3 | 1:F:465:GLY:HA3 | 1.78 | 0.65 |
| 1:G:33:ILE:HB | 1:G:378:LEU:HB3 | 1.78 | 0.65 |
| 1:G:118:SER:HB2 | 1:G:151:TYR:CE1 | 2.32 | 0.65 |
| 1:G:305:GLN:HE22 | 1:G:337:THR:HG21 | 1.61 | 0.65 |
| 1:H:463:PRO:HA | 1:H:466:ARG:HE | 1.61 | 0.65 |
| 1:J:220:VAL:O | 1:J:221:PRO:C | 2.30 | 0.65 |
| 1:J:323:ILE:HG21 | 1:J:325:TRP:CZ2 | 2.30 | 0.65 |
| 1:K:344:LEU:CB | 1:L:213:LEU:HD12 | 2.25 | 0.65 |
| 1:B:54:LYS:CE | 1:B:55:PRO:HD2 | 2.17 | 0.65 |
| 1:B:75:ILE:CG2 | 1:B:451:LEU:HD12 | 2.26 | 0.65 |
| 1:C:79:ASP:HA | 1:C:327:ASN:ND2 | 2.11 | 0.65 |
| 1:D:31:THR:CG2 | 1:D:378:LEU:O | 2.43 | 0.65 |
| 1:F:216:ASN:CB | 1:J:345:CYS:SG | 2.85 | 0.65 |
| 1:G:260:LEU:HD12 | 1:G:260:LEU:N | 2.11 | 0.65 |
| 1:L:124:ASN:OD1 | 1:L:264:ALA:N | 2.27 | 0.65 |
| 1:B:220:VAL:O | 1:B:221:PRO:O | 2.15 | 0.65 |
| 1:F:183:GLY:O | 1:F:184:ASP:C | 2.35 | 0.65 |
| 1:J:74:ARG:HD2 | 1:J:330:PHE:HE2 | 1.61 | 0.65 |
| 1:J:255:MET:CG | 1:J:256:PHE:N | 2.56 | 0.65 |
| 1:N:172:GLY:O | 1:N:173:SER:C | 2.35 | 0.65 |
| 1:N:188:LEU:HD11 | 1:N:213:LEU:HD11 | 1.79 | 0.65 |
| 1:A:241:PRO:HG2 | 1:A:242:TYR:H | 1.61 | 0.65 |
| 1:D:54:LYS:HG2 | 1:D:57:ASN:HB3 | 1.78 | 0.65 |
| 1:G:151:TYR:OH | 1:G:221:PRO:HB2 | 1.95 | 0.65 |
| 1:I:358:THR:HG22 | 1:J:266:THR:CG2 | 2.27 | 0.65 |
| 1:J:200:MET:O | 1:J:229:CYS:HA | 1.96 | 0.65 |
| 1:O:52:ILE:N | 1:O:52:ILE:HD12 | 2.09 | 0.65 |
| 1:O:92:ASN:HD21 | 1:O:94:ASP:HB2 | 1.62 | 0.65 |
| 1:A:240:GLU:HG3 | 1:A:243:GLY:H | 1.61 | 0.65 |
| 1:B:77:LEU:HB2 | 1:B:327:ASN:HB3 | 1.79 | 0.65 |
| 1:C:49:TYR:HE2 | 1:C:118:SER:HA | 1.60 | 0.65 |
| 1:C:323:ILE:HG21 | 1:C:325:TRP:CE2 | 2.32 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:96:GLN:HE22 | 1:D:380:LYS:HE3 | 1.61 | 0.65 |
| 1:E:189:GLU:O | 1:E:191:ILE:HG13 | 1.96 | 0.65 |
| 1:E:439:ASP:OD2 | 1:E:440:PRO:HD2 | 1.96 | 0.65 |
| 1:G:129:THR:HG21 | 1:G:291:TYR:CD2 | 2.32 | 0.65 |
| 1:I:109:ARG:NH1 | 1:I:370:TYR:CZ | 2.65 | 0.65 |
| 1:K:300:VAL:O | 1:K:300:VAL:HG23 | 1.97 | 0.65 |
| 1:L:373:GLN:CB | 1:L:464:LEU:HD12 | 2.26 | 0.65 |
| 1:M:54:LYS:HE3 | 1:M:55:PRO:HD2 | 1.79 | 0.65 |
| 1:M:299:MET:HA | 1:N:256:PHE:HB3 | 1.78 | 0.65 |
| 1:M:439:ASP:O | 1:M:442:LYS:HB2 | 1.96 | 0.65 |
| 1:O:52:ILE:N | 1:O:52:ILE:CD1 | 2.59 | 0.65 |
| 1:O:92:ASN:HD22 | 1:O:95:THR:H | 1.45 | 0.65 |
| 1:E:49:TYR:CE2 | 1:E:118:SER:HA | 2.32 | 0.65 |
| 1:E:442:LYS:HB3 | 1:E:443:LYS:HD3 | 1.78 | 0.65 |
| 1:F:153:GLN:HE22 | 1:F:300:VAL:HA | 1.62 | 0.65 |
| 1:I:139:ALA:O | 1:I:140:GLY:O | 2.15 | 0.65 |
| 1:J:44:ALA:O | 1:J:45:VAL:CG2 | 2.40 | 0.65 |
| 1:J:166:GLY:HA3 | 1:J:195:ILE:HD11 | 1.79 | 0.65 |
| 1:M:75:ILE:HG23 | 1:M:451:LEU:HD12 | 1.78 | 0.65 |
| 1:N:274:ASP:N | 1:N:274:ASP:OD1 | 2.28 | 0.65 |
| 1:O:49:TYR:CE2 | 1:O:118:SER:HA | 2.30 | 0.65 |
| 1:B:30:ARG:HH11 | 1:B:377:GLN:HE22 | 1.45 | 0.65 |
| 1:B:263:ARG:HG2 | 1:B:292:PHE:HD2 | 1.61 | 0.65 |
| 1:C:123:LEU:HD23 | 1:C:147:ILE:HB | 1.78 | 0.65 |
| 1:C:300:VAL:HG22 | 1:D:255:MET:O | 1.97 | 0.65 |
| 1:D:34:TYR:OH | 1:D:377:GLN:OE1 | 2.11 | 0.65 |
| 1:H:307:PHE:C | 1:H:309:LYS:H | 1.99 | 0.65 |
| 1:H:391:ILE:O | 1:H:391:ILE:HG22 | 1.97 | 0.65 |
| 1:I:111:GLN:HG2 | 1:I:369:GLU:HB3 | 1.79 | 0.65 |
| 1:I:219:GLU:HA | 1:I:263:ARG:HH12 | 1.62 | 0.65 |
| 1:J:372:LEU:HB3 | 1:J:374:PHE:HE1 | 1.61 | 0.65 |
| 1:J:463:PRO:HG2 | 1:J:464:LEU:H | 1.62 | 0.65 |
| 1:K:164:PRO:HG3 | 1:K:332:THR:CG2 | 2.26 | 0.65 |
| 1:K:450:ASN:HD21 | 1:K:452:LYS:HD2 | 1.62 | 0.65 |
| 1:M:220:VAL:O | 1:M:221:PRO:O | 2.15 | 0.65 |
| 1:N:74:ARG:HG3 | 1:N:330:PHE:CE2 | 2.32 | 0.65 |
| 1:N:123:LEU:CD2 | 1:N:123:LEU:HG | 2.16 | 0.65 |
| 1:N:151:TYR:HD2 | 1:N:203:THR:O | 1.79 | 0.65 |
| 1:A:67:GLY:H | 1:A:366:HIS:HE1 | 1.42 | 0.65 |
| 1:B:54:LYS:NZ | 1:B:54:LYS:HA | 2.10 | 0.65 |
| 1:C:67:GLY:C | 1:C:68:LEU:HG | 2.12 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:223:ASP:OD1 | 1:C:224:ILE:HG12 | 1.96 | 0.65 |
| 1:D:72:VAL:HG22 | 1:D:332:THR:CG2 | 2.27 | 0.65 |
| 1:D:142:ASP:O | 1:E:283:THR:HG21 | 1.97 | 0.65 |
| 1:E:77:LEU:HD22 | 1:E:455:PHE:HZ | 1.61 | 0.65 |
| 1:G:70:TYR:HE1 | 1:G:201:VAL:HA | 1.62 | 0.65 |
| 1:H:141:VAL:O | 1:H:142:ASP:HB3 | 1.96 | 0.65 |
| 1:H:166:GLY:HA2 | 1:H:195:ILE:HD11 | 1.77 | 0.65 |
| 1:I:27:TYR:CE2 | 1:I:390:TYR:HE2 | 2.15 | 0.65 |
| 1:J:463:PRO:O | 1:J:467:LYS:HG3 | 1.97 | 0.65 |
| 1:L:228:ILE:CD1 | 1:L:228:ILE:N | 2.60 | 0.65 |
| 1:M:35:TYR:CE2 | 1:M:457:ALA:HB2 | 2.31 | 0.65 |
| 1:O:323:ILE:O | 1:O:325:TRP:N | 2.28 | 0.65 |
| 1:B:373:GLN:HB3 | 1:B:464:LEU:HD12 | 1.79 | 0.65 |
| 1:C:216:ASN:OD1 | 1:C:218:SER:N | 2.29 | 0.65 |
| 1:C:440:PRO:O | 1:C:443:LYS:NZ | 2.29 | 0.65 |
| 1:D:121:PRO:CG | 1:E:289:SER:HB2 | 2.27 | 0.65 |
| 1:H:266:THR:CG2 | 1:H:266:THR:CA | 2.73 | 0.65 |
| 1:K:31:THR:CG2 | 1:K:378:LEU:O | 2.45 | 0.65 |
| 1:M:33:ILE:HB | 1:M:378:LEU:HB3 | 1.77 | 0.65 |
| 1:N:390:TYR:O | 1:N:393:SER:N | 2.30 | 0.65 |
| 1:A:92:ASN:ND2 | 1:A:95:THR:OG1 | 2.30 | 0.64 |
| 1:F:214:GLN:OE1 | 1:F:219:GLU:HB2 | 1.98 | 0.64 |
| 1:J:323:ILE:HG21 | 1:J:325:TRP:CH2 | 2.32 | 0.64 |
| 1:L:361:LYS:HA | 1:M:266:THR:HG1 | 1.62 | 0.64 |
| 1:M:201:VAL:HG23 | 1:M:202:ASP:O | 1.97 | 0.64 |
| 1:M:365:ARG:HH11 | 1:M:365:ARG:HG3 | 1.62 | 0.64 |
| 1:O:171:LYS:HG3 | 1:O:187:PRO:HD2 | 1.78 | 0.64 |
| 1:O:451:LEU:CD2 | 1:O:454:LYS:HG3 | 2.26 | 0.64 |
| 1:A:196:GLN:N | 1:A:199:ASP:OD2 | 2.30 | 0.64 |
| 1:C:188:LEU:HD11 | 1:C:213:LEU:CD1 | 2.27 | 0.64 |
| 1:F:57:ASN:HD21 | 1:F:59:LYS:H | 1.45 | 0.64 |
| 1:J:188:LEU:CD1 | 1:J:213:LEU:HD11 | 2.27 | 0.64 |
| 1:K:52:ILE:HB | 1:K:62:VAL:HB | 1.79 | 0.64 |
| 1:K:192:ASN:ND2 | 1:O:41:ARG:HH22 | 1.95 | 0.64 |
| 1:L:70:TYR:CE1 | 1:L:201:VAL:HA | 2.33 | 0.64 |
| 1:M:217:LYS:HD3 | 1:N:274:ASP:O | 1.97 | 0.64 |
| 1:N:77:LEU:HD22 | 1:N:455:PHE:CZ | 2.33 | 0.64 |
| 1:A:60:ILE:O | 1:A:60:ILE:HG13 | 1.98 | 0.64 |
| 1:B:257:VAL:HG12 | 1:B:293:PRO:HB2 | 1.79 | 0.64 |
| 1:H:24:THR:HG23 | 1:H:320:ASN:HA | 1.78 | 0.64 |
| 1:H:36:HIS:ND1 | 1:H:36:HIS:C | 2.50 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:65:VAL:HA | 1:I:69:GLN:NE2 | 2.13 | 0.64 |
| 1:I:80:PRO:O | 1:I:85:PHE:HE1 | 1.79 | 0.64 |
| 1:J:88:THR:CG2 | 1:J:88:THR:CA | 2.72 | 0.64 |
| 1:K:70:TYR:OH | 1:K:230:LYS:O | 2.10 | 0.64 |
| 1:O:156:LEU:HG | 1:O:334:VAL:HB | 1.77 | 0.64 |
| 1:A:240:GLU:OE1 | 1:A:241:PRO:HG2 | 1.98 | 0.64 |
| 1:B:80:PRO:C | 1:B:82:LYS:H | 2.01 | 0.64 |
| 1:B:391:ILE:CG2 | 1:B:391:ILE:O | 2.45 | 0.64 |
| 1:E:71:ARG:HA | 1:E:71:ARG:NH1 | 2.08 | 0.64 |
| 1:H:250:LEU:N | 1:H:250:LEU:HD12 | 2.10 | 0.64 |
| 1:I:151:TYR:CD2 | 1:I:203:THR:HB | 2.32 | 0.64 |
| 1:J:242:TYR:CD2 | 1:J:394:MET:CG | 2.71 | 0.64 |
| 1:J:307:PHE:O | 1:J:308:ASN:HB2 | 1.97 | 0.64 |
| 1:L:110:GLY:O | 1:L:111:GLN:HG2 | 1.97 | 0.64 |
| 1:N:148:SER:OG | 1:O:129:THR:HB | 1.97 | 0.64 |
| 1:N:363:TYR:CE1 | 1:O:185:CYS:HB2 | 2.31 | 0.64 |
| 1:A:54:LYS:HA | 1:A:54:LYS:NZ | 2.11 | 0.64 |
| 1:B:461:GLN:HA | 1:B:461:GLN:HE21 | 1.61 | 0.64 |
| 1:C:116:GLY:N | 1:C:339:SER:OG | 2.31 | 0.64 |
| 1:D:344:LEU:HD13 | 1:E:213:LEU:HD12 | 1.79 | 0.64 |
| 1:F:54:LYS:HG2 | 1:F:56:ASN:OD1 | 1.96 | 0.64 |
| 1:F:67:GLY:O | 1:F:68:LEU:HG | 1.97 | 0.64 |
| 1:F:158:LEU:HD23 | 1:F:249:TYR:HB2 | 1.79 | 0.64 |
| 1:G:158:LEU:HB2 | 1:G:332:THR:OG1 | 1.97 | 0.64 |
| 1:G:345:CYS:HG | 1:H:216:ASN:HB2 | 1.62 | 0.64 |
| 1:H:384:THR:HG23 | 1:H:387:VAL:CG2 | 2.28 | 0.64 |
| 1:J:391:ILE:HG21 | 1:J:402:TRP:HZ3 | 1.59 | 0.64 |
| 1:L:279:GLY:HA3 | 1:L:283:THR:O | 1.98 | 0.64 |
| 1:N:77:LEU:HD22 | 1:N:455:PHE:HZ | 1.61 | 0.64 |
| 1:N:193:THR:HG21 | 1:N:230:LYS:HD3 | 1.79 | 0.64 |
| 1:O:384:THR:H | 1:O:387:VAL:HB | 1.62 | 0.64 |
| 1:C:60:ILE:CD1 | 1:C:60:ILE:CG2 | 2.75 | 0.64 |
| 1:F:271:VAL:HG12 | 1:F:276:TYR:CE2 | 2.32 | 0.64 |
| 1:H:153:GLN:HE22 | 1:H:300:VAL:HA | 1.63 | 0.64 |
| 1:I:329:LEU:HD13 | 1:I:374:PHE:CE2 | 2.33 | 0.64 |
| 1:K:96:GLN:HB3 | 1:K:382:THR:HG22 | 1.79 | 0.64 |
| 1:L:363:TYR:CE2 | 1:M:185:CYS:HB2 | 2.33 | 0.64 |
| 1:M:147:ILE:HG22 | 1:M:148:SER:N | 2.11 | 0.64 |
| 1:M:440:PRO:O | 1:M:443:LYS:NZ | 2.30 | 0.64 |
| 1:O:317:GLN:HE21 | 1:O:317:GLN:C | 2.00 | 0.64 |
| 1:D:80:PRO:C | 1:D:82:LYS:H | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:68:LEU:HD23 | 1:F:201:VAL:HG21 | 1.80 | 0.64 |
| 1:F:344:LEU:HD21 | 1:F:365:ARG:HG2 | 1.79 | 0.64 |
| 1:G:470:LEU:HD23 | 1:G:470:LEU:O | 1.96 | 0.64 |
| 1:M:65:VAL:HA | 1:M:69:GLN:NE2 | 2.12 | 0.64 |
| 1:M:166:GLY:HA3 | 1:M:195:ILE:HD11 | 1.80 | 0.64 |
| 1:O:110:GLY:O | 1:O:111:GLN:NE2 | 2.31 | 0.64 |
| 1:O:163:PRO:N | 1:O:330:PHE:CD1 | 2.65 | 0.64 |
| 1:A:91:TYR:HD1 | 1:A:96:GLN:HG3 | 1.63 | 0.64 |
| 1:C:467:LYS:CD | 1:C:467:LYS:CB | 2.76 | 0.64 |
| 1:D:176:THR:C | 1:D:177:GLN:HG3 | 2.15 | 0.64 |
| 1:J:54:LYS:HB3 | 1:J:57:ASN:HD22 | 1.62 | 0.64 |
| 1:J:74:ARG:HG2 | 1:J:76:HIS:NE2 | 2.13 | 0.64 |
| 1:K:99:VAL:HG11 | 1:K:323:ILE:HG22 | 1.80 | 0.64 |
| 1:L:24:THR:HG21 | 1:L:323:ILE:CG1 | 2.28 | 0.64 |
| 1:L:123:LEU:O | 1:L:125:LYS:N | 2.30 | 0.64 |
| 1:M:21:VAL:O | 1:M:22:VAL:HG13 | 1.97 | 0.64 |
| 1:N:54:LYS:CB | 1:N:57:ASN:HD22 | 2.09 | 0.64 |
| 1:B:35:TYR:CE2 | 1:B:457:ALA:HB2 | 2.33 | 0.64 |
| 1:C:105:VAL:HA | 1:C:373:GLN:O | 1.98 | 0.64 |
| 1:C:114:GLY:HA2 | 1:D:255:MET:SD | 2.38 | 0.64 |
| 1:C:320:ASN:HD21 | 1:C:323:ILE:HB | 1.63 | 0.64 |
| 1:D:21:VAL:HG13 | 1:D:390:TYR:OH | 1.98 | 0.64 |
| 1:D:42:LEU:CD1 | 1:D:73:PHE:HE2 | 2.10 | 0.64 |
| 1:D:67:GLY:O | 1:D:68:LEU:HG | 1.97 | 0.64 |
| 1:D:110:GLY:O | 1:D:111:GLN:NE2 | 2.29 | 0.64 |
| 1:E:79:ASP:OD2 | 1:E:81:ASN:HB2 | 1.98 | 0.64 |
| 1:E:274:ASP:OD1 | 1:E:274:ASP:N | 2.30 | 0.64 |
| 1:F:180:VAL:CG1 | 1:F:184:ASP:CB | 2.75 | 0.64 |
| 1:F:363:TYR:CD2 | 1:G:185:CYS:HB2 | 2.32 | 0.64 |
| 1:G:280:SER:CA | 1:G:284:ALA:HB2 | 2.28 | 0.64 |
| 1:G:323:ILE:HD13 | 1:G:323:ILE:N | 2.12 | 0.64 |
| 1:I:57:ASN:HD21 | 1:I:59:LYS:H | 1.44 | 0.64 |
| 1:J:36:HIS:CG | 1:J:462:PHE:CD1 | 2.86 | 0.64 |
| 1:J:152:LYS:HB2 | 1:J:255:MET:HB2 | 1.79 | 0.64 |
| 1:J:348:ILE:HG22 | 1:J:359:ASN:OD1 | 1.98 | 0.64 |
| 1:J:444:TYR:CB | 1:J:446:PHE:CZ | 2.81 | 0.64 |
| 1:L:250:LEU:N | 1:L:250:LEU:CD1 | 2.44 | 0.64 |
| 1:M:64:LYS:CB | 1:M:64:LYS:CD | 2.75 | 0.64 |
| 1:M:320:ASN:OD1 | 1:M:321:ASN:N | 2.31 | 0.64 |
| 1:N:30:ARG:HH11 | 1:N:377:GLN:HE22 | 1.45 | 0.64 |
| 1:N:52:ILE:HB | 1:N:62:VAL:HB | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:78:PRO:HD3 | 1:C:452:LYS:HA | 1.80 | 0.64 |
| 1:E:439:ASP:O | 1:E:442:LYS:HB2 | 1.98 | 0.64 |
| 1:F:440:PRO:HA | 1:F:443:LYS:NZ | 2.12 | 0.64 |
| 1:J:49:TYR:O | 1:J:64:LYS:HE2 | 1.97 | 0.64 |
| 1:L:65:VAL:HA | 1:L:69:GLN:HE22 | 1.61 | 0.64 |
| 1:A:323:ILE:HG21 | 1:A:325:TRP:CZ2 | 2.32 | 0.63 |
| 1:B:180:VAL:CG1 | 1:B:184:ASP:HB2 | 2.28 | 0.63 |
| 1:D:66:SER:N | 1:D:69:GLN:NE2 | 2.43 | 0.63 |
| 1:G:143:ASN:O | 1:G:145:GLU:HG2 | 1.98 | 0.63 |
| 1:I:262:ASN:HD22 | 1:I:263:ARG:N | 1.95 | 0.63 |
| 1:J:81:ASN:O | 1:J:82:LYS:HG3 | 1.97 | 0.63 |
| 1:K:255:MET:HG2 | 1:K:256:PHE:N | 2.13 | 0.63 |
| 1:K:452:LYS:CD | 1:K:452:LYS:CB | 2.73 | 0.63 |
| 1:N:104:GLY:HA3 | 1:N:375:ILE:HB | 1.80 | 0.63 |
| 1:O:158:LEU:CD2 | 1:O:249:TYR:HB2 | 2.29 | 0.63 |
| 1:A:262:ASN:HD21 | 1:A:288:SER:CB | 2.08 | 0.63 |
| 1:C:54:LYS:NZ | 1:C:55:PRO:HD2 | 2.13 | 0.63 |
| 1:C:74:ARG:CG | 1:C:330:PHE:HE2 | 2.11 | 0.63 |
| 1:D:194:VAL:CG2 | 1:D:194:VAL:CA | 2.74 | 0.63 |
| 1:F:280:SER:C | 1:F:284:ALA:HB2 | 2.18 | 0.63 |
| 1:H:255:MET:HG2 | 1:H:256:PHE:N | 2.12 | 0.63 |
| 1:I:208:MET:SD | 1:I:210:PHE:HE2 | 2.21 | 0.63 |
| 1:I:363:TYR:CG | 1:J:185:CYS:HB2 | 2.34 | 0.63 |
| 1:K:266:THR:HG23 | 1:O:358:THR:HA | 1.80 | 0.63 |
| 1:N:237:MET:O | 1:N:240:GLU:HB3 | 1.98 | 0.63 |
| 1:B:325:TRP:CE2 | 1:B:394:MET:HE1 | 2.32 | 0.63 |
| 1:C:240:GLU:HG3 | 1:C:243:GLY:H | 1.62 | 0.63 |
| 1:F:250:LEU:HD22 | 1:F:306:ILE:HG23 | 1.80 | 0.63 |
| 1:F:255:MET:CE | 1:J:115:VAL:HG22 | 2.27 | 0.63 |
| 1:F:471:GLN:O | 1:F:472:LEU:OXT | 2.17 | 0.63 |
| 1:I:54:LYS:CB | 1:I:57:ASN:HD22 | 2.10 | 0.63 |
| 1:I:99:VAL:HG11 | 1:I:323:ILE:HG22 | 1.79 | 0.63 |
| 1:K:375:ILE:HG12 | 1:K:464:LEU:HD22 | 1.80 | 0.63 |
| 1:L:273:ASP:OD2 | 1:L:273:ASP:N | 2.30 | 0.63 |
| 1:A:67:GLY:H | 1:A:366:HIS:CE1 | 2.16 | 0.63 |
| 1:A:67:GLY:N | 1:A:366:HIS:HE1 | 1.95 | 0.63 |
| 1:A:363:TYR:CE2 | 1:B:185:CYS:HB2 | 2.33 | 0.63 |
| 1:D:54:LYS:CE | 1:D:55:PRO:HD2 | 2.22 | 0.63 |
| 1:D:228:ILE:N | 1:D:228:ILE:HD12 | 2.14 | 0.63 |
| 1:F:122:LEU:HD13 | 1:F:144:ARG:NH2 | 2.14 | 0.63 |
| 1:G:216:ASN:OD1 | 1:G:218:SER:C | 2.37 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:228:ILE:N | 1:G:228:ILE:HD12 | 2.13 | 0.63 |
| 1:G:230:LYS:NZ | 1:G:230:LYS:CD | 2.59 | 0.63 |
| 1:H:260:LEU:O | 1:H:261:PHE:CD2 | 2.51 | 0.63 |
| 1:K:52:ILE:HG12 | 1:L:269:GLU:CD | 2.19 | 0.63 |
| 1:K:180:VAL:HG13 | 1:K:184:ASP:HB2 | 1.80 | 0.63 |
| 1:K:342:MET:HB2 | 1:L:208:MET:CE | 2.28 | 0.63 |
| 1:L:458:ASP:OD2 | 1:L:458:ASP:N | 2.30 | 0.63 |
| 1:M:147:ILE:HA | 1:N:129:THR:O | 1.99 | 0.63 |
| 1:N:91:TYR:C | 1:N:91:TYR:CD2 | 2.69 | 0.63 |
| 1:O:54:LYS:HG3 | 1:O:55:PRO:CD | 2.28 | 0.63 |
| 1:D:43:LEU:HD12 | 1:D:369:GLU:HA | 1.79 | 0.63 |
| 1:F:248:PHE:CZ | 1:F:311:TYR:HB3 | 2.33 | 0.63 |
| 1:F:280:SER:N | 1:F:284:ALA:HB2 | 2.14 | 0.63 |
| 1:G:29:ALA:HB3 | 1:G:380:LYS:O | 1.98 | 0.63 |
| 1:H:162:LYS:C | 1:H:330:PHE:HD1 | 2.02 | 0.63 |
| 1:I:358:THR:CG2 | 1:J:266:THR:HG22 | 2.28 | 0.63 |
| 1:J:103:VAL:HA | 1:J:313:LEU:HB2 | 1.80 | 0.63 |
| 1:K:220:VAL:O | 1:K:221:PRO:O | 2.16 | 0.63 |
| 1:L:461:GLN:HE22 | 1:M:21:VAL:HG23 | 1.64 | 0.63 |
| 1:M:220:VAL:O | 1:M:221:PRO:C | 2.35 | 0.63 |
| 1:B:105:VAL:HG11 | 1:B:159:ILE:CD1 | 2.29 | 0.63 |
| 1:B:467:LYS:CD | 1:B:467:LYS:CB | 2.72 | 0.63 |
| 1:E:75:ILE:CG2 | 1:E:451:LEU:HD12 | 2.28 | 0.63 |
| 1:E:80:PRO:HG2 | 1:E:98:LEU:O | 1.99 | 0.63 |
| 1:G:193:THR:CG2 | 1:G:230:LYS:HD3 | 2.28 | 0.63 |
| 1:H:188:LEU:HD13 | 1:H:213:LEU:HD11 | 1.80 | 0.63 |
| 1:I:33:ILE:HB | 1:I:378:LEU:HB3 | 1.79 | 0.63 |
| 1:I:151:TYR:OH | 1:I:221:PRO:HB2 | 1.99 | 0.63 |
| 1:I:397:THR:HB | 1:I:401:ASP:OD2 | 1.99 | 0.63 |
| 1:J:242:TYR:CE2 | 1:J:394:MET:CB | 2.82 | 0.63 |
| 1:K:29:ALA:HB3 | 1:K:380:LYS:O | 1.99 | 0.63 |
| 1:K:363:TYR:CD2 | 1:L:185:CYS:HB2 | 2.33 | 0.63 |
| 1:M:262:ASN:C | 1:M:262:ASN:ND2 | 2.51 | 0.63 |
| 1:D:196:GLN:NE2 | 1:D:444:TYR:HD2 | 1.96 | 0.63 |
| 1:D:464:LEU:O | 1:D:464:LEU:HD23 | 1.98 | 0.63 |
| 1:G:115:VAL:HG21 | 1:H:257:VAL:HG13 | 1.81 | 0.63 |
| 1:J:75:ILE:HG21 | 1:J:451:LEU:HD12 | 1.81 | 0.63 |
| 1:K:153:GLN:HE22 | 1:K:300:VAL:HA | 1.63 | 0.63 |
| 1:K:266:THR:CG2 | 1:K:266:THR:CA | 2.72 | 0.63 |
| 1:A:345:CYS:SG | 1:B:216:ASN:CB | 2.80 | 0.63 |
| 1:B:391:ILE:HG22 | 1:B:399:LEU:CD2 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:170:GLY:O | 1:D:188:LEU:HA | 1.98 | 0.63 |
| 1:E:471:GLN:OE1 | 1:E:472:LEU:N | 2.32 | 0.63 |
| 1:I:378:LEU:HD12 | 1:I:379:CYS:H | 1.62 | 0.63 |
| 1:J:459:LEU:HB3 | 1:J:465:GLY:HA3 | 1.81 | 0.63 |
| 1:K:159:ILE:CD1 | 1:K:159:ILE:CB | 2.74 | 0.63 |
| 1:L:92:ASN:C | 1:L:94:ASP:H | 2.02 | 0.63 |
| 1:N:250:LEU:N | 1:N:250:LEU:HD12 | 2.14 | 0.63 |
| 1:A:381:ILE:CG2 | 1:A:381:ILE:CA | 2.74 | 0.63 |
| 1:C:30:ARG:HH11 | 1:C:377:GLN:HE22 | 1.45 | 0.63 |
| 1:C:185:CYS:SG | 1:C:186:PRO:HD2 | 2.39 | 0.63 |
| 1:D:52:ILE:HB | 1:D:62:VAL:HB | 1.81 | 0.63 |
| 1:F:176:THR:C | 1:F:177:GLN:HG3 | 2.19 | 0.63 |
| 1:G:96:GLN:HE21 | 1:G:382:THR:HG23 | 1.64 | 0.63 |
| 1:H:141:VAL:O | 1:H:142:ASP:CB | 2.41 | 0.63 |
| 1:J:60:ILE:O | 1:J:60:ILE:HG13 | 1.97 | 0.63 |
| 1:K:49:TYR:HA | 1:K:223:ASP:HB3 | 1.81 | 0.63 |
| 1:L:36:HIS:ND1 | 1:L:37:ALA:N | 2.46 | 0.63 |
| 1:N:365:ARG:NH2 | 1:O:269:GLU:OE1 | 2.32 | 0.63 |
| 1:O:375:ILE:HG21 | 1:O:468:PHE:CD2 | 2.33 | 0.63 |
| 1:C:77:LEU:CD2 | 1:C:77:LEU:HG | 2.14 | 0.62 |
| 1:D:107:VAL:HG21 | 1:D:157:CYS:SG | 2.39 | 0.62 |
| 1:F:240:GLU:HG3 | 1:F:243:GLY:HA2 | 1.81 | 0.62 |
| 1:G:36:HIS:CG | 1:G:462:PHE:CD1 | 2.87 | 0.62 |
| 1:H:69:GLN:HA | 1:H:199:ASP:O | 1.98 | 0.62 |
| 1:I:193:THR:CG2 | 1:I:193:THR:N | 2.61 | 0.62 |
| 1:J:325:TRP:HB3 | 1:J:398:ILE:HD12 | 1.79 | 0.62 |
| 1:K:443:LYS:N | 1:K:443:LYS:CD | 2.56 | 0.62 |
| 1:M:113:LEU:N | 1:M:113:LEU:HD12 | 2.14 | 0.62 |
| 1:M:395:ASN:HB3 | 1:M:398:ILE:CG1 | 2.28 | 0.62 |
| 1:O:45:VAL:C | 1:O:65:VAL:HG21 | 2.19 | 0.62 |
| 1:A:64:LYS:CG | 1:A:64:LYS:CE | 2.77 | 0.62 |
| 1:A:75:ILE:HB | 1:A:329:LEU:HB3 | 1.80 | 0.62 |
| 1:B:21:VAL:HG13 | 1:B:390:TYR:OH | 1.99 | 0.62 |
| 1:B:57:ASN:ND2 | 1:B:59:LYS:H | 1.97 | 0.62 |
| 1:B:150:ASP:OD2 | 1:B:150:ASP:N | 2.33 | 0.62 |
| 1:C:81:ASN:ND2 | 1:C:402:TRP:HD1 | 1.97 | 0.62 |
| 1:F:257:VAL:HG21 | 1:J:150:ASP:HB3 | 1.81 | 0.62 |
| 1:G:46:GLY:HA3 | 1:G:63:PRO:O | 1.98 | 0.62 |
| 1:K:266:THR:CG2 | 1:K:266:THR:HB | 2.16 | 0.62 |
| 1:M:141:VAL:HG12 | 1:M:142:ASP:N | 2.14 | 0.62 |
| 1:M:149:MET:HE3 | 1:M:294:THR:HG22 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:217:LYS:HG2 | 1:O:276:TYR:HA | 1.81 | 0.62 |
| 1:N:343:SER:HB3 | 1:N:364:LEU:HD23 | 1.80 | 0.62 |
| 1:N:384:THR:H | 1:N:387:VAL:HB | 1.64 | 0.62 |
| 1:A:99:VAL:HG11 | 1:A:323:ILE:CG2 | 2.29 | 0.62 |
| 1:E:395:ASN:HB3 | 1:E:398:ILE:HG12 | 1.80 | 0.62 |
| 1:F:255:MET:SD | 1:J:115:VAL:HG22 | 2.38 | 0.62 |
| 1:J:71:ARG:HH11 | 1:J:71:ARG:CA | 2.13 | 0.62 |
| 1:J:79:ASP:HA | 1:J:327:ASN:HD21 | 1.65 | 0.62 |
| 1:L:180:VAL:HG13 | 1:L:184:ASP:CB | 2.28 | 0.62 |
| 1:M:71:ARG:NH1 | 1:M:197:ASP:OD1 | 2.32 | 0.62 |
| 1:A:117:ILE:HG21 | 1:B:293:PRO:HD3 | 1.81 | 0.62 |
| 1:B:96:GLN:HE21 | 1:B:382:THR:HG23 | 1.63 | 0.62 |
| 1:D:73:PHE:N | 1:D:73:PHE:CD1 | 2.66 | 0.62 |
| 1:D:262:ASN:HD21 | 1:D:288:SER:HB3 | 1.64 | 0.62 |
| 1:E:160:GLY:O | 1:E:329:LEU:HD23 | 2.00 | 0.62 |
| 1:F:66:SER:N | 1:F:69:GLN:NE2 | 2.48 | 0.62 |
| 1:F:112:PRO:HD3 | 1:G:231:TYR:CD2 | 2.34 | 0.62 |
| 1:I:79:ASP:OD2 | 1:I:81:ASN:HB2 | 1.99 | 0.62 |
| 1:I:142:ASP:O | 1:J:283:THR:HG21 | 1.98 | 0.62 |
| 1:I:259:HIS:CE1 | 1:J:130:GLU:HG2 | 2.35 | 0.62 |
| 1:K:48:PRO:HB3 | 1:K:341:ASN:HD22 | 1.64 | 0.62 |
| 1:L:440:PRO:O | 1:L:443:LYS:NZ | 2.32 | 0.62 |
| 1:M:305:GLN:HE22 | 1:M:337:THR:HG21 | 1.64 | 0.62 |
| 1:N:220:VAL:O | 1:N:221:PRO:C | 2.37 | 0.62 |
| 1:N:390:TYR:C | 1:N:392:HIS:N | 2.50 | 0.62 |
| 1:A:34:TYR:CE2 | 1:A:377:GLN:CG | 2.72 | 0.62 |
| 1:F:451:LEU:O | 1:F:454:LYS:HB2 | 1.99 | 0.62 |
| 1:H:176:THR:O | 1:H:177:GLN:HG2 | 1.99 | 0.62 |
| 1:I:85:PHE:CE2 | 1:I:378:LEU:HD22 | 2.34 | 0.62 |
| 1:I:237:MET:O | 1:I:240:GLU:HB3 | 1.99 | 0.62 |
| 1:K:308:ASN:HD22 | 1:L:251:ARG:HH22 | 1.47 | 0.62 |
| 1:L:21:VAL:HG12 | 1:L:22:VAL:N | 2.14 | 0.62 |
| 1:M:27:TYR:CE2 | 1:M:390:TYR:CE2 | 2.87 | 0.62 |
| 1:M:74:ARG:CZ | 1:M:441:LEU:CD1 | 2.76 | 0.62 |
| 1:N:259:HIS:HE1 | 1:O:130:GLU:CG | 2.12 | 0.62 |
| 1:O:74:ARG:NH2 | 1:O:441:LEU:HD12 | 2.14 | 0.62 |
| 1:A:125:LYS:NZ | 1:B:132:ALA:O | 2.30 | 0.62 |
| 1:C:77:LEU:CD2 | 1:C:77:LEU:CB | 2.75 | 0.62 |
| 1:C:92:ASN:ND2 | 1:C:95:THR:OG1 | 2.32 | 0.62 |
| 1:C:471:GLN:OE1 | 1:C:472:LEU:N | 2.32 | 0.62 |
| 1:E:280:SER:N | 1:E:284:ALA:HB2 | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:373:GLN:HB3 | 1:E:464:LEU:HD12 | 1.81 | 0.62 |
| 1:F:61:LEU:HD12 | 1:F:61:LEU:O | 1.98 | 0.62 |
| 1:G:54:LYS:CB | 1:G:57:ASN:HD22 | 2.13 | 0.62 |
| 1:G:463:PRO:HB3 | 1:G:466:ARG:NH2 | 2.15 | 0.62 |
| 1:I:220:VAL:HB | 1:I:224:ILE:HD12 | 1.80 | 0.62 |
| 1:J:107:VAL:HG23 | 1:J:311:TYR:CE1 | 2.34 | 0.62 |
| 1:K:29:ALA:HB3 | 1:K:380:LYS:HG3 | 1.81 | 0.62 |
| 1:K:290:ASN:HA | 1:O:364:LEU:HD11 | 1.82 | 0.62 |
| 1:M:348:ILE:HG22 | 1:M:359:ASN:OD1 | 1.99 | 0.62 |
| 1:N:381:ILE:O | 1:N:381:ILE:HG22 | 2.00 | 0.62 |
| 1:O:443:LYS:H | 1:O:443:LYS:CD | 2.13 | 0.62 |
| 1:D:73:PHE:N | 1:D:331:VAL:O | 2.30 | 0.62 |
| 1:D:167:GLU:O | 1:D:168:HIS:HB3 | 1.99 | 0.62 |
| 1:E:266:THR:O | 1:E:267:VAL:C | 2.36 | 0.62 |
| 1:E:397:THR:HB | 1:E:401:ASP:OD2 | 1.99 | 0.62 |
| 1:F:96:GLN:CA | 1:F:383:LEU:HD12 | 2.29 | 0.62 |
| 1:F:153:GLN:NE2 | 1:F:300:VAL:HG12 | 2.14 | 0.62 |
| 1:F:358:THR:HG22 | 1:G:266:THR:HG22 | 1.80 | 0.62 |
| 1:I:36:HIS:ND1 | 1:I:36:HIS:C | 2.52 | 0.62 |
| 1:J:163:PRO:HG2 | 1:J:163:PRO:O | 2.00 | 0.62 |
| 1:L:54:LYS:HE3 | 1:L:55:PRO:HD2 | 1.81 | 0.62 |
| 1:C:117:ILE:HG13 | 1:C:149:MET:O | 2.00 | 0.62 |
| 1:C:158:LEU:CD2 | 1:C:249:TYR:HB2 | 2.29 | 0.62 |
| 1:C:237:MET:HB3 | 1:C:246:LEU:CD2 | 2.29 | 0.62 |
| 1:E:178:VAL:CG1 | 1:E:178:VAL:CG2 | 2.76 | 0.62 |
| 1:G:250:LEU:HD12 | 1:G:250:LEU:H | 1.63 | 0.62 |
| 1:H:44:ALA:HB3 | 1:H:368:GLU:HB2 | 1.80 | 0.62 |
| 1:I:97:ARG:HH11 | 1:I:97:ARG:HA | 1.63 | 0.62 |
| 1:J:262:ASN:HD21 | 1:J:288:SER:HB3 | 1.64 | 0.62 |
| 1:L:53:LYS:HD3 | 1:L:58:ASN:HA | 1.82 | 0.62 |
| 1:L:105:VAL:HG11 | 1:L:159:ILE:HD11 | 1.81 | 0.62 |
| 1:M:344:LEU:CD1 | 1:N:188:LEU:HD21 | 2.30 | 0.62 |
| 1:A:27:TYR:CE2 | 1:A:390:TYR:HE2 | 2.18 | 0.62 |
| 1:A:115:VAL:HG22 | 1:B:255:MET:SD | 2.40 | 0.62 |
| 1:C:122:LEU:HD13 | 1:C:144:ARG:NH2 | 2.14 | 0.62 |
| 1:C:391:ILE:O | 1:C:391:ILE:HG22 | 1.99 | 0.62 |
| 1:D:66:SER:N | 1:D:69:GLN:HE21 | 1.98 | 0.62 |
| 1:F:122:LEU:HD11 | 1:G:286:LEU:HD11 | 1.82 | 0.62 |
| 1:G:54:LYS:CG | 1:G:55:PRO:HD2 | 2.26 | 0.62 |
| 1:H:302:SER:HB2 | 1:I:253:GLU:H | 1.64 | 0.62 |
| 1:H:384:THR:H | 1:H:387:VAL:HB | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:208:MET:SD | 1:J:210:PHE:HE2 | 2.22 | 0.62 |
| 1:L:28:VAL:HA | 1:L:381:ILE:HG12 | 1.81 | 0.62 |
| 1:N:115:VAL:HG21 | 1:O:257:VAL:HG13 | 1.81 | 0.62 |
| 1:A:49:TYR:HE2 | 1:A:118:SER:HA | 1.65 | 0.62 |
| 1:B:33:ILE:CD1 | 1:B:33:ILE:HG23 | 2.29 | 0.62 |
| 1:B:72:VAL:HG21 | 1:B:195:ILE:O | 2.00 | 0.62 |
| 1:C:464:LEU:C | 1:C:464:LEU:HD22 | 2.20 | 0.62 |
| 1:D:54:LYS:CG | 1:D:57:ASN:HB3 | 2.30 | 0.62 |
| 1:D:159:ILE:HG22 | 1:D:247:PHE:CE1 | 2.35 | 0.62 |
| 1:E:151:TYR:CG | 1:E:203:THR:HB | 2.33 | 0.62 |
| 1:G:65:VAL:HA | 1:G:69:GLN:NE2 | 2.14 | 0.62 |
| 1:I:260:LEU:HD12 | 1:I:260:LEU:N | 2.14 | 0.62 |
| 1:I:316:ALA:HB3 | 1:I:321:ASN:OD1 | 1.99 | 0.62 |
| 1:J:54:LYS:HA | 1:J:54:LYS:HZ3 | 1.64 | 0.62 |
| 1:K:79:ASP:OD2 | 1:K:82:LYS:HG3 | 2.00 | 0.62 |
| 1:K:152:LYS:CB | 1:K:255:MET:HB2 | 2.24 | 0.62 |
| 1:K:323:ILE:HG21 | 1:K:325:TRP:CZ3 | 2.35 | 0.62 |
| 1:L:23:SER:OG | 1:L:25:ASP:HB2 | 2.00 | 0.62 |
| 1:N:139:ALA:O | 1:N:140:GLY:O | 2.18 | 0.62 |
| 1:O:54:LYS:HB2 | 1:O:57:ASN:HD22 | 1.63 | 0.62 |
| 1:O:323:ILE:HD13 | 1:O:323:ILE:N | 2.15 | 0.62 |
| 1:B:92:ASN:ND2 | 1:B:95:THR:OG1 | 2.33 | 0.61 |
| 1:D:30:ARG:NH1 | 1:D:377:GLN:NE2 | 2.44 | 0.61 |
| 1:E:165:ILE:O | 1:E:165:ILE:HG22 | 1.98 | 0.61 |
| 1:E:262:ASN:HD21 | 1:E:288:SER:HB3 | 1.65 | 0.61 |
| 1:F:365:ARG:CD | 1:F:365:ARG:CB | 2.73 | 0.61 |
| 1:G:149:MET:HE3 | 1:G:295:PRO:HD2 | 1.82 | 0.61 |
| 1:I:159:ILE:HD12 | 1:I:248:PHE:CD2 | 2.35 | 0.61 |
| 1:J:33:ILE:HB | 1:J:378:LEU:HB3 | 1.81 | 0.61 |
| 1:J:163:PRO:N | 1:J:330:PHE:CD1 | 2.68 | 0.61 |
| 1:K:193:THR:OG1 | 1:K:194:VAL:N | 2.33 | 0.61 |
| 1:L:54:LYS:CB | 1:L:57:ASN:HD22 | 2.14 | 0.61 |
| 1:L:74:ARG:CG | 1:L:330:PHE:HE2 | 2.12 | 0.61 |
| 1:M:46:GLY:HA3 | 1:M:63:PRO:O | 1.99 | 0.61 |
| 1:M:69:GLN:HA | 1:M:199:ASP:O | 2.00 | 0.61 |
| 1:M:172:GLY:O | 1:M:173:SER:C | 2.38 | 0.61 |
| 1:N:367:GLY:O | 1:N:368:GLU:HG2 | 2.00 | 0.61 |
| 1:O:24:THR:HG21 | 1:O:320:ASN:HA | 1.81 | 0.61 |
| 1:A:248:PHE:CZ | 1:A:311:TYR:HB3 | 2.35 | 0.61 |
| 1:C:171:LYS:HA | 1:C:187:PRO:O | 1.98 | 0.61 |
| 1:C:255:MET:CG | 1:C:256:PHE:N | 2.63 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:384:THR:HG23 | 1:D:387:VAL:CG2 | 2.30 | 0.61 |
| 1:E:389:THR:CG2 | 1:E:389:THR:HB | 2.13 | 0.61 |
| 1:F:365:ARG:CD | 1:F:365:ARG:CA | 2.77 | 0.61 |
| 1:G:96:GLN:HB3 | 1:G:382:THR:CG2 | 2.29 | 0.61 |
| 1:H:57:ASN:HD21 | 1:H:59:LYS:CB | 2.13 | 0.61 |
| 1:J:67:GLY:C | 1:J:68:LEU:HG | 2.19 | 0.61 |
| 1:L:344:LEU:CD1 | 1:M:186:PRO:HD2 | 2.29 | 0.61 |
| 1:M:114:GLY:HA2 | 1:N:255:MET:SD | 2.40 | 0.61 |
| 1:N:149:MET:HA | 1:O:260:LEU:HD21 | 1.81 | 0.61 |
| 1:D:54:LYS:HB2 | 1:D:57:ASN:HD22 | 1.65 | 0.61 |
| 1:D:80:PRO:HD2 | 1:D:81:ASN:H | 1.64 | 0.61 |
| 1:D:141:VAL:CG1 | 1:D:142:ASP:N | 2.59 | 0.61 |
| 1:E:30:ARG:HD3 | 1:E:377:GLN:HE22 | 1.65 | 0.61 |
| 1:E:235:ILE:CD1 | 1:E:235:ILE:CB | 2.73 | 0.61 |
| 1:F:274:ASP:N | 1:F:274:ASP:OD1 | 2.32 | 0.61 |
| 1:J:91:TYR:OH | 1:J:97:ARG:NH2 | 2.33 | 0.61 |
| 1:L:312:TRP:CH2 | 1:L:468:PHE:HB2 | 2.35 | 0.61 |
| 1:L:373:GLN:HB3 | 1:L:464:LEU:HD12 | 1.82 | 0.61 |
| 1:M:27:TYR:CE2 | 1:M:390:TYR:HE2 | 2.18 | 0.61 |
| 1:M:115:VAL:HG22 | 1:N:255:MET:CE | 2.31 | 0.61 |
| 1:N:21:VAL:HG12 | 1:N:22:VAL:N | 2.15 | 0.61 |
| 1:N:65:VAL:O | 1:N:366:HIS:HB3 | 2.00 | 0.61 |
| 1:O:442:LYS:NZ | 1:O:442:LYS:CG | 2.64 | 0.61 |
| 1:A:381:ILE:CG2 | 1:A:381:ILE:HB | 2.14 | 0.61 |
| 1:A:397:THR:HB | 1:A:401:ASP:OD2 | 2.00 | 0.61 |
| 1:B:66:SER:O | 1:B:69:GLN:HG3 | 2.00 | 0.61 |
| 1:B:126:LEU:HB3 | 1:B:262:ASN:HB3 | 1.82 | 0.61 |
| 1:D:49:TYR:HA | 1:D:223:ASP:HB3 | 1.81 | 0.61 |
| 1:G:24:THR:CG2 | 1:G:320:ASN:HA | 2.30 | 0.61 |
| 1:H:124:ASN:OD1 | 1:H:264:ALA:N | 2.33 | 0.61 |
| 1:J:54:LYS:CB | 1:J:57:ASN:HD22 | 2.13 | 0.61 |
| 1:J:163:PRO:HB3 | 1:J:330:PHE:CE1 | 2.36 | 0.61 |
| 1:K:306:ILE:HD13 | 1:K:306:ILE:N | 2.15 | 0.61 |
| 1:M:74:ARG:HH22 | 1:M:441:LEU:HD12 | 1.58 | 0.61 |
| 1:M:250:LEU:HD12 | 1:M:250:LEU:H | 1.65 | 0.61 |
| 1:N:70:TYR:OH | 1:N:232:PRO:HD3 | 2.00 | 0.61 |
| 1:O:30:ARG:HH11 | 1:O:377:GLN:HE22 | 1.48 | 0.61 |
| 1:A:21:VAL:HB | 1:E:461:GLN:HE22 | 1.64 | 0.61 |
| 1:A:63:PRO:O | 1:A:65:VAL:HG23 | 2.01 | 0.61 |
| 1:D:80:PRO:CD | 1:D:81:ASN:H | 2.14 | 0.61 |
| 1:D:464:LEU:O | 1:D:464:LEU:CD2 | 2.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:167:GLU:HG3 | 1:E:231:TYR:O | 2.00 | 0.61 |
| 1:E:172:GLY:O | 1:E:173:SER:O | 2.19 | 0.61 |
| 1:F:274:ASP:O | 1:J:217:LYS:HD3 | 2.00 | 0.61 |
| 1:G:96:GLN:HE21 | 1:G:382:THR:CG2 | 2.13 | 0.61 |
| 1:G:255:MET:CG | 1:G:256:PHE:N | 2.60 | 0.61 |
| 1:H:104:GLY:HA3 | 1:H:375:ILE:HB | 1.82 | 0.61 |
| 1:H:137:ALA:O | 1:H:138:ASN:O | 2.19 | 0.61 |
| 1:I:344:LEU:HD11 | 1:J:185:CYS:SG | 2.41 | 0.61 |
| 1:I:399:LEU:O | 1:I:402:TRP:HB2 | 1.99 | 0.61 |
| 1:J:166:GLY:CA | 1:J:195:ILE:HD11 | 2.30 | 0.61 |
| 1:K:57:ASN:HD21 | 1:K:59:LYS:HB3 | 1.64 | 0.61 |
| 1:K:109:ARG:NH1 | 1:K:370:TYR:CE1 | 2.68 | 0.61 |
| 1:K:254:GLN:HA | 1:O:300:VAL:O | 2.00 | 0.61 |
| 1:L:320:ASN:OD1 | 1:L:321:ASN:N | 2.34 | 0.61 |
| 1:M:323:ILE:HG21 | 1:M:325:TRP:CZ2 | 2.34 | 0.61 |
| 1:B:44:ALA:HB3 | 1:B:368:GLU:HB2 | 1.81 | 0.61 |
| 1:B:358:THR:HA | 1:C:266:THR:CG2 | 2.30 | 0.61 |
| 1:C:355:TYR:CD1 | 1:D:144:ARG:HD3 | 2.35 | 0.61 |
| 1:C:375:ILE:CG1 | 1:C:464:LEU:HD13 | 2.31 | 0.61 |
| 1:F:175:CYS:SG | 1:F:175:CYS:CA | 2.87 | 0.61 |
| 1:I:42:LEU:HD13 | 1:I:447:TRP:CE2 | 2.35 | 0.61 |
| 1:O:237:MET:HB3 | 1:O:246:LEU:CD2 | 2.30 | 0.61 |
| 1:O:331:VAL:CG1 | 1:O:331:VAL:HB | 2.18 | 0.61 |
| 1:A:323:ILE:HG21 | 1:A:325:TRP:CH2 | 2.35 | 0.61 |
| 1:B:110:GLY:C | 1:B:111:GLN:HG2 | 2.20 | 0.61 |
| 1:B:219:GLU:C | 1:B:220:VAL:HG13 | 2.21 | 0.61 |
| 1:C:122:LEU:HD11 | 1:D:286:LEU:HD11 | 1.83 | 0.61 |
| 1:C:151:TYR:CG | 1:C:203:THR:HB | 2.35 | 0.61 |
| 1:D:80:PRO:C | 1:D:82:LYS:N | 2.54 | 0.61 |
| 1:H:300:VAL:O | 1:I:254:GLN:HA | 1.99 | 0.61 |
| 1:I:82:LYS:CD | 1:I:82:LYS:NZ | 2.61 | 0.61 |
| 1:K:117:ILE:HD11 | 1:L:260:LEU:HD23 | 1.81 | 0.61 |
| 1:L:227:SER:C | 1:L:228:ILE:HD12 | 2.20 | 0.61 |
| 1:L:298:SER:OG | 1:L:299:MET:N | 2.33 | 0.61 |
| 1:N:344:LEU:HD12 | 1:O:186:PRO:HD2 | 1.83 | 0.61 |
| 1:O:71:ARG:HH12 | 1:O:198:GLY:N | 1.97 | 0.61 |
| 1:A:163:PRO:N | 1:A:330:PHE:CD1 | 2.69 | 0.61 |
| 1:D:98:LEU:HD22 | 1:D:379:CYS:O | 2.00 | 0.61 |
| 1:G:219:GLU:HB3 | 1:G:263:ARG:NH2 | 2.16 | 0.61 |
| 1:K:219:GLU:C | 1:K:220:VAL:HG13 | 2.21 | 0.61 |
| 1:L:374:PHE:O | 1:L:375:ILE:HD13 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:323:ILE:HD13 | 1:M:323:ILE:CA | 2.30 | 0.61 |
| 1:N:96:GLN:NE2 | 1:N:382:THR:CG2 | 2.63 | 0.61 |
| 1:O:117:ILE:CD1 | 1:O:117:ILE:CB | 2.72 | 0.61 |
| 1:A:280:SER:CA | 1:A:284:ALA:HB2 | 2.31 | 0.61 |
| 1:A:345:CYS:HG | 1:B:216:ASN:HB2 | 1.66 | 0.61 |
| 1:B:208:MET:SD | 1:B:210:PHE:CE2 | 2.94 | 0.61 |
| 1:B:391:ILE:O | 1:B:391:ILE:HG22 | 1.99 | 0.61 |
| 1:D:36:HIS:CG | 1:D:462:PHE:CD1 | 2.89 | 0.61 |
| 1:E:24:THR:HG23 | 1:E:320:ASN:HA | 1.83 | 0.61 |
| 1:E:70:TYR:O | 1:E:71:ARG:NH1 | 2.34 | 0.61 |
| 1:F:121:PRO:HG3 | 1:G:289:SER:HB2 | 1.83 | 0.61 |
| 1:I:157:CYS:HB3 | 1:I:250:LEU:CD1 | 2.31 | 0.61 |
| 1:I:208:MET:SD | 1:I:210:PHE:CE2 | 2.94 | 0.61 |
| 1:I:281:GLY:O | 1:I:284:ALA:N | 2.30 | 0.61 |
| 1:J:163:PRO:HD3 | 1:J:330:PHE:CE1 | 2.31 | 0.61 |
| 1:N:54:LYS:HG2 | 1:N:56:ASN:OD1 | 2.00 | 0.61 |
| 1:N:216:ASN:ND2 | 1:N:219:GLU:OE2 | 2.34 | 0.61 |
| 1:E:344:LEU:HD21 | 1:E:365:ARG:CG | 2.31 | 0.61 |
| 1:G:147:ILE:HG22 | 1:G:148:SER:N | 2.15 | 0.61 |
| 1:H:223:ASP:OD1 | 1:H:224:ILE:N | 2.34 | 0.61 |
| 1:I:126:LEU:HB3 | 1:I:262:ASN:HB3 | 1.82 | 0.61 |
| 1:K:166:GLY:CA | 1:K:195:ILE:HD11 | 2.31 | 0.61 |
| 1:L:463:PRO:HG2 | 1:L:464:LEU:H | 1.66 | 0.61 |
| 1:M:169:TRP:H | 1:M:208:MET:HA | 1.66 | 0.61 |
| 1:O:149:MET:HE1 | 1:O:294:THR:HG22 | 1.82 | 0.61 |
| 1:A:357:ASN:HB2 | 1:B:141:VAL:HA | 1.83 | 0.60 |
| 1:B:299:MET:HA | 1:C:256:PHE:HB3 | 1.83 | 0.60 |
| 1:D:159:ILE:HD12 | 1:D:248:PHE:HD2 | 1.65 | 0.60 |
| 1:D:344:LEU:HD13 | 1:E:213:LEU:HD13 | 1.83 | 0.60 |
| 1:F:217:LYS:O | 1:G:276:TYR:HA | 2.01 | 0.60 |
| 1:G:361:LYS:CA | 1:H:266:THR:OG1 | 2.45 | 0.60 |
| 1:H:172:GLY:O | 1:H:173:SER:C | 2.40 | 0.60 |
| 1:L:248:PHE:CZ | 1:L:311:TYR:HB3 | 2.36 | 0.60 |
| 1:M:154:THR:O | 1:M:336:THR:HG23 | 2.01 | 0.60 |
| 1:M:378:LEU:HD12 | 1:M:379:CYS:H | 1.66 | 0.60 |
| 1:O:130:GLU:HB2 | 1:O:260:LEU:HD13 | 1.82 | 0.60 |
| 1:A:75:ILE:CG2 | 1:A:451:LEU:HD12 | 2.26 | 0.60 |
| 1:A:257:VAL:HG13 | 1:E:115:VAL:CG2 | 2.31 | 0.60 |
| 1:A:276:TYR:HA | 1:E:217:LYS:HG2 | 1.82 | 0.60 |
| 1:E:83:PHE:HD2 | 1:E:85:PHE:CE2 | 2.19 | 0.60 |
| 1:E:119:GLY:HA3 | 1:E:148:SER:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:117:ILE:N | 1:F:117:ILE:HG22 | 2.16 | 0.60 |
| 1:H:123:LEU:HD23 | 1:H:147:ILE:HB | 1.81 | 0.60 |
| 1:I:101:ALA:HB3 | 1:I:377:GLN:O | 2.01 | 0.60 |
| 1:I:322:GLY:C | 1:I:323:ILE:HD13 | 2.21 | 0.60 |
| 1:K:99:VAL:HG11 | 1:K:323:ILE:CG2 | 2.31 | 0.60 |
| 1:L:464:LEU:HD23 | 1:L:464:LEU:C | 2.21 | 0.60 |
| 1:M:241:PRO:HG2 | 1:M:242:TYR:H | 1.66 | 0.60 |
| 1:M:299:MET:HE2 | 1:N:298:SER:HB2 | 1.83 | 0.60 |
| 1:M:383:LEU:CD2 | 1:M:388:MET:CE | 2.79 | 0.60 |
| 1:O:24:THR:O | 1:O:25:ASP:C | 2.38 | 0.60 |
| 1:O:442:LYS:NZ | 1:O:442:LYS:CD | 2.64 | 0.60 |
| 1:B:24:THR:HA | 1:B:27:TYR:CE2 | 2.37 | 0.60 |
| 1:B:29:ALA:HB3 | 1:B:380:LYS:O | 2.02 | 0.60 |
| 1:C:250:LEU:HD12 | 1:C:250:LEU:O | 2.01 | 0.60 |
| 1:D:122:LEU:HD13 | 1:D:144:ARG:NH2 | 2.16 | 0.60 |
| 1:G:43:LEU:HD12 | 1:G:368:GLU:O | 2.02 | 0.60 |
| 1:G:178:VAL:O | 1:G:180:VAL:N | 2.22 | 0.60 |
| 1:H:79:ASP:OD2 | 1:H:81:ASN:HB2 | 2.02 | 0.60 |
| 1:H:82:LYS:NZ | 1:H:403:ASN:HD22 | 1.99 | 0.60 |
| 1:H:109:ARG:NH1 | 1:H:370:TYR:CE1 | 2.69 | 0.60 |
| 1:H:180:VAL:HG13 | 1:H:184:ASP:CB | 2.30 | 0.60 |
| 1:H:365:ARG:NH2 | 1:I:269:GLU:OE1 | 2.34 | 0.60 |
| 1:I:375:ILE:HG12 | 1:I:464:LEU:HD13 | 1.83 | 0.60 |
| 1:K:96:GLN:HA | 1:K:382:THR:HA | 1.83 | 0.60 |
| 1:L:21:VAL:HG13 | 1:L:390:TYR:OH | 2.01 | 0.60 |
| 1:L:142:ASP:OD2 | 1:L:144:ARG:HG3 | 2.00 | 0.60 |
| 1:L:217:LYS:HG2 | 1:M:276:TYR:HA | 1.83 | 0.60 |
| 1:N:240:GLU:HG3 | 1:N:243:GLY:H | 1.66 | 0.60 |
| 1:A:82:LYS:NZ | 1:A:82:LYS:CD | 2.64 | 0.60 |
| 1:C:54:LYS:CB | 1:C:57:ASN:HD22 | 2.14 | 0.60 |
| 1:C:79:ASP:HA | 1:C:327:ASN:HD21 | 1.66 | 0.60 |
| 1:C:228:ILE:HD12 | 1:C:228:ILE:N | 2.16 | 0.60 |
| 1:C:374:PHE:HB2 | 1:C:376:PHE:CE1 | 2.36 | 0.60 |
| 1:D:61:LEU:HG | 1:D:62:VAL:HG23 | 1.83 | 0.60 |
| 1:I:193:THR:HG23 | 1:I:230:LYS:HD2 | 1.83 | 0.60 |
| 1:J:27:TYR:O | 1:J:381:ILE:HG23 | 2.02 | 0.60 |
| 1:J:47:HIS:CE1 | 1:J:49:TYR:HD1 | 2.19 | 0.60 |
| 1:M:35:TYR:O | 1:M:376:PHE:N | 2.21 | 0.60 |
| 1:M:180:VAL:HG12 | 1:M:181:GLN:N | 2.16 | 0.60 |
| 1:A:302:SER:HB2 | 1:B:253:GLU:N | 2.16 | 0.60 |
| 1:B:280:SER:O | 1:B:280:SER:OG | 2.19 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:391:ILE:HG22 | 1:B:399:LEU:HD21 | 1.84 | 0.60 |
| 1:C:451:LEU:HA | 1:C:454:LYS:CG | 2.32 | 0.60 |
| 1:D:465:GLY:O | 1:D:467:LYS:N | 2.34 | 0.60 |
| 1:F:171:LYS:HG3 | 1:F:187:PRO:HD2 | 1.82 | 0.60 |
| 1:G:42:LEU:HD13 | 1:G:447:TRP:CZ2 | 2.36 | 0.60 |
| 1:J:126:LEU:HB3 | 1:J:262:ASN:HB3 | 1.82 | 0.60 |
| 1:J:248:PHE:CZ | 1:J:311:TYR:HB3 | 2.36 | 0.60 |
| 1:K:226:THR:CG2 | 1:L:275:LEU:HD22 | 2.30 | 0.60 |
| 1:N:24:THR:HG21 | 1:N:320:ASN:HA | 1.82 | 0.60 |
| 1:B:77:LEU:HD22 | 1:B:455:PHE:HZ | 1.62 | 0.60 |
| 1:B:458:ASP:OD1 | 1:B:461:GLN:HG3 | 2.01 | 0.60 |
| 1:C:348:ILE:CD1 | 1:C:348:ILE:CB | 2.75 | 0.60 |
| 1:D:361:LYS:CD | 1:D:361:LYS:CB | 2.78 | 0.60 |
| 1:D:391:ILE:HG21 | 1:D:402:TRP:CZ3 | 2.36 | 0.60 |
| 1:H:74:ARG:CG | 1:H:330:PHE:HE2 | 2.15 | 0.60 |
| 1:I:21:VAL:CG1 | 1:I:390:TYR:OH | 2.49 | 0.60 |
| 1:J:329:LEU:HD13 | 1:J:374:PHE:CE2 | 2.36 | 0.60 |
| 1:L:65:VAL:HA | 1:L:69:GLN:NE2 | 2.17 | 0.60 |
| 1:O:246:LEU:CD2 | 1:O:246:LEU:N | 2.60 | 0.60 |
| 1:B:234:TYR:O | 1:B:237:MET:N | 2.34 | 0.60 |
| 1:F:80:PRO:HB2 | 1:F:98:LEU:HB3 | 1.82 | 0.60 |
| 1:G:172:GLY:O | 1:G:173:SER:C | 2.39 | 0.60 |
| 1:G:178:VAL:CG1 | 1:G:178:VAL:CA | 2.77 | 0.60 |
| 1:H:272:PRO:HD2 | 1:H:275:LEU:CD1 | 2.31 | 0.60 |
| 1:I:274:ASP:N | 1:I:274:ASP:OD1 | 2.34 | 0.60 |
| 1:J:167:GLU:HG2 | 1:J:231:TYR:O | 2.01 | 0.60 |
| 1:K:266:THR:OG1 | 1:O:361:LYS:HA | 2.00 | 0.60 |
| 1:L:305:GLN:HE22 | 1:L:337:THR:HG21 | 1.67 | 0.60 |
| 1:N:91:TYR:CD1 | 1:N:98:LEU:HD21 | 2.37 | 0.60 |
| 1:N:97:ARG:HA | 1:N:97:ARG:NH1 | 2.16 | 0.60 |
| 1:O:458:ASP:OD2 | 1:O:458:ASP:N | 2.34 | 0.60 |
| 1:A:439:ASP:OD2 | 1:A:440:PRO:HD2 | 2.02 | 0.60 |
| 1:B:363:TYR:CG | 1:C:185:CYS:HB2 | 2.36 | 0.60 |
| 1:D:345:CYS:SG | 1:E:216:ASN:CB | 2.89 | 0.60 |
| 1:D:361:LYS:HA | 1:E:266:THR:HG1 | 1.66 | 0.60 |
| 1:G:120:HIS:NE2 | 1:G:218:SER:CB | 2.63 | 0.60 |
| 1:I:163:PRO:N | 1:I:330:PHE:HD1 | 1.99 | 0.60 |
| 1:I:356:LYS:NZ | 1:I:356:LYS:CD | 2.65 | 0.60 |
| 1:J:160:GLY:HA3 | 1:J:245:SER:O | 2.01 | 0.60 |
| 1:J:216:ASN:OD1 | 1:J:218:SER:N | 2.34 | 0.60 |
| 1:M:112:PRO:HB3 | 1:N:231:TYR:CG | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:170:GLY:O | 1:N:188:LEU:HA | 2.01 | 0.60 |
| 1:A:46:GLY:HA3 | 1:A:65:VAL:CG2 | 2.31 | 0.60 |
| 1:B:97:ARG:HG3 | 1:B:383:LEU:CD1 | 2.31 | 0.60 |
| 1:C:81:ASN:ND2 | 1:C:402:TRP:CD1 | 2.70 | 0.60 |
| 1:D:121:PRO:HD3 | 1:D:222:LEU:HD13 | 1.84 | 0.60 |
| 1:E:219:GLU:HB3 | 1:E:263:ARG:CZ | 2.32 | 0.60 |
| 1:F:172:GLY:O | 1:F:173:SER:O | 2.19 | 0.60 |
| 1:G:103:VAL:HG22 | 1:G:375:ILE:O | 2.02 | 0.60 |
| 1:G:399:LEU:HA | 1:G:402:TRP:HE3 | 1.66 | 0.60 |
| 1:H:302:SER:CB | 1:I:253:GLU:H | 2.15 | 0.60 |
| 1:M:122:LEU:HD13 | 1:M:144:ARG:NH2 | 2.17 | 0.60 |
| 1:M:178:VAL:CG1 | 1:M:178:VAL:HB | 2.17 | 0.60 |
| 1:O:103:VAL:HA | 1:O:313:LEU:HB2 | 1.83 | 0.60 |
| 1:B:105:VAL:HG11 | 1:B:159:ILE:HD11 | 1.84 | 0.60 |
| 1:C:247:PHE:HD1 | 1:C:248:PHE:N | 2.00 | 0.60 |
| 1:D:121:PRO:O | 1:D:122:LEU:HD23 | 2.01 | 0.60 |
| 1:E:139:ALA:O | 1:E:140:GLY:O | 2.20 | 0.60 |
| 1:F:50:PHE:CD1 | 1:F:50:PHE:O | 2.55 | 0.60 |
| 1:F:105:VAL:HG11 | 1:F:159:ILE:HD11 | 1.83 | 0.60 |
| 1:I:237:MET:HB3 | 1:I:246:LEU:HD22 | 1.82 | 0.60 |
| 1:J:98:LEU:HD23 | 1:J:379:CYS:O | 2.02 | 0.60 |
| 1:L:320:ASN:OD1 | 1:L:322:GLY:N | 2.35 | 0.60 |
| 1:O:235:ILE:CD1 | 1:O:235:ILE:HG23 | 2.31 | 0.60 |
| 1:A:182:PRO:O | 1:E:348:ILE:HD12 | 2.02 | 0.59 |
| 1:A:255:MET:HG2 | 1:A:256:PHE:CA | 2.27 | 0.59 |
| 1:A:345:CYS:HB2 | 1:A:361:LYS:O | 2.02 | 0.59 |
| 1:B:117:ILE:O | 1:B:117:ILE:HG23 | 2.02 | 0.59 |
| 1:B:391:ILE:HG22 | 1:B:399:LEU:HG | 1.83 | 0.59 |
| 1:F:71:ARG:HB3 | 1:F:73:PHE:CE1 | 2.37 | 0.59 |
| 1:F:121:PRO:HD3 | 1:F:222:LEU:HD22 | 1.84 | 0.59 |
| 1:F:167:GLU:CB | 1:F:190:LEU:HD11 | 2.15 | 0.59 |
| 1:G:162:LYS:C | 1:G:330:PHE:HD1 | 2.06 | 0.59 |
| 1:I:176:THR:O | 1:I:176:THR:HG22 | 2.02 | 0.59 |
| 1:I:234:TYR:O | 1:I:237:MET:N | 2.35 | 0.59 |
| 1:J:246:LEU:CD2 | 1:J:246:LEU:N | 2.61 | 0.59 |
| 1:J:262:ASN:HD22 | 1:J:263:ARG:N | 1.99 | 0.59 |
| 1:K:336:THR:O | 1:K:338:ARG:N | 2.35 | 0.59 |
| 1:A:36:HIS:ND1 | 1:A:36:HIS:C | 2.54 | 0.59 |
| 1:A:42:LEU:HD13 | 1:A:447:TRP:CE2 | 2.37 | 0.59 |
| 1:A:42:LEU:HD12 | 1:A:73:PHE:HE2 | 1.67 | 0.59 |
| 1:A:57:ASN:HD21 | 1:A:59:LYS:HB2 | 1.65 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:57:ASN:HD21 | 1:D:59:LYS:CB | 2.16 | 0.59 |
| 1:D:237:MET:HB3 | 1:D:246:LEU:CD2 | 2.32 | 0.59 |
| 1:D:384:THR:OG1 | 1:D:385:ALA:N | 2.32 | 0.59 |
| 1:E:27:TYR:O | 1:E:381:ILE:HG23 | 2.02 | 0.59 |
| 1:E:220:VAL:HB | 1:E:224:ILE:CD1 | 2.32 | 0.59 |
| 1:F:49:TYR:HA | 1:F:223:ASP:HB3 | 1.84 | 0.59 |
| 1:G:54:LYS:HZ2 | 1:G:55:PRO:HD3 | 1.66 | 0.59 |
| 1:I:208:MET:HG2 | 1:I:210:PHE:CE2 | 2.37 | 0.59 |
| 1:I:355:TYR:CD1 | 1:J:144:ARG:HD3 | 2.37 | 0.59 |
| 1:K:149:MET:CE | 1:K:295:PRO:HD2 | 2.31 | 0.59 |
| 1:L:99:VAL:HG11 | 1:L:323:ILE:HG22 | 1.84 | 0.59 |
| 1:M:383:LEU:HD23 | 1:M:388:MET:HE2 | 1.84 | 0.59 |
| 1:N:167:GLU:HG2 | 1:N:231:TYR:O | 2.02 | 0.59 |
| 1:A:342:MET:HB2 | 1:B:208:MET:HE1 | 1.83 | 0.59 |
| 1:B:72:VAL:HG22 | 1:B:332:THR:CG2 | 2.32 | 0.59 |
| 1:B:162:LYS:C | 1:B:330:PHE:HD1 | 2.05 | 0.59 |
| 1:D:124:ASN:OD1 | 1:D:264:ALA:N | 2.33 | 0.59 |
| 1:F:361:LYS:HA | 1:G:266:THR:HG1 | 1.65 | 0.59 |
| 1:G:29:ALA:HB3 | 1:G:380:LYS:HG3 | 1.83 | 0.59 |
| 1:G:375:ILE:HG21 | 1:G:468:PHE:CD2 | 2.37 | 0.59 |
| 1:I:174:PRO:CD | 1:I:187:PRO:HG2 | 2.32 | 0.59 |
| 1:I:223:ASP:OD1 | 1:I:224:ILE:HG12 | 2.02 | 0.59 |
| 1:K:323:ILE:HG21 | 1:K:325:TRP:CZ2 | 2.37 | 0.59 |
| 1:M:98:LEU:HD22 | 1:M:379:CYS:O | 2.02 | 0.59 |
| 1:M:112:PRO:HB3 | 1:N:231:TYR:CD1 | 2.37 | 0.59 |
| 1:N:66:SER:HA | 1:N:366:HIS:ND1 | 2.17 | 0.59 |
| 1:O:135:TYR:HE2 | 1:O:287:ALA:HB2 | 1.68 | 0.59 |
| 1:D:156:LEU:HG | 1:D:334:VAL:HB | 1.84 | 0.59 |
| 1:D:348:ILE:HD12 | 1:E:182:PRO:O | 2.01 | 0.59 |
| 1:E:68:LEU:O | 1:E:201:VAL:HG13 | 2.01 | 0.59 |
| 1:E:300:VAL:HG23 | 1:E:300:VAL:O | 2.01 | 0.59 |
| 1:H:55:PRO:HG2 | 1:H:56:ASN:ND2 | 2.16 | 0.59 |
| 1:H:344:LEU:HD13 | 1:I:213:LEU:HD12 | 1.82 | 0.59 |
| 1:J:157:CYS:HB2 | 1:J:307:PHE:HE2 | 1.67 | 0.59 |
| 1:J:463:PRO:HB3 | 1:J:466:ARG:HH21 | 1.67 | 0.59 |
| 1:M:98:LEU:CD1 | 1:M:98:LEU:CB | 2.75 | 0.59 |
| 1:M:263:ARG:HD3 | 1:M:292:PHE:CD2 | 2.38 | 0.59 |
| 1:N:79:ASP:OD1 | 1:N:80:PRO:HD2 | 2.03 | 0.59 |
| 1:N:320:ASN:OD1 | 1:N:320:ASN:C | 2.41 | 0.59 |
| 1:A:279:GLY:C | 1:A:284:ALA:HB2 | 2.22 | 0.59 |
| 1:D:54:LYS:HB3 | 1:D:57:ASN:CB | 2.29 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:115:VAL:HG22 | 1:E:255:MET:SD | 2.42 | 0.59 |
| 1:D:361:LYS:HG2 | 1:E:268:GLY:HA2 | 1.85 | 0.59 |
| 1:E:24:THR:HA | 1:E:27:TYR:CE2 | 2.37 | 0.59 |
| 1:E:381:ILE:O | 1:E:383:LEU:HD12 | 2.02 | 0.59 |
| 1:F:117:ILE:CG2 | 1:F:117:ILE:H | 2.13 | 0.59 |
| 1:F:160:GLY:HA3 | 1:F:245:SER:O | 2.02 | 0.59 |
| 1:F:250:LEU:HD12 | 1:F:250:LEU:H | 1.66 | 0.59 |
| 1:F:278:LYS:HB2 | 1:I:353:THR:O | 2.02 | 0.59 |
| 1:I:105:VAL:HG22 | 1:I:374:PHE:CD2 | 2.38 | 0.59 |
| 1:I:163:PRO:CA | 1:I:330:PHE:CD1 | 2.86 | 0.59 |
| 1:J:151:TYR:OH | 1:J:221:PRO:HB2 | 2.02 | 0.59 |
| 1:J:260:LEU:N | 1:J:260:LEU:CD1 | 2.61 | 0.59 |
| 1:J:300:VAL:HG11 | 1:J:337:THR:HA | 1.84 | 0.59 |
| 1:L:55:PRO:HG2 | 1:L:56:ASN:ND2 | 2.17 | 0.59 |
| 1:L:280:SER:O | 1:L:280:SER:OG | 2.20 | 0.59 |
| 1:B:391:ILE:CG2 | 1:B:399:LEU:HD21 | 2.33 | 0.59 |
| 1:G:210:PHE:O | 1:G:214:GLN:HB2 | 2.03 | 0.59 |
| 1:H:75:ILE:CG2 | 1:H:451:LEU:HD12 | 2.28 | 0.59 |
| 1:H:466:ARG:HD2 | 1:I:317:GLN:O | 2.01 | 0.59 |
| 1:L:160:GLY:HA3 | 1:L:245:SER:O | 2.03 | 0.59 |
| 1:L:247:PHE:HD1 | 1:L:248:PHE:N | 1.99 | 0.59 |
| 1:L:378:LEU:HD12 | 1:L:379:CYS:N | 2.17 | 0.59 |
| 1:M:383:LEU:HD23 | 1:M:388:MET:CE | 2.33 | 0.59 |
| 1:N:188:LEU:CD1 | 1:N:213:LEU:HD11 | 2.33 | 0.59 |
| 1:A:77:LEU:HD11 | 1:A:376:PHE:CE2 | 2.38 | 0.59 |
| 1:A:216:ASN:OD1 | 1:A:218:SER:N | 2.36 | 0.59 |
| 1:E:178:VAL:CG1 | 1:E:178:VAL:CA | 2.78 | 0.59 |
| 1:F:52:ILE:N | 1:F:52:ILE:CD1 | 2.64 | 0.59 |
| 1:F:107:VAL:HG23 | 1:F:311:TYR:CE1 | 2.34 | 0.59 |
| 1:G:57:ASN:ND2 | 1:G:59:LYS:H | 2.00 | 0.59 |
| 1:G:66:SER:N | 1:G:69:GLN:NE2 | 2.50 | 0.59 |
| 1:H:28:VAL:HG12 | 1:H:29:ALA:H | 1.65 | 0.59 |
| 1:I:82:LYS:NZ | 1:I:403:ASN:HD22 | 2.00 | 0.59 |
| 1:J:397:THR:HB | 1:J:401:ASP:OD2 | 2.02 | 0.59 |
| 1:K:90:PHE:O | 1:K:380:LYS:NZ | 2.35 | 0.59 |
| 1:K:344:LEU:CD1 | 1:L:185:CYS:SG | 2.91 | 0.59 |
| 1:L:111:GLN:HG2 | 1:L:369:GLU:HB3 | 1.85 | 0.59 |
| 1:L:120:HIS:NE2 | 1:L:218:SER:HB3 | 2.18 | 0.59 |
| 1:N:66:SER:N | 1:N:69:GLN:NE2 | 2.39 | 0.59 |
| 1:A:399:LEU:HA | 1:A:402:TRP:HE3 | 1.66 | 0.59 |
| 1:B:45:VAL:HA | 1:B:366:HIS:O | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:49:TYR:HE1 | 1:C:364:LEU:HD13 | 1.68 | 0.59 |
| 1:D:223:ASP:OD1 | 1:D:224:ILE:N | 2.35 | 0.59 |
| 1:E:205:PHE:CD1 | 1:E:220:VAL:HG12 | 2.38 | 0.59 |
| 1:F:96:GLN:HB3 | 1:F:382:THR:HA | 1.84 | 0.59 |
| 1:F:125:LYS:HD2 | 1:F:147:ILE:HD11 | 1.84 | 0.59 |
| 1:G:98:LEU:CD1 | 1:G:98:LEU:CB | 2.76 | 0.59 |
| 1:G:391:ILE:HG21 | 1:G:402:TRP:CZ3 | 2.38 | 0.59 |
| 1:H:174:PRO:HG3 | 1:H:187:PRO:HG2 | 1.84 | 0.59 |
| 1:H:248:PHE:CZ | 1:H:311:TYR:HB3 | 2.37 | 0.59 |
| 1:H:259:HIS:HB2 | 1:H:294:THR:OG1 | 2.02 | 0.59 |
| 1:K:391:ILE:HG21 | 1:K:402:TRP:CZ3 | 2.37 | 0.59 |
| 1:L:237:MET:HB3 | 1:L:246:LEU:HD22 | 1.83 | 0.59 |
| 1:M:323:ILE:CD1 | 1:M:323:ILE:HA | 2.31 | 0.59 |
| 1:N:61:LEU:CD1 | 1:N:61:LEU:HG | 2.17 | 0.59 |
| 1:N:255:MET:HG2 | 1:N:256:PHE:H | 1.67 | 0.59 |
| 1:A:465:GLY:O | 1:A:466:ARG:C | 2.41 | 0.59 |
| 1:B:152:LYS:HE3 | 1:B:154:THR:OG1 | 2.03 | 0.59 |
| 1:C:70:TYR:CE1 | 1:C:201:VAL:HA | 2.38 | 0.59 |
| 1:E:149:MET:HE2 | 1:E:205:PHE:CE1 | 2.38 | 0.59 |
| 1:F:129:THR:HB | 1:J:148:SER:OG | 2.03 | 0.59 |
| 1:F:257:VAL:HG21 | 1:J:150:ASP:CB | 2.33 | 0.59 |
| 1:I:49:TYR:CE2 | 1:I:118:SER:HA | 2.37 | 0.59 |
| 1:I:384:THR:HG23 | 1:I:387:VAL:CG2 | 2.33 | 0.59 |
| 1:K:391:ILE:HG21 | 1:K:402:TRP:HZ3 | 1.68 | 0.59 |
| 1:L:101:ALA:HA | 1:L:322:GLY:O | 2.02 | 0.59 |
| 1:L:470:LEU:O | 1:L:470:LEU:CD2 | 2.50 | 0.59 |
| 1:M:57:ASN:HD21 | 1:M:59:LYS:H | 1.49 | 0.59 |
| 1:N:183:GLY:O | 1:N:184:ASP:C | 2.40 | 0.59 |
| 1:N:237:MET:HB3 | 1:N:246:LEU:HD22 | 1.85 | 0.59 |
| 1:O:23:SER:OG | 1:O:25:ASP:HB2 | 2.03 | 0.59 |
| 1:O:378:LEU:HD12 | 1:O:379:CYS:N | 2.18 | 0.59 |
| 1:A:155:GLN:OE1 | 1:A:305:GLN:HA | 2.03 | 0.59 |
| 1:A:384:THR:H | 1:A:387:VAL:HB | 1.68 | 0.59 |
| 1:B:357:ASN:H | 1:C:141:VAL:HG13 | 1.67 | 0.59 |
| 1:C:98:LEU:HD22 | 1:C:379:CYS:O | 2.03 | 0.59 |
| 1:C:110:GLY:O | 1:C:111:GLN:NE2 | 2.35 | 0.59 |
| 1:G:98:LEU:HD22 | 1:G:379:CYS:O | 2.03 | 0.59 |
| 1:H:54:LYS:HZ2 | 1:H:55:PRO:CD | 2.13 | 0.59 |
| 1:H:92:ASN:ND2 | 1:H:95:THR:H | 2.00 | 0.59 |
| 1:K:113:LEU:HB2 | 1:L:253:GLU:OE1 | 2.03 | 0.59 |
| 1:K:117:ILE:HG21 | 1:L:293:PRO:HD3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:316:ALA:HB3 | 1:L:321:ASN:OD1 | 2.03 | 0.59 |
| 1:M:66:SER:HA | 1:M:366:HIS:ND1 | 2.18 | 0.59 |
| 1:M:71:ARG:HH12 | 1:M:198:GLY:H | 1.49 | 0.59 |
| 1:M:113:LEU:N | 1:M:113:LEU:CD1 | 2.66 | 0.59 |
| 1:B:356:LYS:O | 1:B:357:ASN:C | 2.39 | 0.58 |
| 1:C:358:THR:HA | 1:D:266:THR:HG23 | 1.85 | 0.58 |
| 1:D:98:LEU:CD1 | 1:D:378:LEU:HD11 | 2.13 | 0.58 |
| 1:E:234:TYR:CD1 | 1:E:251:ARG:NH2 | 2.70 | 0.58 |
| 1:E:399:LEU:O | 1:E:402:TRP:HB2 | 2.03 | 0.58 |
| 1:G:163:PRO:N | 1:G:330:PHE:CD1 | 2.71 | 0.58 |
| 1:G:172:GLY:O | 1:G:173:SER:O | 2.21 | 0.58 |
| 1:G:234:TYR:CD1 | 1:G:251:ARG:NH2 | 2.71 | 0.58 |
| 1:H:154:THR:H | 1:H:336:THR:HG21 | 1.68 | 0.58 |
| 1:H:176:THR:O | 1:H:177:GLN:CG | 2.51 | 0.58 |
| 1:H:178:VAL:CG1 | 1:H:178:VAL:HB | 2.21 | 0.58 |
| 1:H:200:MET:HB2 | 1:H:228:ILE:O | 2.03 | 0.58 |
| 1:I:28:VAL:HA | 1:I:381:ILE:HG12 | 1.83 | 0.58 |
| 1:J:153:GLN:HE22 | 1:J:300:VAL:HA | 1.67 | 0.58 |
| 1:J:183:GLY:O | 1:J:185:CYS:N | 2.36 | 0.58 |
| 1:K:149:MET:HE3 | 1:K:295:PRO:HD2 | 1.83 | 0.58 |
| 1:K:307:PHE:C | 1:K:309:LYS:H | 2.06 | 0.58 |
| 1:L:80:PRO:HG2 | 1:L:81:ASN:H | 1.68 | 0.58 |
| 1:L:468:PHE:O | 1:L:468:PHE:CD1 | 2.56 | 0.58 |
| 1:N:49:TYR:CE2 | 1:N:118:SER:HA | 2.36 | 0.58 |
| 1:O:129:THR:OG1 | 1:O:260:LEU:O | 2.19 | 0.58 |
| 1:A:156:LEU:HD12 | 1:A:157:CYS:N | 2.18 | 0.58 |
| 1:B:74:ARG:NH2 | 1:B:441:LEU:HD12 | 2.17 | 0.58 |
| 1:C:274:ASP:OD2 | 1:C:275:LEU:HD23 | 2.03 | 0.58 |
| 1:D:53:LYS:CG | 1:D:53:LYS:CA | 2.77 | 0.58 |
| 1:E:316:ALA:C | 1:E:318:GLY:H | 2.07 | 0.58 |
| 1:G:71:ARG:NH1 | 1:G:197:ASP:OD1 | 2.36 | 0.58 |
| 1:H:466:ARG:HD3 | 1:I:319:HIS:CE1 | 2.38 | 0.58 |
| 1:I:54:LYS:HE3 | 1:I:55:PRO:HD2 | 1.85 | 0.58 |
| 1:I:250:LEU:HD12 | 1:I:250:LEU:N | 2.18 | 0.58 |
| 1:J:50:PHE:HB2 | 1:J:51:PRO:CD | 2.31 | 0.58 |
| 1:J:65:VAL:HA | 1:J:69:GLN:NE2 | 2.16 | 0.58 |
| 1:L:152:LYS:HE2 | 1:L:202:ASP:CG | 2.23 | 0.58 |
| 1:L:309:LYS:CD | 1:L:309:LYS:NZ | 2.64 | 0.58 |
| 1:L:323:ILE:N | 1:L:323:ILE:HD13 | 2.17 | 0.58 |
| 1:O:274:ASP:OD1 | 1:O:274:ASP:N | 2.35 | 0.58 |
| 1:A:374:PHE:HB3 | 1:A:376:PHE:CE1 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:201:VAL:C | 1:B:202:ASP:O | 2.35 | 0.58 |
| 1:B:312:TRP:CH2 | 1:B:468:PHE:HB2 | 2.38 | 0.58 |
| 1:C:196:GLN:N | 1:C:199:ASP:OD2 | 2.35 | 0.58 |
| 1:D:459:LEU:HB3 | 1:D:465:GLY:HA3 | 1.84 | 0.58 |
| 1:E:52:ILE:HD12 | 1:E:52:ILE:N | 2.18 | 0.58 |
| 1:F:391:ILE:HG21 | 1:F:402:TRP:HZ3 | 1.68 | 0.58 |
| 1:F:461:GLN:HE22 | 1:G:21:VAL:HB | 1.67 | 0.58 |
| 1:G:29:ALA:O | 1:G:379:CYS:HB3 | 2.02 | 0.58 |
| 1:H:358:THR:HA | 1:I:266:THR:CG2 | 2.32 | 0.58 |
| 1:I:24:THR:HA | 1:I:27:TYR:CE2 | 2.38 | 0.58 |
| 1:K:461:GLN:HE22 | 1:L:21:VAL:H | 1.50 | 0.58 |
| 1:L:262:ASN:HD22 | 1:L:263:ARG:N | 2.01 | 0.58 |
| 1:A:190:LEU:HD12 | 1:A:191:ILE:N | 2.18 | 0.58 |
| 1:B:22:VAL:O | 1:B:23:SER:C | 2.42 | 0.58 |
| 1:B:96:GLN:HA | 1:B:382:THR:HA | 1.84 | 0.58 |
| 1:B:364:LEU:O | 1:B:365:ARG:HD3 | 2.03 | 0.58 |
| 1:D:75:ILE:N | 1:D:75:ILE:HD12 | 2.17 | 0.58 |
| 1:E:167:GLU:HB2 | 1:E:190:LEU:HD11 | 1.84 | 0.58 |
| 1:F:307:PHE:CE2 | 1:F:333:VAL:HG13 | 2.38 | 0.58 |
| 1:H:46:GLY:HA3 | 1:H:63:PRO:O | 2.04 | 0.58 |
| 1:I:179:ALA:CB | 1:I:179:ALA:C | 2.67 | 0.58 |
| 1:I:180:VAL:CG1 | 1:I:184:ASP:CB | 2.79 | 0.58 |
| 1:J:223:ASP:OD1 | 1:J:224:ILE:HG12 | 2.04 | 0.58 |
| 1:M:214:GLN:OE1 | 1:M:219:GLU:HB2 | 2.03 | 0.58 |
| 1:N:30:ARG:HH11 | 1:N:377:GLN:NE2 | 2.00 | 0.58 |
| 1:N:176:THR:O | 1:N:177:GLN:HG3 | 2.03 | 0.58 |
| 1:N:220:VAL:O | 1:N:221:PRO:O | 2.22 | 0.58 |
| 1:O:183:GLY:O | 1:O:185:CYS:N | 2.37 | 0.58 |
| 1:O:344:LEU:O | 1:O:363:TYR:N | 2.34 | 0.58 |
| 1:A:27:TYR:CE2 | 1:A:390:TYR:CE2 | 2.91 | 0.58 |
| 1:A:155:GLN:HB3 | 1:A:252:ARG:HB3 | 1.85 | 0.58 |
| 1:C:281:GLY:O | 1:C:284:ALA:N | 2.34 | 0.58 |
| 1:D:68:LEU:HD23 | 1:D:201:VAL:HG21 | 1.85 | 0.58 |
| 1:E:21:VAL:HG13 | 1:E:390:TYR:OH | 2.04 | 0.58 |
| 1:G:149:MET:CE | 1:G:205:PHE:CE1 | 2.86 | 0.58 |
| 1:H:301:THR:CG2 | 1:H:301:THR:CA | 2.79 | 0.58 |
| 1:I:384:THR:O | 1:I:388:MET:HB3 | 2.03 | 0.58 |
| 1:L:123:LEU:CD2 | 1:L:147:ILE:HB | 2.23 | 0.58 |
| 1:L:272:PRO:HD2 | 1:L:275:LEU:HG | 1.85 | 0.58 |
| 1:M:30:ARG:HH11 | 1:M:377:GLN:NE2 | 2.02 | 0.58 |
| 1:M:162:LYS:O | 1:M:330:PHE:HD1 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:171:LYS:HA | 1:M:187:PRO:O | 2.04 | 0.58 |
| 1:M:358:THR:HA | 1:N:266:THR:HG22 | 1.85 | 0.58 |
| 1:M:383:LEU:HD22 | 1:M:388:MET:HE3 | 1.85 | 0.58 |
| 1:O:162:LYS:C | 1:O:330:PHE:HD1 | 2.07 | 0.58 |
| 1:A:151:TYR:CG | 1:A:203:THR:HB | 2.39 | 0.58 |
| 1:A:169:TRP:H | 1:A:208:MET:HA | 1.68 | 0.58 |
| 1:A:390:TYR:O | 1:A:393:SER:N | 2.36 | 0.58 |
| 1:C:344:LEU:CD1 | 1:D:213:LEU:HD12 | 2.32 | 0.58 |
| 1:D:120:HIS:ND1 | 1:D:122:LEU:N | 2.47 | 0.58 |
| 1:D:122:LEU:HD11 | 1:E:286:LEU:CD1 | 2.34 | 0.58 |
| 1:D:152:LYS:NZ | 1:D:152:LYS:CD | 2.64 | 0.58 |
| 1:E:391:ILE:HG21 | 1:E:402:TRP:HZ3 | 1.68 | 0.58 |
| 1:F:344:LEU:CD1 | 1:G:185:CYS:SG | 2.91 | 0.58 |
| 1:G:471:GLN:OE1 | 1:G:472:LEU:N | 2.36 | 0.58 |
| 1:H:162:LYS:HB3 | 1:H:163:PRO:HD2 | 1.86 | 0.58 |
| 1:H:272:PRO:HD2 | 1:H:275:LEU:HD12 | 1.86 | 0.58 |
| 1:H:343:SER:HB3 | 1:H:364:LEU:HD23 | 1.86 | 0.58 |
| 1:I:117:ILE:HD11 | 1:J:260:LEU:HB3 | 1.86 | 0.58 |
| 1:J:211:THR:O | 1:J:211:THR:HG22 | 2.03 | 0.58 |
| 1:K:57:ASN:HD21 | 1:K:59:LYS:CB | 2.16 | 0.58 |
| 1:O:54:LYS:CG | 1:O:55:PRO:HD2 | 2.34 | 0.58 |
| 1:A:104:GLY:HA3 | 1:A:375:ILE:HB | 1.86 | 0.58 |
| 1:B:120:HIS:ND1 | 1:B:122:LEU:N | 2.49 | 0.58 |
| 1:B:156:LEU:HG | 1:B:334:VAL:HB | 1.86 | 0.58 |
| 1:C:452:LYS:NZ | 1:C:452:LYS:CD | 2.63 | 0.58 |
| 1:D:49:TYR:HE2 | 1:D:118:SER:HA | 1.67 | 0.58 |
| 1:G:443:LYS:HD3 | 1:G:443:LYS:N | 2.18 | 0.58 |
| 1:H:34:TYR:CE2 | 1:H:377:GLN:HG3 | 2.38 | 0.58 |
| 1:K:153:GLN:NE2 | 1:K:300:VAL:CG1 | 2.67 | 0.58 |
| 1:K:302:SER:HB2 | 1:L:253:GLU:H | 1.69 | 0.58 |
| 1:K:373:GLN:HB2 | 1:K:464:LEU:HD12 | 1.84 | 0.58 |
| 1:M:188:LEU:CD1 | 1:M:213:LEU:HD11 | 2.34 | 0.58 |
| 1:N:72:VAL:HG22 | 1:N:332:THR:CG2 | 2.34 | 0.58 |
| 1:N:398:ILE:HG22 | 1:N:402:TRP:CZ3 | 2.39 | 0.58 |
| 1:O:158:LEU:HD23 | 1:O:249:TYR:HB2 | 1.85 | 0.58 |
| 1:O:159:ILE:HG22 | 1:O:160:GLY:N | 2.18 | 0.58 |
| 1:A:46:GLY:O | 1:A:365:ARG:HD3 | 2.04 | 0.58 |
| 1:A:317:GLN:O | 1:E:466:ARG:HD2 | 2.03 | 0.58 |
| 1:A:463:PRO:HA | 1:A:466:ARG:HE | 1.69 | 0.58 |
| 1:B:23:SER:HG | 1:B:25:ASP:HB2 | 1.67 | 0.58 |
| 1:C:361:LYS:HA | 1:D:266:THR:HG1 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:76:HIS:HB2 | 1:D:450:ASN:HA | 1.86 | 0.58 |
| 1:D:465:GLY:O | 1:D:466:ARG:C | 2.42 | 0.58 |
| 1:E:24:THR:CG2 | 1:E:320:ASN:HA | 2.34 | 0.58 |
| 1:E:96:GLN:HE21 | 1:E:382:THR:CG2 | 2.17 | 0.58 |
| 1:E:157:CYS:HB2 | 1:E:307:PHE:CE2 | 2.38 | 0.58 |
| 1:F:231:TYR:CG | 1:J:112:PRO:HD3 | 2.38 | 0.58 |
| 1:H:250:LEU:HD12 | 1:H:250:LEU:H | 1.68 | 0.58 |
| 1:I:75:ILE:HD12 | 1:I:75:ILE:H | 1.68 | 0.58 |
| 1:I:120:HIS:NE2 | 1:I:218:SER:HB3 | 2.18 | 0.58 |
| 1:I:122:LEU:HD13 | 1:I:144:ARG:NH2 | 2.18 | 0.58 |
| 1:I:363:TYR:CD2 | 1:J:185:CYS:HB2 | 2.39 | 0.58 |
| 1:K:250:LEU:HD13 | 1:K:306:ILE:CG2 | 2.33 | 0.58 |
| 1:L:391:ILE:O | 1:L:391:ILE:HG22 | 2.02 | 0.58 |
| 1:M:34:TYR:HE2 | 1:M:377:GLN:HB2 | 1.60 | 0.58 |
| 1:N:344:LEU:HD11 | 1:O:185:CYS:SG | 2.44 | 0.58 |
| 1:C:157:CYS:HB2 | 1:C:307:PHE:HE2 | 1.69 | 0.58 |
| 1:C:180:VAL:CG1 | 1:C:184:ASP:HB3 | 2.33 | 0.58 |
| 1:C:451:LEU:O | 1:C:454:LYS:HB2 | 2.04 | 0.58 |
| 1:E:68:LEU:O | 1:E:201:VAL:HG22 | 2.04 | 0.58 |
| 1:F:364:LEU:O | 1:F:365:ARG:HD3 | 2.04 | 0.58 |
| 1:G:103:VAL:O | 1:G:313:LEU:N | 2.28 | 0.58 |
| 1:G:168:HIS:H | 1:G:190:LEU:HD11 | 1.68 | 0.58 |
| 1:G:387:VAL:HG12 | 1:G:388:MET:N | 2.19 | 0.58 |
| 1:H:217:LYS:NZ | 1:H:217:LYS:CD | 2.67 | 0.58 |
| 1:I:183:GLY:O | 1:I:185:CYS:N | 2.37 | 0.58 |
| 1:I:358:THR:HA | 1:J:266:THR:CG2 | 2.33 | 0.58 |
| 1:J:341:ASN:HB3 | 1:J:366:HIS:HB2 | 1.85 | 0.58 |
| 1:K:33:ILE:HB | 1:K:378:LEU:HB3 | 1.85 | 0.58 |
| 1:K:144:ARG:HD3 | 1:O:355:TYR:CE1 | 2.39 | 0.58 |
| 1:M:144:ARG:C | 1:M:145:GLU:HG2 | 2.24 | 0.58 |
| 1:N:22:VAL:O | 1:N:23:SER:C | 2.42 | 0.58 |
| 1:O:99:VAL:HG11 | 1:O:323:ILE:HG22 | 1.85 | 0.58 |
| 1:A:345:CYS:O | 1:B:215:ALA:N | 2.29 | 0.58 |
| 1:A:363:TYR:CG | 1:B:185:CYS:HB2 | 2.39 | 0.58 |
| 1:B:117:ILE:HD12 | 1:C:293:PRO:HB3 | 1.84 | 0.58 |
| 1:B:123:LEU:CD2 | 1:B:123:LEU:CD1 | 2.73 | 0.58 |
| 1:B:344:LEU:HD23 | 1:B:344:LEU:H | 1.69 | 0.58 |
| 1:C:24:THR:HG23 | 1:C:320:ASN:HA | 1.84 | 0.58 |
| 1:C:440:PRO:HA | 1:C:443:LYS:NZ | 2.19 | 0.58 |
| 1:E:67:GLY:C | 1:E:68:LEU:HG | 2.23 | 0.58 |
| 1:E:180:VAL:CG1 | 1:E:184:ASP:CB | 2.82 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:117:ILE:CG1 | 1:F:149:MET:O | 2.52 | 0.58 |
| 1:H:105:VAL:HG22 | 1:H:374:PHE:CD2 | 2.38 | 0.58 |
| 1:J:163:PRO:N | 1:J:330:PHE:HD1 | 2.01 | 0.58 |
| 1:K:97:ARG:HG3 | 1:K:383:LEU:CD1 | 2.34 | 0.58 |
| 1:K:98:LEU:HD22 | 1:K:378:LEU:HD11 | 1.86 | 0.58 |
| 1:K:375:ILE:HG13 | 1:K:464:LEU:HD22 | 1.86 | 0.58 |
| 1:L:61:LEU:CD1 | 1:L:61:LEU:CD2 | 2.79 | 0.58 |
| 1:L:139:ALA:HB1 | 1:L:143:ASN:ND2 | 2.19 | 0.58 |
| 1:M:456:SER:O | 1:M:457:ALA:C | 2.37 | 0.58 |
| 1:C:54:LYS:HG2 | 1:C:57:ASN:HB3 | 1.86 | 0.57 |
| 1:C:157:CYS:O | 1:C:158:LEU:HD23 | 2.03 | 0.57 |
| 1:C:440:PRO:HA | 1:C:443:LYS:HZ1 | 1.68 | 0.57 |
| 1:F:151:TYR:OH | 1:F:221:PRO:HB2 | 2.04 | 0.57 |
| 1:F:157:CYS:HB2 | 1:F:307:PHE:HE2 | 1.68 | 0.57 |
| 1:F:266:THR:HG1 | 1:J:361:LYS:HA | 1.69 | 0.57 |
| 1:F:358:THR:HA | 1:G:266:THR:CG2 | 2.33 | 0.57 |
| 1:F:363:TYR:CE1 | 1:G:185:CYS:HB2 | 2.39 | 0.57 |
| 1:G:194:VAL:HG21 | 1:G:444:TYR:CE2 | 2.39 | 0.57 |
| 1:H:180:VAL:HG12 | 1:H:184:ASP:HB2 | 1.86 | 0.57 |
| 1:I:361:LYS:HA | 1:J:266:THR:OG1 | 2.04 | 0.57 |
| 1:J:190:LEU:HD12 | 1:J:191:ILE:H | 1.68 | 0.57 |
| 1:J:262:ASN:C | 1:J:262:ASN:ND2 | 2.58 | 0.57 |
| 1:K:174:PRO:HG3 | 1:K:187:PRO:HG2 | 1.86 | 0.57 |
| 1:K:391:ILE:HD13 | 1:K:402:TRP:CH2 | 2.38 | 0.57 |
| 1:L:257:VAL:HG12 | 1:L:293:PRO:HB2 | 1.86 | 0.57 |
| 1:M:188:LEU:HD22 | 1:M:188:LEU:N | 2.18 | 0.57 |
| 1:M:247:PHE:HD1 | 1:M:248:PHE:N | 2.00 | 0.57 |
| 1:M:361:LYS:CA | 1:N:266:THR:HG1 | 2.10 | 0.57 |
| 1:M:383:LEU:CD2 | 1:M:388:MET:HE3 | 2.34 | 0.57 |
| 1:O:34:TYR:HE2 | 1:O:377:GLN:HB2 | 1.67 | 0.57 |
| 1:O:151:TYR:CG | 1:O:203:THR:HB | 2.39 | 0.57 |
| 1:O:398:ILE:CD1 | 1:O:398:ILE:CB | 2.78 | 0.57 |
| 1:A:92:ASN:ND2 | 1:A:95:THR:N | 2.49 | 0.57 |
| 1:B:66:SER:N | 1:B:69:GLN:NE2 | 2.50 | 0.57 |
| 1:B:274:ASP:OD1 | 1:B:274:ASP:N | 2.36 | 0.57 |
| 1:C:320:ASN:OD1 | 1:C:321:ASN:N | 2.37 | 0.57 |
| 1:D:68:LEU:HD23 | 1:D:201:VAL:CG2 | 2.34 | 0.57 |
| 1:D:365:ARG:NH2 | 1:E:269:GLU:OE1 | 2.37 | 0.57 |
| 1:E:333:VAL:HG12 | 1:E:334:VAL:N | 2.20 | 0.57 |
| 1:F:31:THR:OG1 | 1:F:33:ILE:HB | 2.04 | 0.57 |
| 1:F:253:GLU:HG3 | 1:J:113:LEU:HD22 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:439:ASP:HB3 | 1:F:442:LYS:HE3 | 1.85 | 0.57 |
| 1:G:149:MET:HE1 | 1:G:205:PHE:CE1 | 2.39 | 0.57 |
| 1:G:150:ASP:OD2 | 1:G:150:ASP:N | 2.36 | 0.57 |
| 1:G:259:HIS:CE1 | 1:H:130:GLU:HG3 | 2.38 | 0.57 |
| 1:H:46:GLY:N | 1:H:65:VAL:HB | 2.19 | 0.57 |
| 1:I:22:VAL:HG23 | 1:I:22:VAL:O | 2.02 | 0.57 |
| 1:I:104:GLY:HA3 | 1:I:375:ILE:HB | 1.86 | 0.57 |
| 1:L:464:LEU:O | 1:L:464:LEU:CD2 | 2.52 | 0.57 |
| 1:O:68:LEU:HD22 | 1:O:203:THR:HG22 | 1.85 | 0.57 |
| 1:O:163:PRO:CA | 1:O:330:PHE:CD1 | 2.87 | 0.57 |
| 1:A:71:ARG:HB3 | 1:A:73:PHE:CE1 | 2.38 | 0.57 |
| 1:A:124:ASN:OD1 | 1:A:264:ALA:N | 2.37 | 0.57 |
| 1:A:246:LEU:H | 1:A:246:LEU:CD2 | 2.16 | 0.57 |
| 1:A:355:TYR:O | 1:A:356:LYS:CG | 2.52 | 0.57 |
| 1:D:149:MET:HE1 | 1:D:205:PHE:CZ | 2.39 | 0.57 |
| 1:F:29:ALA:HB3 | 1:F:380:LYS:HG3 | 1.87 | 0.57 |
| 1:F:171:LYS:HA | 1:F:187:PRO:O | 2.02 | 0.57 |
| 1:F:391:ILE:HG21 | 1:F:402:TRP:CZ3 | 2.39 | 0.57 |
| 1:H:262:ASN:HD21 | 1:H:288:SER:HB3 | 1.68 | 0.57 |
| 1:H:361:LYS:CB | 1:H:361:LYS:CD | 2.82 | 0.57 |
| 1:I:166:GLY:H | 1:I:195:ILE:HG13 | 1.69 | 0.57 |
| 1:J:157:CYS:HB2 | 1:J:307:PHE:CE2 | 2.38 | 0.57 |
| 1:J:201:VAL:O | 1:J:229:CYS:SG | 2.53 | 0.57 |
| 1:K:112:PRO:HD3 | 1:L:231:TYR:CG | 2.39 | 0.57 |
| 1:L:70:TYR:CD2 | 1:L:195:ILE:HG21 | 2.40 | 0.57 |
| 1:L:80:PRO:HD3 | 1:L:100:TRP:CD1 | 2.39 | 0.57 |
| 1:L:155:GLN:O | 1:L:252:ARG:N | 2.37 | 0.57 |
| 1:L:352:GLU:HG2 | 1:L:356:LYS:HD2 | 1.85 | 0.57 |
| 1:M:97:ARG:NH1 | 1:M:97:ARG:HA | 2.19 | 0.57 |
| 1:M:185:CYS:SG | 1:M:186:PRO:CD | 2.88 | 0.57 |
| 1:N:323:ILE:HD13 | 1:N:323:ILE:N | 2.19 | 0.57 |
| 1:N:329:LEU:HD13 | 1:N:374:PHE:CE2 | 2.38 | 0.57 |
| 1:O:223:ASP:OD1 | 1:O:224:ILE:HG23 | 2.05 | 0.57 |
| 1:B:241:PRO:O | 1:B:243:GLY:N | 2.38 | 0.57 |
| 1:C:66:SER:O | 1:C:69:GLN:HG3 | 2.03 | 0.57 |
| 1:G:166:GLY:O | 1:G:192:ASN:HA | 2.04 | 0.57 |
| 1:H:463:PRO:HB3 | 1:H:466:ARG:HH21 | 1.70 | 0.57 |
| 1:I:149:MET:CE | 1:I:205:PHE:CE1 | 2.87 | 0.57 |
| 1:L:355:TYR:CE1 | 1:M:144:ARG:HD3 | 2.40 | 0.57 |
| 1:M:29:ALA:HB3 | 1:M:380:LYS:HG3 | 1.85 | 0.57 |
| 1:M:320:ASN:HD21 | 1:M:323:ILE:HB | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:61:LEU:CD1 | 1:N:61:LEU:CD2 | 2.79 | 0.57 |
| 1:A:64:LYS:CD | 1:A:64:LYS:NZ | 2.68 | 0.57 |
| 1:A:172:GLY:O | 1:A:173:SER:C | 2.41 | 0.57 |
| 1:C:162:LYS:C | 1:C:330:PHE:CD1 | 2.74 | 0.57 |
| 1:D:120:HIS:NE2 | 1:D:218:SER:CB | 2.68 | 0.57 |
| 1:F:391:ILE:O | 1:F:395:ASN:O | 2.23 | 0.57 |
| 1:H:24:THR:OG1 | 1:H:25:ASP:N | 2.38 | 0.57 |
| 1:H:218:SER:O | 1:H:219:GLU:HG2 | 2.03 | 0.57 |
| 1:J:320:ASN:ND2 | 1:J:325:TRP:NE1 | 2.53 | 0.57 |
| 1:K:143:ASN:O | 1:K:144:ARG:C | 2.42 | 0.57 |
| 1:L:165:ILE:CD1 | 1:L:165:ILE:CB | 2.80 | 0.57 |
| 1:M:121:PRO:HG2 | 1:N:289:SER:HB2 | 1.85 | 0.57 |
| 1:O:124:ASN:OD1 | 1:O:264:ALA:N | 2.35 | 0.57 |
| 1:A:98:LEU:HD13 | 1:A:378:LEU:HD11 | 1.86 | 0.57 |
| 1:A:107:VAL:HG11 | 1:A:333:VAL:HG21 | 1.87 | 0.57 |
| 1:A:467:LYS:O | 1:A:470:LEU:N | 2.37 | 0.57 |
| 1:B:176:THR:O | 1:B:177:GLN:HG3 | 2.05 | 0.57 |
| 1:B:250:LEU:HD12 | 1:B:250:LEU:N | 2.19 | 0.57 |
| 1:C:66:SER:HA | 1:C:366:HIS:ND1 | 2.20 | 0.57 |
| 1:D:451:LEU:HD23 | 1:D:454:LYS:HG3 | 1.87 | 0.57 |
| 1:E:272:PRO:O | 1:E:275:LEU:HG | 2.04 | 0.57 |
| 1:F:117:ILE:CG2 | 1:F:117:ILE:HB | 2.16 | 0.57 |
| 1:H:260:LEU:O | 1:H:261:PHE:HD2 | 1.87 | 0.57 |
| 1:H:465:GLY:C | 1:H:467:LYS:N | 2.58 | 0.57 |
| 1:J:47:HIS:CG | 1:J:48:PRO:HD2 | 2.40 | 0.57 |
| 1:J:242:TYR:HE2 | 1:J:394:MET:HB2 | 1.66 | 0.57 |
| 1:J:472:LEU:HD23 | 1:N:138:ASN:HD22 | 1.68 | 0.57 |
| 1:K:74:ARG:CG | 1:K:330:PHE:HE2 | 2.18 | 0.57 |
| 1:K:81:ASN:ND2 | 1:K:402:TRP:HD1 | 2.00 | 0.57 |
| 1:K:226:THR:HG21 | 1:L:275:LEU:CD2 | 2.32 | 0.57 |
| 1:K:274:ASP:N | 1:K:274:ASP:OD1 | 2.37 | 0.57 |
| 1:L:41:ARG:HH22 | 1:M:192:ASN:HD21 | 1.52 | 0.57 |
| 1:L:96:GLN:HA | 1:L:382:THR:HA | 1.85 | 0.57 |
| 1:L:252:ARG:HD2 | 1:L:306:ILE:HD11 | 1.87 | 0.57 |
| 1:L:345:CYS:SG | 1:M:216:ASN:HB2 | 2.45 | 0.57 |
| 1:N:96:GLN:HE21 | 1:N:382:THR:HG22 | 1.70 | 0.57 |
| 1:A:55:PRO:HG2 | 1:A:56:ASN:ND2 | 2.19 | 0.57 |
| 1:B:81:ASN:ND2 | 1:B:402:TRP:CD1 | 2.73 | 0.57 |
| 1:B:97:ARG:HA | 1:B:97:ARG:HH11 | 1.69 | 0.57 |
| 1:C:353:THR:O | 1:E:278:LYS:HB2 | 2.04 | 0.57 |
| 1:D:456:SER:OG | 1:D:458:ASP:OD2 | 2.23 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:185:CYS:SG | 1:F:186:PRO:CD | 2.93 | 0.57 |
| 1:F:255:MET:HG2 | 1:F:256:PHE:N | 2.20 | 0.57 |
| 1:G:316:ALA:C | 1:G:318:GLY:H | 2.06 | 0.57 |
| 1:J:274:ASP:OD1 | 1:J:274:ASP:N | 2.37 | 0.57 |
| 1:M:49:TYR:HE1 | 1:M:364:LEU:HD13 | 1.69 | 0.57 |
| 1:M:49:TYR:HE2 | 1:M:118:SER:HA | 1.68 | 0.57 |
| 1:N:146:CYS:O | 1:O:129:THR:HG22 | 2.05 | 0.57 |
| 1:O:65:VAL:CA | 1:O:69:GLN:NE2 | 2.62 | 0.57 |
| 1:O:126:LEU:HB3 | 1:O:262:ASN:HB3 | 1.86 | 0.57 |
| 1:A:183:GLY:O | 1:A:185:CYS:N | 2.38 | 0.57 |
| 1:A:242:TYR:CD2 | 1:A:394:MET:CG | 2.84 | 0.57 |
| 1:B:50:PHE:HB2 | 1:B:51:PRO:HD2 | 1.85 | 0.57 |
| 1:B:142:ASP:CG | 1:C:283:THR:OG1 | 2.43 | 0.57 |
| 1:C:36:HIS:CG | 1:C:462:PHE:CD1 | 2.92 | 0.57 |
| 1:D:241:PRO:HG2 | 1:D:242:TYR:H | 1.70 | 0.57 |
| 1:D:344:LEU:N | 1:D:344:LEU:HD23 | 2.20 | 0.57 |
| 1:G:196:GLN:N | 1:G:199:ASP:OD2 | 2.37 | 0.57 |
| 1:G:372:LEU:HB3 | 1:G:374:PHE:HE1 | 1.68 | 0.57 |
| 1:H:117:ILE:HG13 | 1:H:149:MET:O | 2.04 | 0.57 |
| 1:I:384:THR:HG23 | 1:I:387:VAL:HG21 | 1.87 | 0.57 |
| 1:I:399:LEU:HA | 1:I:402:TRP:HE3 | 1.69 | 0.57 |
| 1:I:463:PRO:HA | 1:I:466:ARG:HH21 | 1.69 | 0.57 |
| 1:J:281:GLY:O | 1:J:284:ALA:N | 2.29 | 0.57 |
| 1:L:121:PRO:HD3 | 1:L:222:LEU:HD13 | 1.87 | 0.57 |
| 1:N:149:MET:HE3 | 1:N:294:THR:HG22 | 1.87 | 0.57 |
| 1:N:300:VAL:HG11 | 1:N:337:THR:HA | 1.86 | 0.57 |
| 1:O:176:THR:CG2 | 1:O:176:THR:CA | 2.82 | 0.57 |
| 1:A:92:ASN:HD22 | 1:A:95:THR:H | 1.50 | 0.57 |
| 1:B:61:LEU:CD1 | 1:B:61:LEU:HG | 2.17 | 0.57 |
| 1:B:75:ILE:HG23 | 1:B:451:LEU:HD12 | 1.84 | 0.57 |
| 1:B:439:ASP:O | 1:B:442:LYS:HB2 | 2.05 | 0.57 |
| 1:C:24:THR:HG21 | 1:C:320:ASN:HA | 1.87 | 0.57 |
| 1:D:123:LEU:HD23 | 1:D:147:ILE:HB | 1.87 | 0.57 |
| 1:D:380:LYS:CE | 1:D:380:LYS:HG3 | 2.33 | 0.57 |
| 1:E:180:VAL:HG13 | 1:E:184:ASP:CB | 2.34 | 0.57 |
| 1:F:77:LEU:HD22 | 1:F:455:PHE:CZ | 2.40 | 0.57 |
| 1:G:54:LYS:HG3 | 1:G:55:PRO:CD | 2.28 | 0.57 |
| 1:G:220:VAL:O | 1:G:221:PRO:O | 2.23 | 0.57 |
| 1:G:391:ILE:HG23 | 1:G:398:ILE:HG21 | 1.86 | 0.57 |
| 1:I:54:LYS:HA | 1:I:54:LYS:NZ | 2.20 | 0.57 |
| 1:K:342:MET:HB2 | 1:L:208:MET:HE1 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:22:VAL:HG23 | 1:L:22:VAL:O | 2.05 | 0.57 |
| 1:N:259:HIS:CE1 | 1:O:130:GLU:CG | 2.88 | 0.57 |
| 1:O:81:ASN:ND2 | 1:O:402:TRP:CD1 | 2.73 | 0.57 |
| 1:A:196:GLN:O | 1:A:199:ASP:OD2 | 2.22 | 0.57 |
| 1:C:59:LYS:CE | 1:C:59:LYS:CG | 2.78 | 0.57 |
| 1:C:149:MET:HE2 | 1:C:205:PHE:CE1 | 2.40 | 0.57 |
| 1:D:210:PHE:CD1 | 1:D:224:ILE:HB | 2.40 | 0.57 |
| 1:E:470:LEU:O | 1:E:470:LEU:CD2 | 2.52 | 0.57 |
| 1:G:115:VAL:CG2 | 1:H:257:VAL:HG13 | 2.35 | 0.57 |
| 1:H:28:VAL:CG1 | 1:H:29:ALA:N | 2.66 | 0.57 |
| 1:I:113:LEU:HB2 | 1:J:253:GLU:OE1 | 2.04 | 0.57 |
| 1:J:303:ASP:N | 1:J:303:ASP:OD1 | 2.36 | 0.57 |
| 1:K:21:VAL:HG12 | 1:K:22:VAL:N | 2.19 | 0.57 |
| 1:L:54:LYS:HB2 | 1:L:57:ASN:HD22 | 1.70 | 0.57 |
| 1:L:96:GLN:HB3 | 1:L:382:THR:HG22 | 1.87 | 0.57 |
| 1:M:96:GLN:HE21 | 1:M:382:THR:HG22 | 1.70 | 0.57 |
| 1:M:126:LEU:CD1 | 1:M:264:ALA:HB2 | 2.35 | 0.57 |
| 1:N:36:HIS:C | 1:N:36:HIS:ND1 | 2.58 | 0.57 |
| 1:N:172:GLY:O | 1:N:173:SER:O | 2.22 | 0.57 |
| 1:O:49:TYR:HA | 1:O:223:ASP:HB3 | 1.86 | 0.57 |
| 1:O:398:ILE:HG23 | 1:O:398:ILE:HD12 | 1.85 | 0.57 |
| 1:A:99:VAL:HG12 | 1:A:100:TRP:O | 2.04 | 0.56 |
| 1:B:151:TYR:OH | 1:B:221:PRO:HB2 | 2.05 | 0.56 |
| 1:D:97:ARG:HA | 1:D:97:ARG:NH1 | 2.20 | 0.56 |
| 1:D:250:LEU:N | 1:D:250:LEU:CD1 | 2.63 | 0.56 |
| 1:F:69:GLN:HA | 1:F:199:ASP:O | 2.05 | 0.56 |
| 1:F:220:VAL:O | 1:F:221:PRO:C | 2.40 | 0.56 |
| 1:G:20:ALA:CB | 1:G:20:ALA:HA | 2.20 | 0.56 |
| 1:G:70:TYR:CD2 | 1:G:195:ILE:HG21 | 2.40 | 0.56 |
| 1:I:88:THR:CG2 | 1:I:88:THR:CA | 2.78 | 0.56 |
| 1:I:149:MET:HE2 | 1:I:205:PHE:CE1 | 2.39 | 0.56 |
| 1:J:147:ILE:HG22 | 1:J:148:SER:N | 2.18 | 0.56 |
| 1:K:167:GLU:OE1 | 1:K:190:LEU:HD21 | 2.04 | 0.56 |
| 1:L:363:TYR:CG | 1:M:185:CYS:HB2 | 2.40 | 0.56 |
| 1:M:151:TYR:O | 1:M:152:LYS:C | 2.41 | 0.56 |
| 1:O:201:VAL:O | 1:O:229:CYS:SG | 2.61 | 0.56 |
| 1:A:271:VAL:HG13 | 1:A:275:LEU:HD12 | 1.86 | 0.56 |
| 1:A:272:PRO:HB2 | 1:A:275:LEU:HG | 1.87 | 0.56 |
| 1:B:183:GLY:O | 1:B:184:ASP:C | 2.41 | 0.56 |
| 1:B:234:TYR:O | 1:B:236:LYS:N | 2.37 | 0.56 |
| 1:C:169:TRP:H | 1:C:208:MET:HA | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:112:PRO:CD | 1:E:231:TYR:CD2 | 2.74 | 0.56 |
| 1:D:457:ALA:O | 1:D:459:LEU:CD2 | 2.52 | 0.56 |
| 1:E:188:LEU:CD1 | 1:E:213:LEU:HD11 | 2.35 | 0.56 |
| 1:F:54:LYS:HG2 | 1:F:57:ASN:HB3 | 1.87 | 0.56 |
| 1:F:80:PRO:HG2 | 1:F:98:LEU:O | 2.05 | 0.56 |
| 1:F:188:LEU:CD1 | 1:F:213:LEU:HD11 | 2.35 | 0.56 |
| 1:F:255:MET:O | 1:J:299:MET:HA | 2.05 | 0.56 |
| 1:G:54:LYS:HG2 | 1:G:57:ASN:HB3 | 1.87 | 0.56 |
| 1:G:139:ALA:O | 1:G:140:GLY:O | 2.22 | 0.56 |
| 1:H:299:MET:HA | 1:I:255:MET:O | 2.04 | 0.56 |
| 1:I:355:TYR:HB3 | 1:J:142:ASP:OD1 | 2.05 | 0.56 |
| 1:K:66:SER:H | 1:K:69:GLN:HE21 | 1.53 | 0.56 |
| 1:L:67:GLY:C | 1:L:68:LEU:HG | 2.26 | 0.56 |
| 1:L:74:ARG:CB | 1:L:330:PHE:HE2 | 2.19 | 0.56 |
| 1:M:52:ILE:HB | 1:M:62:VAL:HB | 1.86 | 0.56 |
| 1:N:121:PRO:HD3 | 1:N:222:LEU:HD13 | 1.87 | 0.56 |
| 1:O:49:TYR:HE2 | 1:O:118:SER:CA | 2.16 | 0.56 |
| 1:O:172:GLY:O | 1:O:173:SER:C | 2.43 | 0.56 |
| 1:B:24:THR:C | 1:B:26:GLU:N | 2.56 | 0.56 |
| 1:B:54:LYS:HA | 1:B:54:LYS:HZ1 | 1.70 | 0.56 |
| 1:B:76:HIS:HB2 | 1:B:449:VAL:O | 2.05 | 0.56 |
| 1:D:54:LYS:CB | 1:D:57:ASN:HD22 | 2.19 | 0.56 |
| 1:D:163:PRO:HB3 | 1:D:330:PHE:CE1 | 2.41 | 0.56 |
| 1:D:399:LEU:O | 1:D:402:TRP:HB2 | 2.05 | 0.56 |
| 1:E:101:ALA:CA | 1:E:322:GLY:O | 2.43 | 0.56 |
| 1:F:125:LYS:NZ | 1:G:132:ALA:O | 2.38 | 0.56 |
| 1:F:155:GLN:HG3 | 1:F:307:PHE:HE1 | 1.70 | 0.56 |
| 1:G:103:VAL:CG2 | 1:G:375:ILE:O | 2.53 | 0.56 |
| 1:G:169:TRP:H | 1:G:208:MET:HA | 1.70 | 0.56 |
| 1:G:178:VAL:O | 1:G:178:VAL:HG12 | 2.05 | 0.56 |
| 1:G:306:ILE:HD13 | 1:G:306:ILE:N | 2.20 | 0.56 |
| 1:G:320:ASN:OD1 | 1:G:321:ASN:N | 2.38 | 0.56 |
| 1:H:361:LYS:CG | 1:H:361:LYS:CA | 2.78 | 0.56 |
| 1:I:27:TYR:CE2 | 1:I:390:TYR:CE2 | 2.94 | 0.56 |
| 1:I:344:LEU:CD2 | 1:I:365:ARG:HB2 | 2.35 | 0.56 |
| 1:K:75:ILE:HD12 | 1:K:75:ILE:N | 2.19 | 0.56 |
| 1:K:141:VAL:HA | 1:O:357:ASN:HB2 | 1.87 | 0.56 |
| 1:K:323:ILE:O | 1:K:325:TRP:N | 2.38 | 0.56 |
| 1:L:44:ALA:HB3 | 1:L:368:GLU:HB2 | 1.88 | 0.56 |
| 1:M:80:PRO:HD3 | 1:M:100:TRP:HD1 | 1.70 | 0.56 |
| 1:M:152:LYS:HE2 | 1:M:202:ASP:HB3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:153:GLN:NE2 | 1:M:298:SER:O | 2.39 | 0.56 |
| 1:M:159:ILE:HG22 | 1:M:247:PHE:CE1 | 2.41 | 0.56 |
| 1:M:399:LEU:HA | 1:M:402:TRP:HE3 | 1.70 | 0.56 |
| 1:N:149:MET:CE | 1:N:205:PHE:HE1 | 2.18 | 0.56 |
| 1:N:171:LYS:HA | 1:N:187:PRO:O | 2.06 | 0.56 |
| 1:N:196:GLN:N | 1:N:199:ASP:OD2 | 2.38 | 0.56 |
| 1:O:105:VAL:HG22 | 1:O:374:PHE:CD2 | 2.40 | 0.56 |
| 1:A:237:MET:HB3 | 1:A:246:LEU:HD22 | 1.86 | 0.56 |
| 1:B:80:PRO:HG2 | 1:B:98:LEU:O | 2.05 | 0.56 |
| 1:B:385:ALA:O | 1:B:389:THR:HG23 | 2.05 | 0.56 |
| 1:D:42:LEU:HD13 | 1:D:73:PHE:HE2 | 1.70 | 0.56 |
| 1:G:112:PRO:CB | 1:H:202:ASP:OD2 | 2.53 | 0.56 |
| 1:H:46:GLY:CA | 1:H:65:VAL:HB | 2.36 | 0.56 |
| 1:H:252:ARG:HD2 | 1:H:306:ILE:HD11 | 1.88 | 0.56 |
| 1:J:241:PRO:O | 1:J:243:GLY:N | 2.37 | 0.56 |
| 1:K:36:HIS:C | 1:K:36:HIS:ND1 | 2.59 | 0.56 |
| 1:M:451:LEU:HA | 1:M:454:LYS:HG3 | 1.88 | 0.56 |
| 1:N:80:PRO:HG2 | 1:N:98:LEU:O | 2.06 | 0.56 |
| 1:N:343:SER:C | 1:N:344:LEU:HD23 | 2.25 | 0.56 |
| 1:O:125:LYS:HG3 | 1:O:147:ILE:HD11 | 1.87 | 0.56 |
| 1:B:75:ILE:HD12 | 1:B:75:ILE:N | 2.21 | 0.56 |
| 1:C:363:TYR:CD2 | 1:D:269:GLU:HG3 | 2.40 | 0.56 |
| 1:C:399:LEU:HA | 1:C:402:TRP:HE3 | 1.70 | 0.56 |
| 1:D:77:LEU:HB2 | 1:D:327:ASN:HB3 | 1.88 | 0.56 |
| 1:G:104:GLY:O | 1:G:374:PHE:CA | 2.53 | 0.56 |
| 1:H:75:ILE:HB | 1:H:329:LEU:CB | 2.35 | 0.56 |
| 1:L:75:ILE:N | 1:L:75:ILE:HD12 | 2.20 | 0.56 |
| 1:N:302:SER:O | 1:N:304:ALA:N | 2.38 | 0.56 |
| 1:A:74:ARG:CZ | 1:A:441:LEU:CD1 | 2.84 | 0.56 |
| 1:A:111:GLN:HB2 | 1:A:338:ARG:HD3 | 1.86 | 0.56 |
| 1:A:320:ASN:OD1 | 1:A:321:ASN:N | 2.39 | 0.56 |
| 1:B:41:ARG:HD3 | 1:B:43:LEU:HD13 | 1.87 | 0.56 |
| 1:B:225:CYS:SG | 1:B:225:CYS:CA | 2.90 | 0.56 |
| 1:C:153:GLN:HE22 | 1:C:300:VAL:HA | 1.70 | 0.56 |
| 1:D:194:VAL:CG2 | 1:D:194:VAL:HB | 2.18 | 0.56 |
| 1:D:464:LEU:CD2 | 1:D:464:LEU:C | 2.73 | 0.56 |
| 1:E:111:GLN:HG2 | 1:E:369:GLU:HB3 | 1.88 | 0.56 |
| 1:E:383:LEU:HD23 | 1:E:388:MET:HE2 | 1.86 | 0.56 |
| 1:H:384:THR:OG1 | 1:H:387:VAL:HG23 | 2.05 | 0.56 |
| 1:I:456:SER:HB3 | 1:I:462:PHE:HE1 | 1.70 | 0.56 |
| 1:K:171:LYS:HG3 | 1:K:187:PRO:HD2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:51:PRO:C | 1:N:52:ILE:HD12 | 2.25 | 0.56 |
| 1:N:246:LEU:H | 1:N:246:LEU:CD2 | 2.19 | 0.56 |
| 1:A:24:THR:HG21 | 1:A:320:ASN:HA | 1.87 | 0.56 |
| 1:A:185:CYS:SG | 1:E:344:LEU:HD11 | 2.45 | 0.56 |
| 1:C:75:ILE:CG2 | 1:C:451:LEU:HD12 | 2.36 | 0.56 |
| 1:D:74:ARG:HG3 | 1:D:330:PHE:HE2 | 1.69 | 0.56 |
| 1:D:159:ILE:HG22 | 1:D:247:PHE:HE1 | 1.69 | 0.56 |
| 1:E:247:PHE:HD1 | 1:E:248:PHE:H | 1.53 | 0.56 |
| 1:E:250:LEU:HD22 | 1:E:306:ILE:CG2 | 2.35 | 0.56 |
| 1:G:82:LYS:NZ | 1:G:403:ASN:HD22 | 2.02 | 0.56 |
| 1:G:149:MET:HA | 1:H:260:LEU:HD21 | 1.88 | 0.56 |
| 1:H:464:LEU:O | 1:H:464:LEU:CD2 | 2.53 | 0.56 |
| 1:H:469:LEU:CD2 | 1:H:469:LEU:CD1 | 2.82 | 0.56 |
| 1:I:150:ASP:N | 1:I:150:ASP:OD2 | 2.37 | 0.56 |
| 1:I:363:TYR:CE1 | 1:J:185:CYS:HB2 | 2.41 | 0.56 |
| 1:I:442:LYS:HB3 | 1:I:443:LYS:HD3 | 1.87 | 0.56 |
| 1:K:101:ALA:HA | 1:K:322:GLY:O | 2.06 | 0.56 |
| 1:K:217:LYS:HD3 | 1:L:274:ASP:O | 2.06 | 0.56 |
| 1:L:222:LEU:HA | 1:L:225:CYS:SG | 2.46 | 0.56 |
| 1:M:21:VAL:HG12 | 1:M:22:VAL:H | 1.71 | 0.56 |
| 1:A:163:PRO:N | 1:A:330:PHE:HD1 | 2.03 | 0.56 |
| 1:B:75:ILE:HB | 1:B:329:LEU:HB3 | 1.88 | 0.56 |
| 1:B:223:ASP:OD1 | 1:B:224:ILE:N | 2.39 | 0.56 |
| 1:B:356:LYS:O | 1:B:358:THR:N | 2.39 | 0.56 |
| 1:B:451:LEU:HA | 1:B:454:LYS:HG3 | 1.88 | 0.56 |
| 1:C:266:THR:OG1 | 1:C:266:THR:O | 2.22 | 0.56 |
| 1:D:180:VAL:CG1 | 1:D:184:ASP:CB | 2.83 | 0.56 |
| 1:E:57:ASN:HD21 | 1:E:59:LYS:N | 2.02 | 0.56 |
| 1:F:77:LEU:HB2 | 1:F:327:ASN:HB3 | 1.86 | 0.56 |
| 1:F:95:THR:O | 1:F:383:LEU:CB | 2.53 | 0.56 |
| 1:F:323:ILE:HD13 | 1:F:323:ILE:N | 2.20 | 0.56 |
| 1:G:378:LEU:HD12 | 1:G:379:CYS:N | 2.21 | 0.56 |
| 1:H:320:ASN:OD1 | 1:H:320:ASN:C | 2.44 | 0.56 |
| 1:H:374:PHE:HB3 | 1:H:376:PHE:CE1 | 2.40 | 0.56 |
| 1:I:75:ILE:HG21 | 1:I:451:LEU:HD12 | 1.85 | 0.56 |
| 1:J:73:PHE:N | 1:J:73:PHE:CD1 | 2.72 | 0.56 |
| 1:L:65:VAL:O | 1:L:65:VAL:HG12 | 2.06 | 0.56 |
| 1:M:42:LEU:HD22 | 1:M:447:TRP:CZ2 | 2.40 | 0.56 |
| 1:N:193:THR:CG2 | 1:N:230:LYS:HD3 | 2.36 | 0.56 |
| 1:N:440:PRO:HA | 1:N:443:LYS:NZ | 2.21 | 0.56 |
| 1:A:57:ASN:CG | 1:A:59:LYS:H | 2.09 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:248:PHE:CZ | 1:B:311:TYR:HB3 | 2.41 | 0.56 |
| 1:B:463:PRO:CB | 1:B:466:ARG:HH21 | 2.15 | 0.56 |
| 1:C:22:VAL:N | 1:C:390:TYR:OH | 2.25 | 0.56 |
| 1:C:75:ILE:HG23 | 1:C:451:LEU:HD12 | 1.88 | 0.56 |
| 1:F:156:LEU:HD11 | 1:F:334:VAL:HG23 | 1.87 | 0.56 |
| 1:F:180:VAL:O | 1:F:182:PRO:HD3 | 2.05 | 0.56 |
| 1:F:193:THR:HG21 | 1:F:230:LYS:HD3 | 1.88 | 0.56 |
| 1:G:105:VAL:CG2 | 1:G:105:VAL:CG1 | 2.75 | 0.56 |
| 1:G:153:GLN:NE2 | 1:G:300:VAL:HG12 | 2.21 | 0.56 |
| 1:I:54:LYS:HB3 | 1:I:57:ASN:HD22 | 1.69 | 0.56 |
| 1:K:34:TYR:CE2 | 1:K:377:GLN:HB2 | 2.41 | 0.56 |
| 1:K:170:GLY:HA2 | 1:K:213:LEU:HD21 | 1.88 | 0.56 |
| 1:L:125:LYS:HD3 | 1:L:125:LYS:C | 2.26 | 0.56 |
| 1:M:61:LEU:HG | 1:M:62:VAL:HG23 | 1.88 | 0.56 |
| 1:N:110:GLY:O | 1:N:111:GLN:HG2 | 2.06 | 0.56 |
| 1:N:156:LEU:C | 1:N:156:LEU:HD12 | 2.26 | 0.56 |
| 1:A:77:LEU:HB2 | 1:A:327:ASN:O | 2.06 | 0.56 |
| 1:C:59:LYS:CD | 1:C:59:LYS:NZ | 2.69 | 0.56 |
| 1:D:117:ILE:HD12 | 1:E:293:PRO:HB3 | 1.87 | 0.56 |
| 1:D:176:THR:O | 1:D:177:GLN:CD | 2.44 | 0.56 |
| 1:D:178:VAL:CG2 | 1:D:178:VAL:CA | 2.80 | 0.56 |
| 1:D:325:TRP:HB3 | 1:D:398:ILE:CD1 | 2.35 | 0.56 |
| 1:F:152:LYS:CB | 1:F:255:MET:HB2 | 2.36 | 0.56 |
| 1:G:24:THR:HG21 | 1:G:323:ILE:HG13 | 1.88 | 0.56 |
| 1:H:137:ALA:O | 1:H:138:ASN:C | 2.44 | 0.56 |
| 1:J:300:VAL:CG1 | 1:J:300:VAL:HB | 2.20 | 0.56 |
| 1:K:157:CYS:HB2 | 1:K:307:PHE:HE2 | 1.71 | 0.56 |
| 1:M:178:VAL:CG1 | 1:M:178:VAL:CA | 2.81 | 0.56 |
| 1:O:79:ASP:OD2 | 1:O:81:ASN:HB2 | 2.05 | 0.56 |
| 1:A:71:ARG:HA | 1:A:71:ARG:NH1 | 2.09 | 0.55 |
| 1:A:266:THR:OG1 | 1:A:266:THR:O | 2.20 | 0.55 |
| 1:A:280:SER:O | 1:A:281:GLY:C | 2.45 | 0.55 |
| 1:C:54:LYS:HB2 | 1:C:57:ASN:HD22 | 1.70 | 0.55 |
| 1:D:65:VAL:O | 1:D:366:HIS:HB3 | 2.06 | 0.55 |
| 1:E:104:GLY:O | 1:E:374:PHE:HA | 2.06 | 0.55 |
| 1:F:220:VAL:HG23 | 1:F:225:CYS:HA | 1.88 | 0.55 |
| 1:G:74:ARG:CB | 1:G:330:PHE:HE2 | 2.18 | 0.55 |
| 1:G:210:PHE:CD1 | 1:G:220:VAL:HG21 | 2.41 | 0.55 |
| 1:G:467:LYS:O | 1:G:470:LEU:N | 2.38 | 0.55 |
| 1:H:21:VAL:HG12 | 1:H:22:VAL:N | 2.20 | 0.55 |
| 1:H:259:HIS:CE1 | 1:I:130:GLU:HG2 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:348:ILE:HG22 | 1:H:359:ASN:OD1 | 2.06 | 0.55 |
| 1:I:166:GLY:N | 1:I:195:ILE:CD1 | 2.69 | 0.55 |
| 1:J:126:LEU:HB3 | 1:J:262:ASN:O | 2.06 | 0.55 |
| 1:J:130:GLU:HB2 | 1:J:260:LEU:CD1 | 2.25 | 0.55 |
| 1:K:111:GLN:HG2 | 1:K:369:GLU:HB3 | 1.88 | 0.55 |
| 1:L:139:ALA:HB1 | 1:L:143:ASN:CG | 2.26 | 0.55 |
| 1:M:323:ILE:CD1 | 1:M:323:ILE:N | 2.68 | 0.55 |
| 1:O:235:ILE:CD1 | 1:O:235:ILE:CG2 | 2.85 | 0.55 |
| 1:O:260:LEU:HD12 | 1:O:260:LEU:N | 2.21 | 0.55 |
| 1:A:122:LEU:HD21 | 1:B:286:LEU:HD12 | 1.87 | 0.55 |
| 1:A:372:LEU:HB3 | 1:A:374:PHE:HE1 | 1.71 | 0.55 |
| 1:B:85:PHE:CE2 | 1:B:378:LEU:HD22 | 2.41 | 0.55 |
| 1:C:96:GLN:HE21 | 1:C:382:THR:HG22 | 1.72 | 0.55 |
| 1:D:228:ILE:HG22 | 1:D:230:LYS:HG3 | 1.89 | 0.55 |
| 1:E:40:SER:O | 1:E:371:ASP:OD1 | 2.24 | 0.55 |
| 1:E:302:SER:C | 1:E:304:ALA:H | 2.09 | 0.55 |
| 1:G:384:THR:H | 1:G:387:VAL:HB | 1.70 | 0.55 |
| 1:L:77:LEU:HD22 | 1:L:455:PHE:CZ | 2.40 | 0.55 |
| 1:M:21:VAL:HG12 | 1:M:22:VAL:N | 2.21 | 0.55 |
| 1:N:118:SER:HB2 | 1:N:151:TYR:CE1 | 2.41 | 0.55 |
| 1:N:464:LEU:O | 1:N:464:LEU:HD22 | 2.06 | 0.55 |
| 1:O:65:VAL:CA | 1:O:69:GLN:HE22 | 2.13 | 0.55 |
| 1:O:237:MET:O | 1:O:240:GLU:HB3 | 2.06 | 0.55 |
| 1:O:396:SER:O | 1:O:400:GLU:HG3 | 2.06 | 0.55 |
| 1:C:463:PRO:CB | 1:C:466:ARG:HH21 | 2.19 | 0.55 |
| 1:D:171:LYS:HA | 1:D:187:PRO:O | 2.07 | 0.55 |
| 1:D:400:GLU:O | 1:D:401:ASP:C | 2.44 | 0.55 |
| 1:G:248:PHE:CE2 | 1:G:311:TYR:HB3 | 2.42 | 0.55 |
| 1:L:79:ASP:OD2 | 1:L:81:ASN:HB2 | 2.05 | 0.55 |
| 1:M:108:GLY:O | 1:M:109:ARG:HG2 | 2.07 | 0.55 |
| 1:M:139:ALA:O | 1:M:140:GLY:O | 2.23 | 0.55 |
| 1:M:358:THR:HA | 1:N:266:THR:CG2 | 2.36 | 0.55 |
| 1:N:43:LEU:HD12 | 1:N:369:GLU:HA | 1.87 | 0.55 |
| 1:N:49:TYR:HE1 | 1:N:364:LEU:HD13 | 1.71 | 0.55 |
| 1:O:33:ILE:O | 1:O:377:GLN:HA | 2.07 | 0.55 |
| 1:O:317:GLN:C | 1:O:317:GLN:NE2 | 2.59 | 0.55 |
| 1:O:442:LYS:HG2 | 1:O:442:LYS:HZ2 | 1.71 | 0.55 |
| 1:C:440:PRO:C | 1:C:443:LYS:NZ | 2.60 | 0.55 |
| 1:E:105:VAL:HG22 | 1:E:374:PHE:CD2 | 2.41 | 0.55 |
| 1:F:66:SER:N | 1:F:69:GLN:HE21 | 2.05 | 0.55 |
| 1:F:257:VAL:HG21 | 1:J:150:ASP:CG | 2.26 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:237:MET:O | 1:H:240:GLU:HB3 | 2.07 | 0.55 |
| 1:J:78:PRO:HD2 | 1:J:455:PHE:CZ | 2.42 | 0.55 |
| 1:J:440:PRO:HA | 1:J:443:LYS:NZ | 2.21 | 0.55 |
| 1:K:165:ILE:CD1 | 1:K:165:ILE:CB | 2.78 | 0.55 |
| 1:M:144:ARG:CG | 1:M:144:ARG:CA | 2.80 | 0.55 |
| 1:M:151:TYR:CG | 1:M:203:THR:HB | 2.41 | 0.55 |
| 1:M:389:THR:O | 1:M:392:HIS:HB3 | 2.07 | 0.55 |
| 1:N:92:ASN:O | 1:N:94:ASP:N | 2.39 | 0.55 |
| 1:N:228:ILE:HD12 | 1:N:228:ILE:N | 2.22 | 0.55 |
| 1:A:216:ASN:HA | 1:E:360:PHE:CE2 | 2.42 | 0.55 |
| 1:B:42:LEU:HD22 | 1:B:447:TRP:CZ2 | 2.41 | 0.55 |
| 1:B:273:ASP:OD2 | 1:B:273:ASP:N | 2.40 | 0.55 |
| 1:B:345:CYS:HB2 | 1:B:361:LYS:O | 2.06 | 0.55 |
| 1:C:326:GLY:O | 1:C:327:ASN:HB2 | 2.06 | 0.55 |
| 1:D:36:HIS:ND1 | 1:D:37:ALA:N | 2.55 | 0.55 |
| 1:E:338:ARG:HG3 | 1:E:338:ARG:HH11 | 1.70 | 0.55 |
| 1:F:81:ASN:OD1 | 1:F:97:ARG:NH1 | 2.39 | 0.55 |
| 1:I:305:GLN:HE22 | 1:I:337:THR:HG21 | 1.71 | 0.55 |
| 1:J:397:THR:C | 1:J:401:ASP:OD2 | 2.45 | 0.55 |
| 1:K:144:ARG:C | 1:K:145:GLU:HG2 | 2.26 | 0.55 |
| 1:K:180:VAL:HG13 | 1:K:184:ASP:HB3 | 1.89 | 0.55 |
| 1:K:209:ASP:OD2 | 1:K:212:THR:HG23 | 2.06 | 0.55 |
| 1:K:231:TYR:OH | 1:K:253:GLU:OE2 | 2.15 | 0.55 |
| 1:K:266:THR:HG1 | 1:O:361:LYS:HA | 1.70 | 0.55 |
| 1:M:216:ASN:O | 1:M:216:ASN:OD1 | 2.24 | 0.55 |
| 1:N:168:HIS:CE1 | 1:N:191:ILE:HB | 2.42 | 0.55 |
| 1:N:302:SER:C | 1:N:304:ALA:H | 2.10 | 0.55 |
| 1:N:302:SER:HB2 | 1:O:253:GLU:H | 1.71 | 0.55 |
| 1:O:267:VAL:CG1 | 1:O:269:GLU:O | 2.55 | 0.55 |
| 1:O:373:GLN:CB | 1:O:464:LEU:HD12 | 2.36 | 0.55 |
| 1:A:66:SER:HA | 1:A:366:HIS:ND1 | 2.22 | 0.55 |
| 1:A:95:THR:O | 1:A:383:LEU:N | 2.35 | 0.55 |
| 1:A:120:HIS:CG | 1:A:222:LEU:HD13 | 2.41 | 0.55 |
| 1:A:240:GLU:HG3 | 1:A:243:GLY:N | 2.21 | 0.55 |
| 1:C:162:LYS:O | 1:C:330:PHE:HD1 | 1.89 | 0.55 |
| 1:E:42:LEU:HD13 | 1:E:447:TRP:CZ2 | 2.42 | 0.55 |
| 1:F:24:THR:CG2 | 1:F:320:ASN:HA | 2.35 | 0.55 |
| 1:H:112:PRO:HB2 | 1:I:202:ASP:OD2 | 2.07 | 0.55 |
| 1:I:166:GLY:O | 1:I:192:ASN:HA | 2.07 | 0.55 |
| 1:I:196:GLN:HB3 | 1:I:445:THR:O | 2.06 | 0.55 |
| 1:J:208:MET:SD | 1:J:210:PHE:CE2 | 2.99 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:28:VAL:HG22 | 1:K:381:ILE:HD11 | 1.89 | 0.55 |
| 1:K:54:LYS:CB | 1:K:57:ASN:HD22 | 2.19 | 0.55 |
| 1:L:158:LEU:HD23 | 1:L:249:TYR:HB2 | 1.88 | 0.55 |
| 1:M:102:CYS:N | 1:M:322:GLY:O | 2.38 | 0.55 |
| 1:M:108:GLY:C | 1:M:109:ARG:HG2 | 2.27 | 0.55 |
| 1:N:180:VAL:HG12 | 1:N:181:GLN:O | 2.07 | 0.55 |
| 1:N:259:HIS:CE1 | 1:O:130:GLU:HG2 | 2.42 | 0.55 |
| 1:N:365:ARG:HH11 | 1:N:365:ARG:HG3 | 1.72 | 0.55 |
| 1:A:114:GLY:HA3 | 1:A:340:THR:OG1 | 2.07 | 0.55 |
| 1:A:185:CYS:HB2 | 1:E:363:TYR:CE1 | 2.42 | 0.55 |
| 1:A:259:HIS:HE1 | 1:B:130:GLU:OE1 | 1.90 | 0.55 |
| 1:B:46:GLY:CA | 1:B:65:VAL:CG2 | 2.80 | 0.55 |
| 1:B:441:LEU:CD2 | 1:B:441:LEU:HG | 2.18 | 0.55 |
| 1:C:46:GLY:HA3 | 1:C:63:PRO:O | 2.06 | 0.55 |
| 1:C:96:GLN:HB3 | 1:C:382:THR:HG22 | 1.89 | 0.55 |
| 1:D:361:LYS:HD2 | 1:E:183:GLY:HA3 | 1.88 | 0.55 |
| 1:F:219:GLU:C | 1:F:220:VAL:HG13 | 2.27 | 0.55 |
| 1:F:221:PRO:HD2 | 1:F:224:ILE:HD11 | 1.89 | 0.55 |
| 1:F:344:LEU:HD23 | 1:F:344:LEU:N | 2.21 | 0.55 |
| 1:G:150:ASP:CB | 1:H:257:VAL:HG21 | 2.36 | 0.55 |
| 1:J:42:LEU:HB2 | 1:J:370:TYR:HB2 | 1.87 | 0.55 |
| 1:M:97:ARG:HA | 1:M:97:ARG:HH11 | 1.71 | 0.55 |
| 1:M:113:LEU:CD1 | 1:M:113:LEU:H | 2.19 | 0.55 |
| 1:N:115:VAL:HG22 | 1:O:255:MET:CE | 2.36 | 0.55 |
| 1:N:348:ILE:O | 1:N:349:SER:HB3 | 2.06 | 0.55 |
| 1:N:358:THR:HG22 | 1:O:266:THR:HG22 | 1.88 | 0.55 |
| 1:A:24:THR:CG2 | 1:A:320:ASN:HA | 2.37 | 0.55 |
| 1:A:142:ASP:OD2 | 1:A:144:ARG:HG3 | 2.06 | 0.55 |
| 1:A:185:CYS:HB2 | 1:E:363:TYR:CD1 | 2.42 | 0.55 |
| 1:A:205:PHE:CD1 | 1:A:220:VAL:HG12 | 2.42 | 0.55 |
| 1:A:342:MET:SD | 1:B:208:MET:HE3 | 2.47 | 0.55 |
| 1:C:96:GLN:HE21 | 1:C:382:THR:CG2 | 2.19 | 0.55 |
| 1:D:24:THR:HG23 | 1:D:320:ASN:HA | 1.87 | 0.55 |
| 1:D:109:ARG:NH1 | 1:D:370:TYR:CE1 | 2.74 | 0.55 |
| 1:D:466:ARG:HD2 | 1:E:317:GLN:O | 2.06 | 0.55 |
| 1:E:126:LEU:HB3 | 1:E:262:ASN:HB3 | 1.89 | 0.55 |
| 1:E:260:LEU:N | 1:E:260:LEU:HD12 | 2.22 | 0.55 |
| 1:F:344:LEU:HB2 | 1:G:213:LEU:O | 2.06 | 0.55 |
| 1:G:271:VAL:HG12 | 1:G:276:TYR:HE2 | 1.72 | 0.55 |
| 1:G:395:ASN:C | 1:G:395:ASN:HD22 | 2.09 | 0.55 |
| 1:H:372:LEU:CB | 1:H:374:PHE:HE1 | 2.20 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:70:TYR:CD2 | 1:J:195:ILE:HG21 | 2.42 | 0.55 |
| 1:J:262:ASN:ND2 | 1:J:288:SER:HB3 | 2.21 | 0.55 |
| 1:K:21:VAL:C | 1:K:22:VAL:HG13 | 2.27 | 0.55 |
| 1:K:92:ASN:ND2 | 1:K:95:THR:OG1 | 2.40 | 0.55 |
| 1:K:216:ASN:ND2 | 1:K:219:GLU:OE2 | 2.40 | 0.55 |
| 1:L:121:PRO:HD3 | 1:L:222:LEU:CD1 | 2.37 | 0.55 |
| 1:L:159:ILE:CD1 | 1:L:159:ILE:CB | 2.83 | 0.55 |
| 1:O:216:ASN:CB | 1:O:219:GLU:OE2 | 2.55 | 0.55 |
| 1:O:471:GLN:O | 1:O:472:LEU:OXT | 2.25 | 0.55 |
| 1:A:299:MET:HA | 1:B:255:MET:O | 2.07 | 0.55 |
| 1:A:325:TRP:HB3 | 1:A:398:ILE:CD1 | 2.37 | 0.55 |
| 1:A:395:ASN:HB3 | 1:A:398:ILE:CG1 | 2.37 | 0.55 |
| 1:B:49:TYR:HA | 1:B:223:ASP:HB3 | 1.88 | 0.55 |
| 1:B:240:GLU:HG3 | 1:B:243:GLY:HA2 | 1.88 | 0.55 |
| 1:B:387:VAL:O | 1:B:390:TYR:N | 2.40 | 0.55 |
| 1:C:112:PRO:HD3 | 1:D:231:TYR:CD2 | 2.41 | 0.55 |
| 1:D:149:MET:HE1 | 1:D:205:PHE:CE1 | 2.41 | 0.55 |
| 1:D:152:LYS:HE3 | 1:D:253:GLU:HB2 | 1.89 | 0.55 |
| 1:D:163:PRO:CA | 1:D:330:PHE:CD1 | 2.90 | 0.55 |
| 1:F:144:ARG:HD3 | 1:J:355:TYR:CD1 | 2.42 | 0.55 |
| 1:F:391:ILE:HG22 | 1:F:399:LEU:HG | 1.89 | 0.55 |
| 1:G:234:TYR:O | 1:G:235:ILE:C | 2.41 | 0.55 |
| 1:K:164:PRO:HG3 | 1:K:332:THR:HG23 | 1.88 | 0.55 |
| 1:K:255:MET:CE | 1:O:115:VAL:H | 2.20 | 0.55 |
| 1:K:450:ASN:ND2 | 1:K:452:LYS:HD2 | 2.21 | 0.55 |
| 1:M:80:PRO:HB3 | 1:M:100:TRP:NE1 | 2.22 | 0.55 |
| 1:M:399:LEU:O | 1:M:402:TRP:HB2 | 2.07 | 0.55 |
| 1:N:66:SER:O | 1:N:69:GLN:HG3 | 2.06 | 0.55 |
| 1:N:280:SER:CA | 1:N:284:ALA:HB2 | 2.37 | 0.55 |
| 1:N:382:THR:CG2 | 1:N:382:THR:HB | 2.17 | 0.55 |
| 1:O:280:SER:C | 1:O:284:ALA:HB2 | 2.26 | 0.55 |
| 1:A:68:LEU:HB3 | 1:A:201:VAL:HG22 | 1.89 | 0.55 |
| 1:B:193:THR:HG23 | 1:B:230:LYS:HD2 | 1.88 | 0.55 |
| 1:B:325:TRP:CE2 | 1:B:394:MET:CE | 2.89 | 0.55 |
| 1:C:21:VAL:HG12 | 1:C:22:VAL:N | 2.22 | 0.55 |
| 1:C:323:ILE:HD13 | 1:C:323:ILE:N | 2.22 | 0.55 |
| 1:C:372:LEU:HB3 | 1:C:374:PHE:CE1 | 2.42 | 0.55 |
| 1:D:247:PHE:HD1 | 1:D:248:PHE:N | 2.04 | 0.55 |
| 1:F:256:PHE:HB3 | 1:J:299:MET:CA | 2.37 | 0.55 |
| 1:F:353:THR:CG2 | 1:F:353:THR:CA | 2.79 | 0.55 |
| 1:F:374:PHE:O | 1:F:375:ILE:HD13 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:151:TYR:CG | 1:H:203:THR:HB | 2.41 | 0.55 |
| 1:H:237:MET:SD | 1:H:237:MET:CB | 2.91 | 0.55 |
| 1:I:259:HIS:HE1 | 1:J:130:GLU:HG2 | 1.71 | 0.55 |
| 1:J:54:LYS:CG | 1:J:55:PRO:HD2 | 2.33 | 0.55 |
| 1:J:184:ASP:O | 1:J:185:CYS:O | 2.25 | 0.55 |
| 1:K:163:PRO:HD3 | 1:K:330:PHE:HE1 | 1.72 | 0.55 |
| 1:K:170:GLY:HA2 | 1:K:213:LEU:CD2 | 2.37 | 0.55 |
| 1:K:207:ALA:O | 1:K:208:MET:HB3 | 2.05 | 0.55 |
| 1:L:27:TYR:OH | 1:L:390:TYR:HE2 | 1.90 | 0.55 |
| 1:L:98:LEU:HA | 1:L:379:CYS:O | 2.07 | 0.55 |
| 1:L:122:LEU:HD11 | 1:M:286:LEU:CD1 | 2.33 | 0.55 |
| 1:M:150:ASP:OD1 | 1:N:257:VAL:HG21 | 2.07 | 0.55 |
| 1:N:299:MET:HA | 1:O:256:PHE:HB3 | 1.88 | 0.55 |
| 1:O:122:LEU:O | 1:O:218:SER:HB2 | 2.07 | 0.55 |
| 1:A:286:LEU:CD1 | 1:E:122:LEU:CD1 | 2.70 | 0.54 |
| 1:B:344:LEU:HD12 | 1:C:186:PRO:CG | 2.37 | 0.54 |
| 1:C:247:PHE:CD1 | 1:C:248:PHE:N | 2.75 | 0.54 |
| 1:C:451:LEU:HA | 1:C:454:LYS:HG3 | 1.88 | 0.54 |
| 1:D:92:ASN:HD21 | 1:D:94:ASP:HB2 | 1.70 | 0.54 |
| 1:D:358:THR:HA | 1:E:266:THR:HG22 | 1.85 | 0.54 |
| 1:E:54:LYS:CB | 1:E:57:ASN:HD22 | 2.20 | 0.54 |
| 1:E:345:CYS:SG | 1:E:345:CYS:O | 2.64 | 0.54 |
| 1:E:378:LEU:HD12 | 1:E:379:CYS:H | 1.71 | 0.54 |
| 1:F:389:THR:CG2 | 1:F:389:THR:CA | 2.77 | 0.54 |
| 1:G:52:ILE:N | 1:G:52:ILE:CD1 | 2.70 | 0.54 |
| 1:G:163:PRO:CA | 1:G:330:PHE:CD1 | 2.90 | 0.54 |
| 1:G:193:THR:HG21 | 1:G:230:LYS:HD3 | 1.87 | 0.54 |
| 1:G:214:GLN:CD | 1:G:219:GLU:HG3 | 2.27 | 0.54 |
| 1:G:246:LEU:HD12 | 1:G:249:TYR:CB | 2.38 | 0.54 |
| 1:H:219:GLU:C | 1:H:220:VAL:HG13 | 2.27 | 0.54 |
| 1:I:179:ALA:O | 1:I:180:VAL:O | 2.25 | 0.54 |
| 1:I:246:LEU:HD23 | 1:I:246:LEU:N | 2.16 | 0.54 |
| 1:K:72:VAL:HG21 | 1:K:195:ILE:O | 2.06 | 0.54 |
| 1:K:159:ILE:HG22 | 1:K:247:PHE:HE1 | 1.72 | 0.54 |
| 1:K:463:PRO:HD3 | 1:K:466:ARG:NH2 | 2.22 | 0.54 |
| 1:L:344:LEU:HD23 | 1:L:344:LEU:H | 1.69 | 0.54 |
| 1:M:50:PHE:HB2 | 1:M:51:PRO:HD2 | 1.90 | 0.54 |
| 1:N:250:LEU:HD13 | 1:N:306:ILE:CG2 | 2.36 | 0.54 |
| 1:O:107:VAL:HG23 | 1:O:311:TYR:HE1 | 1.72 | 0.54 |
| 1:O:170:GLY:HA2 | 1:O:213:LEU:CD2 | 2.34 | 0.54 |
| 1:O:443:LYS:N | 1:O:443:LYS:CD | 2.70 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:67:GLY:N | 1:A:366:HIS:CE1 | 2.74 | 0.54 |
| 1:A:115:VAL:HG22 | 1:B:255:MET:HE1 | 1.88 | 0.54 |
| 1:A:397:THR:O | 1:A:398:ILE:C | 2.45 | 0.54 |
| 1:C:160:GLY:HA3 | 1:C:245:SER:O | 2.07 | 0.54 |
| 1:D:222:LEU:HA | 1:D:225:CYS:SG | 2.47 | 0.54 |
| 1:E:99:VAL:CG1 | 1:E:323:ILE:HG22 | 2.30 | 0.54 |
| 1:H:68:LEU:O | 1:H:201:VAL:HG13 | 2.06 | 0.54 |
| 1:H:151:TYR:CZ | 1:H:221:PRO:HG2 | 2.42 | 0.54 |
| 1:I:41:ARG:HD3 | 1:I:43:LEU:HD13 | 1.88 | 0.54 |
| 1:I:463:PRO:CB | 1:I:466:ARG:HH21 | 2.20 | 0.54 |
| 1:J:223:ASP:OD1 | 1:J:224:ILE:N | 2.39 | 0.54 |
| 1:J:305:GLN:HE22 | 1:J:337:THR:HG21 | 1.72 | 0.54 |
| 1:K:77:LEU:HB2 | 1:K:327:ASN:O | 2.07 | 0.54 |
| 1:M:300:VAL:O | 1:N:254:GLN:HA | 2.06 | 0.54 |
| 1:N:381:ILE:O | 1:N:383:LEU:HD12 | 2.07 | 0.54 |
| 1:O:149:MET:HE2 | 1:O:205:PHE:CE1 | 2.42 | 0.54 |
| 1:B:33:ILE:CD1 | 1:B:33:ILE:CG2 | 2.85 | 0.54 |
| 1:C:305:GLN:HE22 | 1:C:337:THR:HG21 | 1.72 | 0.54 |
| 1:D:117:ILE:HG23 | 1:D:117:ILE:O | 2.06 | 0.54 |
| 1:G:22:VAL:HG23 | 1:G:22:VAL:O | 2.07 | 0.54 |
| 1:G:395:ASN:O | 1:G:398:ILE:HG12 | 2.07 | 0.54 |
| 1:H:258:ARG:NH2 | 1:I:257:VAL:O | 2.41 | 0.54 |
| 1:I:61:LEU:CD1 | 1:I:61:LEU:CD2 | 2.80 | 0.54 |
| 1:M:54:LYS:HG3 | 1:M:55:PRO:HD2 | 1.89 | 0.54 |
| 1:N:207:ALA:HB1 | 1:N:229:CYS:O | 2.07 | 0.54 |
| 1:O:439:ASP:O | 1:O:442:LYS:HB2 | 2.08 | 0.54 |
| 1:D:162:LYS:HG2 | 1:D:244:ASP:HB3 | 1.87 | 0.54 |
| 1:D:461:GLN:HE22 | 1:E:21:VAL:HB | 1.72 | 0.54 |
| 1:F:59:LYS:NZ | 1:F:59:LYS:CD | 2.68 | 0.54 |
| 1:F:90:PHE:HD1 | 1:F:91:TYR:HB3 | 1.73 | 0.54 |
| 1:F:178:VAL:CG1 | 1:F:178:VAL:CA | 2.81 | 0.54 |
| 1:F:185:CYS:HB2 | 1:J:363:TYR:CD1 | 2.42 | 0.54 |
| 1:G:272:PRO:HD2 | 1:G:275:LEU:CD1 | 2.37 | 0.54 |
| 1:G:300:VAL:HG23 | 1:G:300:VAL:O | 2.06 | 0.54 |
| 1:I:222:LEU:HA | 1:I:225:CYS:SG | 2.47 | 0.54 |
| 1:K:96:GLN:CA | 1:K:382:THR:HA | 2.38 | 0.54 |
| 1:L:96:GLN:NE2 | 1:L:382:THR:HG22 | 2.22 | 0.54 |
| 1:O:398:ILE:CD1 | 1:O:398:ILE:HG23 | 2.38 | 0.54 |
| 1:A:30:ARG:HH11 | 1:A:377:GLN:HE22 | 1.55 | 0.54 |
| 1:C:373:GLN:C | 1:C:374:PHE:CD1 | 2.81 | 0.54 |
| 1:D:153:GLN:HE22 | 1:D:300:VAL:HA | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:166:GLY:CA | 1:D:195:ILE:HD11 | 2.37 | 0.54 |
| 1:E:105:VAL:HA | 1:E:373:GLN:O | 2.08 | 0.54 |
| 1:E:150:ASP:OD1 | 1:E:296:SER:HA | 2.06 | 0.54 |
| 1:E:152:LYS:CE | 1:E:202:ASP:HB3 | 2.37 | 0.54 |
| 1:E:153:GLN:HE22 | 1:E:300:VAL:HA | 1.71 | 0.54 |
| 1:E:180:VAL:O | 1:E:182:PRO:HD3 | 2.08 | 0.54 |
| 1:F:273:ASP:OD2 | 1:F:273:ASP:N | 2.39 | 0.54 |
| 1:H:49:TYR:HE2 | 1:H:118:SER:CA | 2.12 | 0.54 |
| 1:H:175:CYS:O | 1:H:177:GLN:N | 2.41 | 0.54 |
| 1:K:97:ARG:HA | 1:K:97:ARG:NH1 | 2.21 | 0.54 |
| 1:L:162:LYS:C | 1:L:330:PHE:HD1 | 2.11 | 0.54 |
| 1:N:151:TYR:OH | 1:N:221:PRO:CG | 2.43 | 0.54 |
| 1:O:152:LYS:O | 1:O:152:LYS:HG3 | 2.07 | 0.54 |
| 1:B:74:ARG:CG | 1:B:330:PHE:HE2 | 2.20 | 0.54 |
| 1:B:114:GLY:HA3 | 1:B:340:THR:OG1 | 2.08 | 0.54 |
| 1:C:80:PRO:HB3 | 1:C:100:TRP:NE1 | 2.23 | 0.54 |
| 1:C:374:PHE:C | 1:C:375:ILE:HG12 | 2.28 | 0.54 |
| 1:D:242:TYR:CD2 | 1:D:394:MET:HG3 | 2.43 | 0.54 |
| 1:D:381:ILE:O | 1:D:383:LEU:HD12 | 2.08 | 0.54 |
| 1:E:162:LYS:C | 1:E:330:PHE:HD1 | 2.11 | 0.54 |
| 1:E:386:ASP:OD2 | 1:E:386:ASP:N | 2.41 | 0.54 |
| 1:E:395:ASN:ND2 | 1:E:397:THR:OG1 | 2.41 | 0.54 |
| 1:F:262:ASN:HD22 | 1:F:263:ARG:N | 2.06 | 0.54 |
| 1:H:79:ASP:OD1 | 1:H:80:PRO:HD2 | 2.08 | 0.54 |
| 1:H:149:MET:HE2 | 1:H:205:PHE:CE1 | 2.42 | 0.54 |
| 1:I:32:ASN:O | 1:I:33:ILE:HD13 | 2.07 | 0.54 |
| 1:I:220:VAL:HB | 1:I:224:ILE:CD1 | 2.37 | 0.54 |
| 1:J:97:ARG:H | 1:J:381:ILE:H | 1.54 | 0.54 |
| 1:J:120:HIS:ND1 | 1:J:122:LEU:N | 2.48 | 0.54 |
| 1:K:42:LEU:HD12 | 1:K:73:PHE:CE2 | 2.39 | 0.54 |
| 1:K:223:ASP:OD1 | 1:K:224:ILE:N | 2.41 | 0.54 |
| 1:K:459:LEU:O | 1:K:461:GLN:N | 2.41 | 0.54 |
| 1:M:36:HIS:CG | 1:M:462:PHE:CD1 | 2.96 | 0.54 |
| 1:M:302:SER:C | 1:M:304:ALA:H | 2.11 | 0.54 |
| 1:N:151:TYR:CZ | 1:N:221:PRO:HG2 | 2.39 | 0.54 |
| 1:O:220:VAL:O | 1:O:221:PRO:C | 2.44 | 0.54 |
| 1:O:261:PHE:CB | 1:O:292:PHE:CE2 | 2.88 | 0.54 |
| 1:C:49:TYR:CE2 | 1:C:118:SER:HA | 2.43 | 0.54 |
| 1:C:117:ILE:HD11 | 1:D:260:LEU:CD2 | 2.35 | 0.54 |
| 1:C:154:THR:O | 1:C:336:THR:HG23 | 2.08 | 0.54 |
| 1:C:234:TYR:CD1 | 1:C:251:ARG:NH2 | 2.76 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:70:TYR:O | 1:D:71:ARG:NH1 | 2.41 | 0.54 |
| 1:F:50:PHE:CD1 | 1:F:50:PHE:C | 2.80 | 0.54 |
| 1:F:94:ASP:C | 1:F:95:THR:HG23 | 2.26 | 0.54 |
| 1:H:189:GLU:O | 1:H:191:ILE:CG1 | 2.55 | 0.54 |
| 1:H:344:LEU:N | 1:H:344:LEU:HD23 | 2.23 | 0.54 |
| 1:I:49:TYR:HA | 1:I:223:ASP:HB3 | 1.90 | 0.54 |
| 1:I:117:ILE:CG1 | 1:I:149:MET:O | 2.56 | 0.54 |
| 1:I:280:SER:N | 1:I:284:ALA:HB2 | 2.22 | 0.54 |
| 1:J:66:SER:HA | 1:J:366:HIS:ND1 | 2.23 | 0.54 |
| 1:J:74:ARG:NH2 | 1:J:441:LEU:HD12 | 2.22 | 0.54 |
| 1:J:77:LEU:O | 1:J:327:ASN:HB3 | 2.08 | 0.54 |
| 1:J:155:GLN:HG2 | 1:J:307:PHE:CE1 | 2.43 | 0.54 |
| 1:L:171:LYS:HA | 1:L:187:PRO:O | 2.08 | 0.54 |
| 1:L:227:SER:HA | 1:L:228:ILE:HD12 | 1.88 | 0.54 |
| 1:M:54:LYS:HG2 | 1:M:57:ASN:HB3 | 1.88 | 0.54 |
| 1:M:66:SER:OG | 1:M:68:LEU:HB2 | 2.07 | 0.54 |
| 1:M:70:TYR:OH | 1:M:232:PRO:HD3 | 2.07 | 0.54 |
| 1:N:92:ASN:HD21 | 1:N:95:THR:N | 2.04 | 0.54 |
| 1:N:121:PRO:HD3 | 1:N:222:LEU:CD1 | 2.38 | 0.54 |
| 1:N:317:GLN:NE2 | 1:N:317:GLN:C | 2.60 | 0.54 |
| 1:A:21:VAL:CG1 | 1:A:22:VAL:N | 2.70 | 0.54 |
| 1:A:75:ILE:N | 1:A:75:ILE:CD1 | 2.64 | 0.54 |
| 1:C:471:GLN:CD | 1:C:472:LEU:N | 2.62 | 0.54 |
| 1:D:391:ILE:HG21 | 1:D:402:TRP:HZ3 | 1.72 | 0.54 |
| 1:F:50:PHE:HB2 | 1:F:51:PRO:HD2 | 1.89 | 0.54 |
| 1:G:50:PHE:HB2 | 1:G:51:PRO:HD2 | 1.90 | 0.54 |
| 1:I:66:SER:OG | 1:I:68:LEU:N | 2.41 | 0.54 |
| 1:J:44:ALA:C | 1:J:45:VAL:HG23 | 2.28 | 0.54 |
| 1:J:53:LYS:HD3 | 1:J:58:ASN:HA | 1.90 | 0.54 |
| 1:K:28:VAL:HA | 1:K:381:ILE:HG12 | 1.90 | 0.54 |
| 1:K:95:THR:O | 1:K:383:LEU:N | 2.30 | 0.54 |
| 1:K:117:ILE:CG2 | 1:L:293:PRO:HD3 | 2.37 | 0.54 |
| 1:L:159:ILE:HD13 | 1:L:159:ILE:HG21 | 1.90 | 0.54 |
| 1:O:52:ILE:HB | 1:O:62:VAL:HB | 1.90 | 0.54 |
| 1:O:96:GLN:NE2 | 1:O:382:THR:HG22 | 2.22 | 0.54 |
| 1:O:216:ASN:ND2 | 1:O:219:GLU:OE2 | 2.41 | 0.54 |
| 1:B:281:GLY:O | 1:B:282:SER:C | 2.47 | 0.54 |
| 1:C:395:ASN:OD1 | 1:C:398:ILE:HD11 | 2.07 | 0.54 |
| 1:D:255:MET:CG | 1:D:256:PHE:N | 2.59 | 0.54 |
| 1:D:451:LEU:CD2 | 1:D:454:LYS:HG3 | 2.38 | 0.54 |
| 1:E:305:GLN:HE22 | 1:E:337:THR:HG21 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:465:GLY:O | 1:E:466:ARG:C | 2.45 | 0.54 |
| 1:F:130:GLU:HG2 | 1:J:259:HIS:CE1 | 2.43 | 0.54 |
| 1:F:157:CYS:HB2 | 1:F:307:PHE:CE2 | 2.43 | 0.54 |
| 1:F:260:LEU:HD21 | 1:J:149:MET:HA | 1.89 | 0.54 |
| 1:G:133:SER:O | 1:G:134:ALA:HB2 | 2.07 | 0.54 |
| 1:G:158:LEU:O | 1:G:331:VAL:HA | 2.07 | 0.54 |
| 1:H:115:VAL:HG22 | 1:I:255:MET:SD | 2.48 | 0.54 |
| 1:I:248:PHE:CZ | 1:I:311:TYR:HB3 | 2.42 | 0.54 |
| 1:J:444:TYR:HB2 | 1:J:446:PHE:CE1 | 2.43 | 0.54 |
| 1:K:159:ILE:HG22 | 1:K:247:PHE:CE1 | 2.42 | 0.54 |
| 1:K:266:THR:CG2 | 1:O:358:THR:HA | 2.38 | 0.54 |
| 1:K:386:ASP:OD2 | 1:K:386:ASP:N | 2.40 | 0.54 |
| 1:L:226:THR:HG21 | 1:M:275:LEU:CD2 | 2.37 | 0.54 |
| 1:L:348:ILE:HD12 | 1:M:182:PRO:O | 2.07 | 0.54 |
| 1:N:75:ILE:H | 1:N:75:ILE:CD1 | 2.09 | 0.54 |
| 1:N:90:PHE:CD1 | 1:N:91:TYR:N | 2.76 | 0.54 |
| 1:A:167:GLU:HB2 | 1:A:190:LEU:HD11 | 1.89 | 0.54 |
| 1:A:170:GLY:O | 1:A:188:LEU:HA | 2.08 | 0.54 |
| 1:A:231:TYR:CG | 1:E:112:PRO:HB3 | 2.43 | 0.54 |
| 1:B:68:LEU:HD23 | 1:B:201:VAL:HG21 | 1.89 | 0.54 |
| 1:C:147:ILE:HG22 | 1:C:148:SER:N | 2.21 | 0.54 |
| 1:D:115:VAL:CG1 | 1:D:115:VAL:CG2 | 2.76 | 0.54 |
| 1:D:237:MET:HB3 | 1:D:246:LEU:HD22 | 1.89 | 0.54 |
| 1:E:320:ASN:OD1 | 1:E:323:ILE:HG12 | 2.08 | 0.54 |
| 1:G:24:THR:HA | 1:G:27:TYR:CE2 | 2.43 | 0.54 |
| 1:G:80:PRO:C | 1:G:82:LYS:H | 2.12 | 0.54 |
| 1:G:168:HIS:O | 1:G:190:LEU:HD12 | 2.08 | 0.54 |
| 1:G:272:PRO:HD2 | 1:G:275:LEU:HD11 | 1.89 | 0.54 |
| 1:H:57:ASN:HD21 | 1:H:59:LYS:HB3 | 1.73 | 0.54 |
| 1:I:54:LYS:CE | 1:I:55:PRO:HD2 | 2.38 | 0.54 |
| 1:K:185:CYS:HB2 | 1:O:363:TYR:CD1 | 2.43 | 0.54 |
| 1:K:346:ALA:CB | 1:K:346:ALA:HA | 2.18 | 0.54 |
| 1:L:80:PRO:C | 1:L:82:LYS:H | 2.10 | 0.54 |
| 1:M:126:LEU:HB3 | 1:M:262:ASN:HB3 | 1.90 | 0.54 |
| 1:A:163:PRO:HD3 | 1:A:330:PHE:HE1 | 1.73 | 0.53 |
| 1:A:257:VAL:HG13 | 1:E:115:VAL:HG23 | 1.90 | 0.53 |
| 1:C:75:ILE:HD12 | 1:C:75:ILE:N | 2.23 | 0.53 |
| 1:C:96:GLN:HA | 1:C:382:THR:HA | 1.90 | 0.53 |
| 1:C:320:ASN:ND2 | 1:C:323:ILE:HB | 2.22 | 0.53 |
| 1:E:72:VAL:HG23 | 1:E:197:ASP:HA | 1.89 | 0.53 |
| 1:F:254:GLN:NE2 | 1:F:298:SER:HB3 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:471:GLN:OE1 | 1:F:472:LEU:N | 2.41 | 0.53 |
| 1:J:139:ALA:HB1 | 1:J:143:ASN:OD1 | 2.07 | 0.53 |
| 1:J:190:LEU:HD12 | 1:J:191:ILE:N | 2.22 | 0.53 |
| 1:K:223:ASP:OD1 | 1:K:224:ILE:HG23 | 2.08 | 0.53 |
| 1:L:152:LYS:HE2 | 1:L:202:ASP:OD2 | 2.08 | 0.53 |
| 1:M:117:ILE:HG13 | 1:M:149:MET:O | 2.07 | 0.53 |
| 1:M:373:GLN:C | 1:M:464:LEU:HD12 | 2.28 | 0.53 |
| 1:N:365:ARG:CG | 1:N:365:ARG:NH1 | 2.68 | 0.53 |
| 1:B:166:GLY:N | 1:B:195:ILE:HG13 | 2.23 | 0.53 |
| 1:B:391:ILE:HG21 | 1:B:402:TRP:CZ3 | 2.43 | 0.53 |
| 1:D:238:VAL:O | 1:D:238:VAL:HG12 | 2.08 | 0.53 |
| 1:D:443:LYS:H | 1:D:443:LYS:CD | 2.07 | 0.53 |
| 1:E:129:THR:HG21 | 1:E:291:TYR:CD2 | 2.43 | 0.53 |
| 1:E:193:THR:HG21 | 1:E:230:LYS:CD | 2.38 | 0.53 |
| 1:F:75:ILE:N | 1:F:75:ILE:CD1 | 2.65 | 0.53 |
| 1:G:52:ILE:N | 1:G:52:ILE:HD12 | 2.22 | 0.53 |
| 1:H:65:VAL:HA | 1:H:69:GLN:NE2 | 2.23 | 0.53 |
| 1:I:49:TYR:HE1 | 1:I:364:LEU:HD13 | 1.72 | 0.53 |
| 1:I:255:MET:CG | 1:I:256:PHE:N | 2.71 | 0.53 |
| 1:I:320:ASN:OD1 | 1:I:321:ASN:N | 2.41 | 0.53 |
| 1:I:465:GLY:O | 1:I:466:ARG:C | 2.45 | 0.53 |
| 1:K:117:ILE:CD1 | 1:L:293:PRO:HB3 | 2.35 | 0.53 |
| 1:K:141:VAL:CG1 | 1:O:357:ASN:H | 2.18 | 0.53 |
| 1:K:169:TRP:H | 1:K:208:MET:HA | 1.73 | 0.53 |
| 1:M:325:TRP:HB3 | 1:M:398:ILE:CD1 | 2.38 | 0.53 |
| 1:N:459:LEU:C | 1:N:461:GLN:H | 2.10 | 0.53 |
| 1:O:99:VAL:HG12 | 1:O:100:TRP:N | 2.21 | 0.53 |
| 1:B:271:VAL:HG13 | 1:B:275:LEU:HD12 | 1.90 | 0.53 |
| 1:D:224:ILE:O | 1:D:227:SER:N | 2.29 | 0.53 |
| 1:E:103:VAL:HG23 | 1:E:104:GLY:N | 2.23 | 0.53 |
| 1:E:383:LEU:HA | 1:E:387:VAL:HG11 | 1.90 | 0.53 |
| 1:E:458:ASP:N | 1:E:458:ASP:OD2 | 2.38 | 0.53 |
| 1:F:363:TYR:CE2 | 1:G:185:CYS:HB2 | 2.44 | 0.53 |
| 1:F:397:THR:HB | 1:F:401:ASP:OD2 | 2.09 | 0.53 |
| 1:J:81:ASN:CB | 1:J:97:ARG:NH1 | 2.72 | 0.53 |
| 1:J:219:GLU:HB3 | 1:J:263:ARG:CZ | 2.39 | 0.53 |
| 1:K:42:LEU:HB3 | 1:K:447:TRP:CZ2 | 2.42 | 0.53 |
| 1:M:36:HIS:ND1 | 1:M:37:ALA:N | 2.56 | 0.53 |
| 1:M:83:PHE:CG | 1:M:84:GLY:N | 2.76 | 0.53 |
| 1:M:96:GLN:HE21 | 1:M:382:THR:CG2 | 2.22 | 0.53 |
| 1:M:150:ASP:CB | 1:N:257:VAL:HG21 | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:91:TYR:CD1 | 1:N:98:LEU:CD2 | 2.91 | 0.53 |
| 1:A:49:TYR:O | 1:A:64:LYS:HD3 | 2.08 | 0.53 |
| 1:A:73:PHE:N | 1:A:73:PHE:CD1 | 2.76 | 0.53 |
| 1:A:156:LEU:C | 1:A:156:LEU:CD1 | 2.72 | 0.53 |
| 1:A:384:THR:O | 1:A:388:MET:HB2 | 2.08 | 0.53 |
| 1:A:450:ASN:HD21 | 1:A:452:LYS:HD2 | 1.73 | 0.53 |
| 1:B:79:ASP:O | 1:B:80:PRO:C | 2.47 | 0.53 |
| 1:C:363:TYR:HE2 | 1:D:269:GLU:HG3 | 1.71 | 0.53 |
| 1:D:188:LEU:HD13 | 1:D:213:LEU:HD11 | 1.89 | 0.53 |
| 1:D:219:GLU:C | 1:D:220:VAL:HG13 | 2.29 | 0.53 |
| 1:E:149:MET:CE | 1:E:205:PHE:CE1 | 2.91 | 0.53 |
| 1:E:273:ASP:OD2 | 1:E:273:ASP:N | 2.37 | 0.53 |
| 1:E:323:ILE:CG2 | 1:E:323:ILE:CG1 | 2.76 | 0.53 |
| 1:G:312:TRP:HA | 1:G:312:TRP:CE3 | 2.44 | 0.53 |
| 1:K:34:TYR:HE2 | 1:K:377:GLN:HB2 | 1.74 | 0.53 |
| 1:K:163:PRO:N | 1:K:330:PHE:CD1 | 2.77 | 0.53 |
| 1:L:49:TYR:HE2 | 1:L:118:SER:HA | 1.73 | 0.53 |
| 1:L:54:LYS:CG | 1:L:55:PRO:HD2 | 2.37 | 0.53 |
| 1:L:80:PRO:HG2 | 1:L:81:ASN:N | 2.21 | 0.53 |
| 1:L:148:SER:HB3 | 1:M:291:TYR:CE2 | 2.43 | 0.53 |
| 1:M:81:ASN:ND2 | 1:M:402:TRP:HD1 | 2.06 | 0.53 |
| 1:N:391:ILE:HG21 | 1:N:402:TRP:CZ3 | 2.44 | 0.53 |
| 1:A:231:TYR:HD2 | 1:E:112:PRO:HD3 | 1.72 | 0.53 |
| 1:B:70:TYR:CZ | 1:B:230:LYS:O | 2.62 | 0.53 |
| 1:B:246:LEU:H | 1:B:246:LEU:HD23 | 1.73 | 0.53 |
| 1:C:208:MET:HG3 | 1:C:210:PHE:CE2 | 2.43 | 0.53 |
| 1:F:183:GLY:O | 1:F:185:CYS:N | 2.42 | 0.53 |
| 1:G:151:TYR:CG | 1:G:203:THR:HB | 2.39 | 0.53 |
| 1:I:117:ILE:CD1 | 1:I:117:ILE:CB | 2.81 | 0.53 |
| 1:K:21:VAL:HB | 1:O:461:GLN:HE22 | 1.71 | 0.53 |
| 1:K:185:CYS:HB2 | 1:O:363:TYR:CE1 | 2.43 | 0.53 |
| 1:K:372:LEU:HB3 | 1:K:374:PHE:CE1 | 2.43 | 0.53 |
| 1:L:74:ARG:NH2 | 1:L:441:LEU:HD12 | 2.24 | 0.53 |
| 1:N:24:THR:OG1 | 1:N:25:ASP:N | 2.41 | 0.53 |
| 1:N:96:GLN:HE21 | 1:N:382:THR:CG2 | 2.22 | 0.53 |
| 1:N:163:PRO:N | 1:N:330:PHE:HD1 | 2.05 | 0.53 |
| 1:O:54:LYS:HB3 | 1:O:57:ASN:HB3 | 1.91 | 0.53 |
| 1:B:36:HIS:ND1 | 1:B:37:ALA:N | 2.57 | 0.53 |
| 1:B:166:GLY:H | 1:B:195:ILE:HG13 | 1.74 | 0.53 |
| 1:B:259:HIS:HE1 | 1:C:130:GLU:CG | 2.21 | 0.53 |
| 1:B:341:ASN:HB3 | 1:B:366:HIS:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:280:SER:CA | 1:C:284:ALA:HB2 | 2.38 | 0.53 |
| 1:C:462:PHE:HB3 | 1:C:463:PRO:HD2 | 1.90 | 0.53 |
| 1:I:280:SER:O | 1:I:280:SER:OG | 2.26 | 0.53 |
| 1:J:42:LEU:HD13 | 1:J:447:TRP:CZ2 | 2.44 | 0.53 |
| 1:J:144:ARG:O | 1:J:145:GLU:HG2 | 2.08 | 0.53 |
| 1:L:262:ASN:HD21 | 1:L:288:SER:CB | 2.12 | 0.53 |
| 1:M:92:ASN:ND2 | 1:M:95:THR:OG1 | 2.40 | 0.53 |
| 1:M:159:ILE:HG22 | 1:M:247:PHE:HE1 | 1.73 | 0.53 |
| 1:N:57:ASN:HD21 | 1:N:59:LYS:H | 1.57 | 0.53 |
| 1:N:281:GLY:O | 1:N:282:SER:C | 2.47 | 0.53 |
| 1:O:96:GLN:HE21 | 1:O:382:THR:HG22 | 1.73 | 0.53 |
| 1:A:97:ARG:HH11 | 1:A:97:ARG:CB | 2.22 | 0.53 |
| 1:B:163:PRO:N | 1:B:330:PHE:CD1 | 2.76 | 0.53 |
| 1:F:250:LEU:HD13 | 1:F:306:ILE:CG2 | 2.38 | 0.53 |
| 1:H:153:GLN:NE2 | 1:H:300:VAL:HA | 2.24 | 0.53 |
| 1:H:217:LYS:C | 1:H:218:SER:OG | 2.47 | 0.53 |
| 1:I:217:LYS:HG2 | 1:J:276:TYR:HA | 1.89 | 0.53 |
| 1:K:49:TYR:HE2 | 1:K:118:SER:HA | 1.74 | 0.53 |
| 1:K:141:VAL:HG13 | 1:O:357:ASN:N | 2.22 | 0.53 |
| 1:L:170:GLY:O | 1:L:188:LEU:HA | 2.09 | 0.53 |
| 1:L:194:VAL:HG21 | 1:L:444:TYR:CZ | 2.44 | 0.53 |
| 1:L:278:LYS:CB | 1:O:354:THR:HG22 | 2.39 | 0.53 |
| 1:N:92:ASN:C | 1:N:94:ASP:H | 2.12 | 0.53 |
| 1:N:153:GLN:NE2 | 1:N:300:VAL:HG12 | 2.23 | 0.53 |
| 1:O:163:PRO:HB3 | 1:O:330:PHE:CE1 | 2.43 | 0.53 |
| 1:B:96:GLN:CA | 1:B:382:THR:HA | 2.38 | 0.53 |
| 1:B:391:ILE:CG2 | 1:B:399:LEU:CD2 | 2.86 | 0.53 |
| 1:D:77:LEU:HD22 | 1:D:455:PHE:CZ | 2.43 | 0.53 |
| 1:D:120:HIS:CE1 | 1:D:122:LEU:H | 2.24 | 0.53 |
| 1:E:154:THR:H | 1:E:336:THR:HG23 | 1.73 | 0.53 |
| 1:F:139:ALA:HB1 | 1:F:143:ASN:OD1 | 2.09 | 0.53 |
| 1:F:154:THR:CG2 | 1:F:154:THR:HB | 2.20 | 0.53 |
| 1:F:317:GLN:O | 1:J:466:ARG:HD2 | 2.08 | 0.53 |
| 1:G:302:SER:C | 1:G:304:ALA:H | 2.09 | 0.53 |
| 1:H:52:ILE:HD12 | 1:H:52:ILE:N | 2.24 | 0.53 |
| 1:H:363:TYR:CD1 | 1:I:185:CYS:HB2 | 2.44 | 0.53 |
| 1:I:163:PRO:HB3 | 1:I:330:PHE:CE1 | 2.44 | 0.53 |
| 1:J:302:SER:O | 1:J:304:ALA:N | 2.40 | 0.53 |
| 1:K:65:VAL:O | 1:K:366:HIS:HB3 | 2.08 | 0.53 |
| 1:K:135:TYR:HE2 | 1:K:287:ALA:HB2 | 1.73 | 0.53 |
| 1:L:150:ASP:OD2 | 1:L:150:ASP:N | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:384:THR:O | 1:L:388:MET:HB2 | 2.09 | 0.53 |
| 1:O:120:HIS:ND1 | 1:O:121:PRO:HD2 | 2.23 | 0.53 |
| 1:O:440:PRO:HA | 1:O:443:LYS:NZ | 2.24 | 0.53 |
| 1:A:207:ALA:O | 1:A:208:MET:HB3 | 2.09 | 0.53 |
| 1:A:242:TYR:CE2 | 1:A:394:MET:CG | 2.91 | 0.53 |
| 1:B:24:THR:C | 1:B:26:GLU:H | 2.11 | 0.53 |
| 1:B:300:VAL:HB | 1:B:337:THR:HG22 | 1.91 | 0.53 |
| 1:C:61:LEU:HD12 | 1:C:61:LEU:O | 2.08 | 0.53 |
| 1:C:113:LEU:N | 1:C:113:LEU:CD1 | 2.72 | 0.53 |
| 1:E:77:LEU:HD22 | 1:E:455:PHE:CZ | 2.43 | 0.53 |
| 1:E:193:THR:CG2 | 1:E:230:LYS:CD | 2.87 | 0.53 |
| 1:F:144:ARG:C | 1:F:145:GLU:HG2 | 2.28 | 0.53 |
| 1:F:208:MET:SD | 1:F:210:PHE:CE2 | 3.02 | 0.53 |
| 1:F:344:LEU:CB | 1:G:213:LEU:O | 2.57 | 0.53 |
| 1:G:157:CYS:HA | 1:G:332:THR:O | 2.09 | 0.53 |
| 1:I:49:TYR:HE1 | 1:I:364:LEU:CD1 | 2.21 | 0.53 |
| 1:I:157:CYS:HB3 | 1:I:250:LEU:HD13 | 1.91 | 0.53 |
| 1:L:39:THR:CG2 | 1:L:372:LEU:HB2 | 2.32 | 0.53 |
| 1:L:227:SER:CA | 1:L:228:ILE:HD12 | 2.39 | 0.53 |
| 1:M:75:ILE:HB | 1:M:329:LEU:CB | 2.38 | 0.53 |
| 1:N:114:GLY:HA3 | 1:N:340:THR:OG1 | 2.09 | 0.53 |
| 1:O:49:TYR:HE1 | 1:O:364:LEU:HD13 | 1.72 | 0.53 |
| 1:O:210:PHE:O | 1:O:214:GLN:HB2 | 2.09 | 0.53 |
| 1:A:200:MET:HB2 | 1:A:228:ILE:O | 2.09 | 0.53 |
| 1:A:228:ILE:HD12 | 1:A:228:ILE:N | 2.24 | 0.53 |
| 1:A:326:GLY:O | 1:A:327:ASN:HB2 | 2.08 | 0.53 |
| 1:B:467:LYS:CG | 1:B:467:LYS:CE | 2.81 | 0.53 |
| 1:C:237:MET:HB3 | 1:C:246:LEU:HD22 | 1.91 | 0.53 |
| 1:C:464:LEU:HD22 | 1:C:464:LEU:O | 2.08 | 0.53 |
| 1:D:87:ASP:O | 1:D:90:PHE:CE2 | 2.62 | 0.53 |
| 1:D:361:LYS:HD3 | 1:D:363:TYR:OH | 2.09 | 0.53 |
| 1:E:315:ARG:O | 1:E:316:ALA:HB2 | 2.09 | 0.53 |
| 1:F:188:LEU:HD21 | 1:J:344:LEU:HD13 | 1.91 | 0.53 |
| 1:F:367:GLY:O | 1:F:368:GLU:HG2 | 2.09 | 0.53 |
| 1:G:99:VAL:HG11 | 1:G:323:ILE:HG23 | 1.91 | 0.53 |
| 1:G:223:ASP:OD1 | 1:G:224:ILE:N | 2.42 | 0.53 |
| 1:H:154:THR:H | 1:H:336:THR:CG2 | 2.21 | 0.53 |
| 1:I:156:LEU:HD12 | 1:I:156:LEU:C | 2.29 | 0.53 |
| 1:I:255:MET:CG | 1:I:256:PHE:H | 2.20 | 0.53 |
| 1:L:126:LEU:HB3 | 1:L:262:ASN:HB3 | 1.89 | 0.53 |
| 1:L:439:ASP:OD2 | 1:L:440:PRO:HD2 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:246:LEU:CD2 | 1:N:246:LEU:N | 2.72 | 0.53 |
| 1:O:53:LYS:HD3 | 1:O:58:ASN:HA | 1.90 | 0.53 |
| 1:A:50:PHE:HB2 | 1:A:51:PRO:HD2 | 1.91 | 0.52 |
| 1:A:451:LEU:HA | 1:A:454:LYS:HG3 | 1.91 | 0.52 |
| 1:B:54:LYS:HG2 | 1:B:57:ASN:HB3 | 1.90 | 0.52 |
| 1:B:76:HIS:HB2 | 1:B:450:ASN:HA | 1.91 | 0.52 |
| 1:B:79:ASP:O | 1:B:82:LYS:N | 2.42 | 0.52 |
| 1:C:47:HIS:HB2 | 1:C:52:ILE:HD11 | 1.91 | 0.52 |
| 1:E:29:ALA:HB3 | 1:E:380:LYS:HG3 | 1.91 | 0.52 |
| 1:E:152:LYS:HG3 | 1:E:152:LYS:O | 2.08 | 0.52 |
| 1:E:154:THR:H | 1:E:336:THR:CG2 | 2.22 | 0.52 |
| 1:E:471:GLN:O | 1:E:472:LEU:OXT | 2.27 | 0.52 |
| 1:F:117:ILE:HG21 | 1:G:293:PRO:HD3 | 1.92 | 0.52 |
| 1:F:283:THR:HG21 | 1:J:142:ASP:O | 2.10 | 0.52 |
| 1:G:46:GLY:CA | 1:G:65:VAL:HB | 2.40 | 0.52 |
| 1:G:272:PRO:HB2 | 1:G:275:LEU:HG | 1.91 | 0.52 |
| 1:G:344:LEU:HD12 | 1:H:186:PRO:HB2 | 1.91 | 0.52 |
| 1:H:112:PRO:HD3 | 1:I:231:TYR:CG | 2.42 | 0.52 |
| 1:H:151:TYR:OH | 1:H:221:PRO:HG2 | 2.09 | 0.52 |
| 1:I:70:TYR:CE1 | 1:I:201:VAL:HA | 2.43 | 0.52 |
| 1:I:130:GLU:HB2 | 1:I:260:LEU:HD13 | 1.89 | 0.52 |
| 1:I:160:GLY:O | 1:I:329:LEU:HD23 | 2.10 | 0.52 |
| 1:I:183:GLY:O | 1:I:184:ASP:C | 2.48 | 0.52 |
| 1:I:358:THR:HA | 1:J:266:THR:HG23 | 1.91 | 0.52 |
| 1:J:30:ARG:HH11 | 1:J:377:GLN:HE22 | 1.57 | 0.52 |
| 1:J:325:TRP:HB3 | 1:J:398:ILE:CD1 | 2.39 | 0.52 |
| 1:M:156:LEU:C | 1:M:156:LEU:CD1 | 2.75 | 0.52 |
| 1:M:366:HIS:CD2 | 1:M:367:GLY:N | 2.78 | 0.52 |
| 1:N:46:GLY:N | 1:N:65:VAL:HB | 2.24 | 0.52 |
| 1:N:123:LEU:CD2 | 1:N:123:LEU:CD1 | 2.80 | 0.52 |
| 1:O:54:LYS:CB | 1:O:57:ASN:HD22 | 2.21 | 0.52 |
| 1:A:459:LEU:HB3 | 1:A:465:GLY:HA3 | 1.92 | 0.52 |
| 1:B:23:SER:N | 1:B:319:HIS:HD2 | 2.07 | 0.52 |
| 1:B:171:LYS:CG | 1:B:171:LYS:CE | 2.81 | 0.52 |
| 1:B:208:MET:CG | 1:B:210:PHE:CE2 | 2.92 | 0.52 |
| 1:C:149:MET:HE3 | 1:C:294:THR:HG22 | 1.91 | 0.52 |
| 1:E:49:TYR:HA | 1:E:223:ASP:HB3 | 1.91 | 0.52 |
| 1:F:90:PHE:CD1 | 1:F:91:TYR:HB3 | 2.43 | 0.52 |
| 1:G:166:GLY:HA3 | 1:G:195:ILE:HD11 | 1.88 | 0.52 |
| 1:G:188:LEU:HD11 | 1:G:213:LEU:CD1 | 2.39 | 0.52 |
| 1:G:353:THR:O | 1:I:278:LYS:HB2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:71:ARG:HH11 | 1:I:71:ARG:CA | 2.18 | 0.52 |
| 1:J:180:VAL:HG12 | 1:J:181:GLN:O | 2.08 | 0.52 |
| 1:K:112:PRO:HB3 | 1:L:231:TYR:CD1 | 2.44 | 0.52 |
| 1:M:81:ASN:ND2 | 1:M:402:TRP:CD1 | 2.77 | 0.52 |
| 1:O:143:ASN:O | 1:O:145:GLU:HG2 | 2.10 | 0.52 |
| 1:A:69:GLN:HA | 1:A:199:ASP:O | 2.09 | 0.52 |
| 1:B:71:ARG:HB3 | 1:B:73:PHE:CE1 | 2.44 | 0.52 |
| 1:B:149:MET:CE | 1:B:205:PHE:CE1 | 2.92 | 0.52 |
| 1:B:246:LEU:H | 1:B:246:LEU:CD2 | 2.23 | 0.52 |
| 1:C:54:LYS:HG2 | 1:C:56:ASN:OD1 | 2.09 | 0.52 |
| 1:C:141:VAL:HG12 | 1:C:142:ASP:N | 2.22 | 0.52 |
| 1:C:172:GLY:O | 1:C:173:SER:O | 2.27 | 0.52 |
| 1:C:220:VAL:O | 1:C:221:PRO:C | 2.46 | 0.52 |
| 1:E:180:VAL:HG13 | 1:E:184:ASP:HB3 | 1.92 | 0.52 |
| 1:E:472:LEU:O | 1:J:138:ASN:HB2 | 2.09 | 0.52 |
| 1:F:81:ASN:ND2 | 1:F:98:LEU:O | 2.42 | 0.52 |
| 1:F:250:LEU:HD13 | 1:F:306:ILE:HG21 | 1.90 | 0.52 |
| 1:F:459:LEU:C | 1:F:461:GLN:N | 2.63 | 0.52 |
| 1:G:105:VAL:HG23 | 1:G:313:LEU:HD11 | 1.90 | 0.52 |
| 1:I:58:ASN:OD1 | 1:I:58:ASN:N | 2.41 | 0.52 |
| 1:I:65:VAL:HA | 1:I:69:GLN:HE22 | 1.73 | 0.52 |
| 1:I:66:SER:H | 1:I:69:GLN:NE2 | 2.07 | 0.52 |
| 1:I:82:LYS:CE | 1:I:82:LYS:HG3 | 2.38 | 0.52 |
| 1:K:216:ASN:CB | 1:O:345:CYS:SG | 2.83 | 0.52 |
| 1:K:242:TYR:CE2 | 1:K:394:MET:CG | 2.93 | 0.52 |
| 1:K:326:GLY:O | 1:K:327:ASN:HB2 | 2.10 | 0.52 |
| 1:A:42:LEU:HD13 | 1:A:447:TRP:CZ2 | 2.44 | 0.52 |
| 1:A:42:LEU:HB2 | 1:A:370:TYR:HB2 | 1.92 | 0.52 |
| 1:B:28:VAL:HA | 1:B:381:ILE:HG12 | 1.91 | 0.52 |
| 1:B:35:TYR:CZ | 1:B:457:ALA:HB2 | 2.44 | 0.52 |
| 1:B:115:VAL:CG2 | 1:C:257:VAL:HG13 | 2.33 | 0.52 |
| 1:C:247:PHE:HD1 | 1:C:248:PHE:H | 1.56 | 0.52 |
| 1:C:464:LEU:CD2 | 1:C:464:LEU:O | 2.57 | 0.52 |
| 1:D:267:VAL:HG11 | 1:D:270:ASN:OD1 | 2.10 | 0.52 |
| 1:F:35:TYR:HD2 | 1:F:456:SER:C | 2.12 | 0.52 |
| 1:F:459:LEU:C | 1:F:461:GLN:H | 2.13 | 0.52 |
| 1:G:344:LEU:HD13 | 1:H:213:LEU:CD1 | 2.34 | 0.52 |
| 1:H:188:LEU:HD11 | 1:H:213:LEU:HD11 | 1.91 | 0.52 |
| 1:K:85:PHE:CZ | 1:K:378:LEU:HD22 | 2.45 | 0.52 |
| 1:N:92:ASN:ND2 | 1:N:95:THR:N | 2.45 | 0.52 |
| 1:N:98:LEU:CD1 | 1:N:378:LEU:HD11 | 2.21 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:101:ALA:HB3 | 1:N:377:GLN:O | 2.10 | 0.52 |
| 1:O:75:ILE:HG23 | 1:O:451:LEU:HD12 | 1.90 | 0.52 |
| 1:A:217:LYS:O | 1:A:218:SER:HB3 | 2.09 | 0.52 |
| 1:B:79:ASP:OD1 | 1:B:80:PRO:HD2 | 2.09 | 0.52 |
| 1:D:397:THR:HB | 1:D:401:ASP:OD2 | 2.09 | 0.52 |
| 1:E:383:LEU:HD23 | 1:E:388:MET:CE | 2.40 | 0.52 |
| 1:F:156:LEU:C | 1:F:156:LEU:HD12 | 2.29 | 0.52 |
| 1:F:185:CYS:HB2 | 1:J:363:TYR:CG | 2.44 | 0.52 |
| 1:F:465:GLY:O | 1:F:466:ARG:C | 2.48 | 0.52 |
| 1:H:66:SER:OG | 1:H:68:LEU:N | 2.42 | 0.52 |
| 1:H:259:HIS:HE1 | 1:I:130:GLU:CG | 2.22 | 0.52 |
| 1:I:342:MET:HB2 | 1:J:208:MET:HE1 | 1.92 | 0.52 |
| 1:J:75:ILE:HB | 1:J:329:LEU:HB2 | 1.90 | 0.52 |
| 1:J:316:ALA:HB3 | 1:J:321:ASN:OD1 | 2.09 | 0.52 |
| 1:L:57:ASN:HD21 | 1:L:59:LYS:H | 1.57 | 0.52 |
| 1:L:180:VAL:HG12 | 1:L:181:GLN:N | 2.25 | 0.52 |
| 1:M:70:TYR:HE1 | 1:M:201:VAL:HA | 1.74 | 0.52 |
| 1:M:120:HIS:NE2 | 1:M:218:SER:HB3 | 2.25 | 0.52 |
| 1:N:22:VAL:N | 1:N:390:TYR:OH | 2.39 | 0.52 |
| 1:N:163:PRO:N | 1:N:330:PHE:CD1 | 2.77 | 0.52 |
| 1:N:374:PHE:CB | 1:N:376:PHE:HE1 | 2.21 | 0.52 |
| 1:O:122:LEU:HD13 | 1:O:144:ARG:NH2 | 2.23 | 0.52 |
| 1:A:149:MET:HG3 | 1:A:295:PRO:HD2 | 1.91 | 0.52 |
| 1:B:397:THR:O | 1:B:401:ASP:N | 2.34 | 0.52 |
| 1:C:249:TYR:O | 1:C:249:TYR:CG | 2.63 | 0.52 |
| 1:F:151:TYR:CD2 | 1:F:203:THR:CB | 2.75 | 0.52 |
| 1:H:226:THR:HG21 | 1:I:275:LEU:HD22 | 1.90 | 0.52 |
| 1:I:153:GLN:HE22 | 1:I:300:VAL:HA | 1.75 | 0.52 |
| 1:I:184:ASP:O | 1:I:185:CYS:C | 2.48 | 0.52 |
| 1:I:459:LEU:HB3 | 1:I:465:GLY:HA3 | 1.92 | 0.52 |
| 1:J:79:ASP:HA | 1:J:327:ASN:ND2 | 2.24 | 0.52 |
| 1:L:99:VAL:HG12 | 1:L:100:TRP:N | 2.23 | 0.52 |
| 1:L:149:MET:CE | 1:L:205:PHE:CE1 | 2.93 | 0.52 |
| 1:O:104:GLY:HA3 | 1:O:375:ILE:HB | 1.92 | 0.52 |
| 1:A:169:TRP:HB3 | 1:A:188:LEU:HD12 | 1.92 | 0.52 |
| 1:B:29:ALA:HB3 | 1:B:380:LYS:HG3 | 1.92 | 0.52 |
| 1:B:151:TYR:CG | 1:B:203:THR:HB | 2.45 | 0.52 |
| 1:B:373:GLN:CB | 1:B:464:LEU:HD12 | 2.40 | 0.52 |
| 1:C:166:GLY:O | 1:C:192:ASN:HA | 2.08 | 0.52 |
| 1:H:120:HIS:NE2 | 1:H:218:SER:HB3 | 2.24 | 0.52 |
| 1:H:255:MET:HG2 | 1:H:256:PHE:H | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:65:VAL:O | 1:I:366:HIS:HB3 | 2.10 | 0.52 |
| 1:I:220:VAL:O | 1:I:221:PRO:C | 2.46 | 0.52 |
| 1:I:255:MET:HG2 | 1:I:256:PHE:N | 2.22 | 0.52 |
| 1:J:155:GLN:HG2 | 1:J:307:PHE:HE1 | 1.75 | 0.52 |
| 1:J:280:SER:N | 1:J:284:ALA:HB2 | 2.25 | 0.52 |
| 1:K:260:LEU:N | 1:K:260:LEU:CD1 | 2.60 | 0.52 |
| 1:K:299:MET:HA | 1:L:255:MET:O | 2.09 | 0.52 |
| 1:L:75:ILE:HB | 1:L:329:LEU:HB3 | 1.91 | 0.52 |
| 1:N:23:SER:OG | 1:N:25:ASP:HB2 | 2.09 | 0.52 |
| 1:N:154:THR:HG23 | 1:N:253:GLU:HB3 | 1.92 | 0.52 |
| 1:N:222:LEU:HA | 1:N:225:CYS:SG | 2.50 | 0.52 |
| 1:A:92:ASN:O | 1:A:94:ASP:N | 2.42 | 0.52 |
| 1:A:124:ASN:HD22 | 1:A:216:ASN:ND2 | 2.06 | 0.52 |
| 1:D:75:ILE:HB | 1:D:329:LEU:HB3 | 1.91 | 0.52 |
| 1:E:46:GLY:HA3 | 1:E:63:PRO:O | 2.10 | 0.52 |
| 1:F:51:PRO:C | 1:F:52:ILE:HD12 | 2.30 | 0.52 |
| 1:F:97:ARG:HG2 | 1:F:383:LEU:HD13 | 1.85 | 0.52 |
| 1:G:163:PRO:HD3 | 1:G:330:PHE:HE1 | 1.73 | 0.52 |
| 1:G:348:ILE:O | 1:G:348:ILE:HG13 | 2.10 | 0.52 |
| 1:H:34:TYR:CE2 | 1:H:377:GLN:HB2 | 2.45 | 0.52 |
| 1:H:95:THR:O | 1:H:383:LEU:N | 2.33 | 0.52 |
| 1:H:124:ASN:OD1 | 1:H:124:ASN:O | 2.28 | 0.52 |
| 1:H:235:ILE:O | 1:H:235:ILE:HG22 | 2.10 | 0.52 |
| 1:H:323:ILE:HD13 | 1:H:323:ILE:N | 2.24 | 0.52 |
| 1:I:80:PRO:HB3 | 1:I:100:TRP:NE1 | 2.25 | 0.52 |
| 1:I:179:ALA:C | 1:I:180:VAL:HG23 | 2.29 | 0.52 |
| 1:K:155:GLN:HB3 | 1:K:252:ARG:HB3 | 1.92 | 0.52 |
| 1:L:96:GLN:HE21 | 1:L:382:THR:HG22 | 1.75 | 0.52 |
| 1:M:79:ASP:OD2 | 1:M:81:ASN:CB | 2.41 | 0.52 |
| 1:M:180:VAL:HG13 | 1:M:184:ASP:HB3 | 1.88 | 0.52 |
| 1:M:443:LYS:N | 1:M:443:LYS:HD3 | 2.25 | 0.52 |
| 1:O:92:ASN:ND2 | 1:O:95:THR:N | 2.55 | 0.52 |
| 1:A:31:THR:HG23 | 1:A:378:LEU:O | 2.10 | 0.52 |
| 1:A:167:GLU:N | 1:A:231:TYR:O | 2.43 | 0.52 |
| 1:B:120:HIS:CE1 | 1:B:122:LEU:H | 2.28 | 0.52 |
| 1:B:384:THR:OG1 | 1:B:385:ALA:N | 2.41 | 0.52 |
| 1:D:61:LEU:HD12 | 1:D:61:LEU:O | 2.09 | 0.52 |
| 1:D:121:PRO:HD3 | 1:D:222:LEU:CD1 | 2.40 | 0.52 |
| 1:E:42:LEU:HD13 | 1:E:447:TRP:CE2 | 2.45 | 0.52 |
| 1:E:66:SER:O | 1:E:69:GLN:HG3 | 2.10 | 0.52 |
| 1:E:155:GLN:HB3 | 1:E:252:ARG:HB3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:72:VAL:HG13 | 1:G:332:THR:HG23 | 1.92 | 0.52 |
| 1:G:166:GLY:HA2 | 1:G:195:ILE:HD11 | 1.92 | 0.52 |
| 1:G:262:ASN:OD1 | 1:G:288:SER:O | 2.28 | 0.52 |
| 1:I:79:ASP:OD2 | 1:I:82:LYS:HE3 | 2.08 | 0.52 |
| 1:I:217:LYS:HG2 | 1:J:276:TYR:CA | 2.40 | 0.52 |
| 1:I:463:PRO:HB3 | 1:I:466:ARG:HH21 | 1.75 | 0.52 |
| 1:K:80:PRO:O | 1:K:98:LEU:HD12 | 2.10 | 0.52 |
| 1:K:329:LEU:HD13 | 1:K:374:PHE:CE2 | 2.45 | 0.52 |
| 1:N:361:LYS:HD3 | 1:N:363:TYR:OH | 2.09 | 0.52 |
| 1:O:42:LEU:HB2 | 1:O:370:TYR:HB2 | 1.90 | 0.52 |
| 1:O:200:MET:HB2 | 1:O:228:ILE:O | 2.10 | 0.52 |
| 1:A:96:GLN:HB3 | 1:A:382:THR:HG22 | 1.91 | 0.52 |
| 1:B:80:PRO:O | 1:B:82:LYS:N | 2.43 | 0.52 |
| 1:D:194:VAL:CG2 | 1:D:194:VAL:CG1 | 2.81 | 0.52 |
| 1:F:46:GLY:HA3 | 1:F:63:PRO:O | 2.11 | 0.52 |
| 1:F:149:MET:CE | 1:F:205:PHE:CE1 | 2.93 | 0.52 |
| 1:G:217:LYS:NZ | 1:G:217:LYS:CD | 2.66 | 0.52 |
| 1:G:228:ILE:N | 1:G:228:ILE:CD1 | 2.72 | 0.52 |
| 1:G:457:ALA:O | 1:G:459:LEU:CD2 | 2.58 | 0.52 |
| 1:I:85:PHE:CZ | 1:I:378:LEU:HD22 | 2.44 | 0.52 |
| 1:I:387:VAL:O | 1:I:391:ILE:HG13 | 2.09 | 0.52 |
| 1:I:451:LEU:HD23 | 1:I:454:LYS:HG3 | 1.92 | 0.52 |
| 1:J:260:LEU:HD12 | 1:J:260:LEU:H | 1.71 | 0.52 |
| 1:L:35:TYR:O | 1:L:376:PHE:N | 2.29 | 0.52 |
| 1:L:459:LEU:HB3 | 1:L:465:GLY:HA3 | 1.92 | 0.52 |
| 1:M:57:ASN:HD21 | 1:M:59:LYS:CB | 2.23 | 0.52 |
| 1:M:106:GLU:HG3 | 1:M:309:LYS:C | 2.30 | 0.52 |
| 1:N:66:SER:OG | 1:N:68:LEU:HD12 | 2.10 | 0.52 |
| 1:N:75:ILE:HB | 1:N:329:LEU:HB3 | 1.92 | 0.52 |
| 1:A:395:ASN:O | 1:A:398:ILE:HG12 | 2.10 | 0.51 |
| 1:C:74:ARG:NH2 | 1:C:441:LEU:HD12 | 2.25 | 0.51 |
| 1:C:307:PHE:O | 1:C:308:ASN:CB | 2.56 | 0.51 |
| 1:C:375:ILE:HG21 | 1:C:468:PHE:CD2 | 2.44 | 0.51 |
| 1:D:119:GLY:HA3 | 1:E:291:TYR:CE1 | 2.46 | 0.51 |
| 1:E:343:SER:HB3 | 1:E:364:LEU:HD23 | 1.92 | 0.51 |
| 1:F:120:HIS:HB3 | 1:F:123:LEU:HB2 | 1.91 | 0.51 |
| 1:F:120:HIS:ND1 | 1:F:122:LEU:N | 2.51 | 0.51 |
| 1:G:121:PRO:HG3 | 1:H:289:SER:OG | 2.10 | 0.51 |
| 1:G:130:GLU:HB2 | 1:G:260:LEU:HD13 | 1.91 | 0.51 |
| 1:G:217:LYS:O | 1:G:218:SER:HB3 | 2.09 | 0.51 |
| 1:H:34:TYR:HE2 | 1:H:377:GLN:HB2 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:54:LYS:HB2 | 1:I:57:ASN:HD22 | 1.74 | 0.51 |
| 1:I:108:GLY:HA3 | 1:I:371:ASP:O | 2.10 | 0.51 |
| 1:I:155:GLN:HB3 | 1:I:252:ARG:HB3 | 1.91 | 0.51 |
| 1:I:280:SER:CA | 1:I:284:ALA:HB2 | 2.40 | 0.51 |
| 1:K:112:PRO:HB2 | 1:L:202:ASP:OD2 | 2.09 | 0.51 |
| 1:K:172:GLY:O | 1:K:173:SER:C | 2.48 | 0.51 |
| 1:L:72:VAL:HG13 | 1:L:332:THR:HG23 | 1.92 | 0.51 |
| 1:L:216:ASN:O | 1:M:277:ILE:HD11 | 2.10 | 0.51 |
| 1:M:323:ILE:HG21 | 1:M:325:TRP:CH2 | 2.45 | 0.51 |
| 1:N:375:ILE:HG12 | 1:N:464:LEU:CD1 | 2.41 | 0.51 |
| 1:O:54:LYS:CG | 1:O:57:ASN:HB3 | 2.40 | 0.51 |
| 1:O:196:GLN:N | 1:O:199:ASP:OD2 | 2.36 | 0.51 |
| 1:O:280:SER:O | 1:O:280:SER:OG | 2.28 | 0.51 |
| 1:A:66:SER:O | 1:A:69:GLN:HG3 | 2.10 | 0.51 |
| 1:A:81:ASN:OD1 | 1:A:98:LEU:N | 2.42 | 0.51 |
| 1:A:122:LEU:O | 1:A:218:SER:HB2 | 2.10 | 0.51 |
| 1:A:260:LEU:HD12 | 1:A:260:LEU:N | 2.25 | 0.51 |
| 1:D:75:ILE:HD12 | 1:D:75:ILE:H | 1.76 | 0.51 |
| 1:F:35:TYR:CD2 | 1:F:456:SER:C | 2.83 | 0.51 |
| 1:F:124:ASN:OD1 | 1:F:264:ALA:N | 2.39 | 0.51 |
| 1:F:208:MET:SD | 1:F:210:PHE:HE2 | 2.32 | 0.51 |
| 1:G:57:ASN:HD21 | 1:G:59:LYS:HB3 | 1.75 | 0.51 |
| 1:G:360:PHE:CE2 | 1:H:216:ASN:HA | 2.46 | 0.51 |
| 1:H:189:GLU:O | 1:H:191:ILE:HG12 | 2.09 | 0.51 |
| 1:H:400:GLU:O | 1:H:401:ASP:C | 2.47 | 0.51 |
| 1:I:181:GLN:O | 1:I:182:PRO:C | 2.48 | 0.51 |
| 1:I:258:ARG:HB2 | 1:I:296:SER:HB2 | 1.91 | 0.51 |
| 1:J:254:GLN:HE22 | 1:J:298:SER:HB3 | 1.76 | 0.51 |
| 1:J:463:PRO:HG2 | 1:J:464:LEU:N | 2.25 | 0.51 |
| 1:K:129:THR:O | 1:O:147:ILE:HA | 2.11 | 0.51 |
| 1:K:298:SER:OG | 1:K:299:MET:N | 2.44 | 0.51 |
| 1:L:96:GLN:HE21 | 1:L:382:THR:CG2 | 2.23 | 0.51 |
| 1:M:70:TYR:CE1 | 1:M:201:VAL:HA | 2.45 | 0.51 |
| 1:A:68:LEU:HB3 | 1:A:201:VAL:CG2 | 2.40 | 0.51 |
| 1:B:167:GLU:HG3 | 1:B:231:TYR:O | 2.11 | 0.51 |
| 1:D:367:GLY:O | 1:D:368:GLU:HG2 | 2.11 | 0.51 |
| 1:E:45:VAL:C | 1:E:65:VAL:HG21 | 2.31 | 0.51 |
| 1:G:158:LEU:O | 1:G:332:THR:N | 2.35 | 0.51 |
| 1:H:112:PRO:CD | 1:I:231:TYR:CD2 | 2.88 | 0.51 |
| 1:I:75:ILE:HD13 | 1:I:329:LEU:HB3 | 1.92 | 0.51 |
| 1:I:464:LEU:C | 1:I:464:LEU:CD2 | 2.77 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:121:PRO:HG3 | 1:L:289:SER:CB | 2.41 | 0.51 |
| 1:K:155:GLN:HG2 | 1:K:306:ILE:HG12 | 1.92 | 0.51 |
| 1:K:220:VAL:O | 1:K:221:PRO:C | 2.48 | 0.51 |
| 1:L:49:TYR:HA | 1:L:223:ASP:HB3 | 1.91 | 0.51 |
| 1:M:160:GLY:HA3 | 1:M:245:SER:O | 2.10 | 0.51 |
| 1:O:395:ASN:O | 1:O:398:ILE:HG12 | 2.10 | 0.51 |
| 1:B:149:MET:HE3 | 1:B:294:THR:HG22 | 1.93 | 0.51 |
| 1:B:397:THR:HB | 1:B:401:ASP:OD2 | 2.10 | 0.51 |
| 1:D:163:PRO:N | 1:D:330:PHE:CD1 | 2.78 | 0.51 |
| 1:F:57:ASN:HD21 | 1:F:59:LYS:HB3 | 1.74 | 0.51 |
| 1:F:96:GLN:HB3 | 1:F:382:THR:HG22 | 1.92 | 0.51 |
| 1:G:150:ASP:CG | 1:H:257:VAL:HG21 | 2.31 | 0.51 |
| 1:I:139:ALA:HB1 | 1:I:143:ASN:OD1 | 2.11 | 0.51 |
| 1:I:150:ASP:CG | 1:I:150:ASP:O | 2.48 | 0.51 |
| 1:I:175:CYS:O | 1:I:177:GLN:N | 2.37 | 0.51 |
| 1:I:228:ILE:N | 1:I:228:ILE:CD1 | 2.64 | 0.51 |
| 1:I:323:ILE:O | 1:I:325:TRP:N | 2.42 | 0.51 |
| 1:I:335:ASP:OD1 | 1:I:337:THR:OG1 | 2.28 | 0.51 |
| 1:I:345:CYS:HA | 1:I:361:LYS:O | 2.10 | 0.51 |
| 1:J:66:SER:N | 1:J:69:GLN:HE21 | 2.06 | 0.51 |
| 1:J:345:CYS:CB | 1:J:362:GLU:OE2 | 2.58 | 0.51 |
| 1:K:163:PRO:N | 1:K:330:PHE:HD1 | 2.08 | 0.51 |
| 1:L:335:ASP:OD1 | 1:L:337:THR:OG1 | 2.28 | 0.51 |
| 1:M:130:GLU:HB2 | 1:M:260:LEU:CD1 | 2.38 | 0.51 |
| 1:M:223:ASP:OD1 | 1:M:224:ILE:HG23 | 2.10 | 0.51 |
| 1:M:390:TYR:O | 1:M:391:ILE:C | 2.48 | 0.51 |
| 1:N:74:ARG:CG | 1:N:330:PHE:HE2 | 2.24 | 0.51 |
| 1:O:54:LYS:HZ1 | 1:O:54:LYS:HA | 1.75 | 0.51 |
| 1:O:300:VAL:O | 1:O:300:VAL:HG23 | 2.09 | 0.51 |
| 1:A:237:MET:HB3 | 1:A:246:LEU:HD21 | 1.92 | 0.51 |
| 1:B:152:LYS:NZ | 1:B:253:GLU:OE1 | 2.42 | 0.51 |
| 1:E:223:ASP:OD1 | 1:E:224:ILE:N | 2.44 | 0.51 |
| 1:F:242:TYR:CE2 | 1:F:394:MET:HB2 | 2.46 | 0.51 |
| 1:G:183:GLY:O | 1:G:184:ASP:C | 2.49 | 0.51 |
| 1:H:143:ASN:O | 1:H:144:ARG:C | 2.48 | 0.51 |
| 1:I:172:GLY:O | 1:I:173:SER:C | 2.49 | 0.51 |
| 1:J:47:HIS:HB3 | 1:J:50:PHE:O | 2.11 | 0.51 |
| 1:K:216:ASN:H | 1:O:345:CYS:HG | 1.57 | 0.51 |
| 1:A:170:GLY:HA2 | 1:A:213:LEU:HD21 | 1.91 | 0.51 |
| 1:A:276:TYR:N | 1:A:276:TYR:CD2 | 2.78 | 0.51 |
| 1:B:20:ALA:O | 1:B:390:TYR:HE1 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:263:ARG:HG2 | 1:B:292:PHE:CD2 | 2.43 | 0.51 |
| 1:C:259:HIS:HE1 | 1:D:130:GLU:OE1 | 1.93 | 0.51 |
| 1:D:159:ILE:CG2 | 1:D:247:PHE:HE1 | 2.23 | 0.51 |
| 1:D:356:LYS:NZ | 1:D:356:LYS:CD | 2.70 | 0.51 |
| 1:F:256:PHE:CD1 | 1:F:257:VAL:N | 2.78 | 0.51 |
| 1:F:389:THR:OG1 | 1:F:390:TYR:N | 2.43 | 0.51 |
| 1:G:65:VAL:O | 1:G:366:HIS:HB3 | 2.10 | 0.51 |
| 1:G:68:LEU:HD23 | 1:G:201:VAL:HG21 | 1.93 | 0.51 |
| 1:G:72:VAL:HG21 | 1:G:195:ILE:O | 2.11 | 0.51 |
| 1:G:220:VAL:O | 1:G:221:PRO:C | 2.47 | 0.51 |
| 1:H:64:LYS:NZ | 1:H:200:MET:CE | 2.74 | 0.51 |
| 1:I:228:ILE:HD12 | 1:I:228:ILE:H | 1.73 | 0.51 |
| 1:I:373:GLN:HB3 | 1:I:464:LEU:HD12 | 1.92 | 0.51 |
| 1:I:391:ILE:HG21 | 1:I:402:TRP:CZ3 | 2.46 | 0.51 |
| 1:J:374:PHE:HB3 | 1:J:376:PHE:CE1 | 2.46 | 0.51 |
| 1:K:105:VAL:HG13 | 1:K:106:GLU:N | 2.24 | 0.51 |
| 1:K:213:LEU:O | 1:O:344:LEU:HB2 | 2.10 | 0.51 |
| 1:L:70:TYR:OH | 1:L:230:LYS:O | 2.18 | 0.51 |
| 1:L:122:LEU:O | 1:L:218:SER:HB2 | 2.10 | 0.51 |
| 1:L:124:ASN:HD22 | 1:L:216:ASN:ND2 | 2.08 | 0.51 |
| 1:L:166:GLY:H | 1:L:195:ILE:HD11 | 1.67 | 0.51 |
| 1:A:200:MET:O | 1:A:229:CYS:HA | 2.11 | 0.51 |
| 1:A:283:THR:OG1 | 1:E:142:ASP:CG | 2.49 | 0.51 |
| 1:B:323:ILE:HG21 | 1:B:325:TRP:CH2 | 2.46 | 0.51 |
| 1:C:194:VAL:HG21 | 1:C:444:TYR:CE2 | 2.46 | 0.51 |
| 1:D:23:SER:OG | 1:D:25:ASP:N | 2.43 | 0.51 |
| 1:D:64:LYS:CB | 1:D:64:LYS:CD | 2.83 | 0.51 |
| 1:D:71:ARG:NH1 | 1:D:71:ARG:HG2 | 2.25 | 0.51 |
| 1:D:137:ALA:CB | 1:D:137:ALA:C | 2.70 | 0.51 |
| 1:E:300:VAL:CG1 | 1:E:337:THR:HG22 | 2.41 | 0.51 |
| 1:F:65:VAL:CA | 1:F:69:GLN:NE2 | 2.72 | 0.51 |
| 1:G:259:HIS:HE1 | 1:H:130:GLU:OE1 | 1.93 | 0.51 |
| 1:H:28:VAL:CG1 | 1:H:29:ALA:H | 2.24 | 0.51 |
| 1:H:66:SER:HA | 1:H:366:HIS:ND1 | 2.26 | 0.51 |
| 1:H:72:VAL:HG21 | 1:H:195:ILE:O | 2.10 | 0.51 |
| 1:J:189:GLU:O | 1:J:191:ILE:HG13 | 2.11 | 0.51 |
| 1:L:122:LEU:CD1 | 1:M:286:LEU:HD11 | 2.34 | 0.51 |
| 1:M:467:LYS:O | 1:M:470:LEU:N | 2.43 | 0.51 |
| 1:N:246:LEU:HD23 | 1:N:246:LEU:H | 1.76 | 0.51 |
| 1:N:466:ARG:HD2 | 1:O:317:GLN:O | 2.11 | 0.51 |
| 1:A:149:MET:CA | 1:B:260:LEU:HD21 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:178:VAL:CG2 | 1:A:178:VAL:CA | 2.81 | 0.51 |
| 1:B:248:PHE:CE2 | 1:B:311:TYR:HB3 | 2.45 | 0.51 |
| 1:C:49:TYR:HE1 | 1:C:364:LEU:CD1 | 2.23 | 0.51 |
| 1:C:115:VAL:HA | 1:C:339:SER:OG | 2.11 | 0.51 |
| 1:C:163:PRO:N | 1:C:330:PHE:CD1 | 2.78 | 0.51 |
| 1:D:123:LEU:CD2 | 1:D:123:LEU:HG | 2.18 | 0.51 |
| 1:D:151:TYR:CG | 1:D:203:THR:HB | 2.46 | 0.51 |
| 1:D:163:PRO:HA | 1:D:330:PHE:CD1 | 2.46 | 0.51 |
| 1:D:188:LEU:HD11 | 1:D:213:LEU:CD1 | 2.39 | 0.51 |
| 1:D:440:PRO:HA | 1:D:443:LYS:HZ1 | 1.73 | 0.51 |
| 1:E:78:PRO:HD2 | 1:E:455:PHE:CE1 | 2.46 | 0.51 |
| 1:E:148:SER:O | 1:E:149:MET:HB3 | 2.09 | 0.51 |
| 1:E:207:ALA:HB1 | 1:E:229:CYS:O | 2.11 | 0.51 |
| 1:F:358:THR:HA | 1:G:266:THR:HG22 | 1.91 | 0.51 |
| 1:H:178:VAL:C | 1:H:180:VAL:H | 2.13 | 0.51 |
| 1:H:344:LEU:CB | 1:I:213:LEU:HD12 | 2.40 | 0.51 |
| 1:K:157:CYS:HB2 | 1:K:307:PHE:CE2 | 2.46 | 0.51 |
| 1:L:185:CYS:SG | 1:L:186:PRO:HD2 | 2.51 | 0.51 |
| 1:L:193:THR:OG1 | 1:L:194:VAL:N | 2.43 | 0.51 |
| 1:O:152:LYS:HE2 | 1:O:202:ASP:HB3 | 1.92 | 0.51 |
| 1:A:101:ALA:O | 1:A:376:PHE:HA | 2.11 | 0.51 |
| 1:A:114:GLY:HA2 | 1:B:255:MET:SD | 2.49 | 0.51 |
| 1:B:49:TYR:HE2 | 1:B:118:SER:CA | 2.15 | 0.51 |
| 1:C:29:ALA:HB3 | 1:C:380:LYS:HG3 | 1.92 | 0.51 |
| 1:C:348:ILE:O | 1:C:349:SER:HB3 | 2.11 | 0.51 |
| 1:D:92:ASN:O | 1:D:94:ASP:N | 2.43 | 0.51 |
| 1:D:247:PHE:HD1 | 1:D:248:PHE:H | 1.58 | 0.51 |
| 1:E:24:THR:C | 1:E:26:GLU:N | 2.64 | 0.51 |
| 1:E:124:ASN:OD1 | 1:E:124:ASN:O | 2.28 | 0.51 |
| 1:E:193:THR:HG21 | 1:E:230:LYS:HD3 | 1.93 | 0.51 |
| 1:F:117:ILE:HG13 | 1:F:149:MET:O | 2.10 | 0.51 |
| 1:F:176:THR:CG2 | 1:F:176:THR:HB | 2.19 | 0.51 |
| 1:F:219:GLU:O | 1:F:220:VAL:HG13 | 2.10 | 0.51 |
| 1:G:42:LEU:HB2 | 1:G:370:TYR:HB2 | 1.92 | 0.51 |
| 1:G:70:TYR:O | 1:G:71:ARG:NH1 | 2.44 | 0.51 |
| 1:G:115:VAL:HG22 | 1:H:255:MET:SD | 2.51 | 0.51 |
| 1:H:142:ASP:O | 1:I:283:THR:HG21 | 2.11 | 0.51 |
| 1:H:162:LYS:CG | 1:H:244:ASP:HB3 | 2.41 | 0.51 |
| 1:I:68:LEU:HD23 | 1:I:201:VAL:CG2 | 2.40 | 0.51 |
| 1:I:189:GLU:O | 1:I:191:ILE:HG13 | 2.11 | 0.51 |
| 1:K:142:ASP:O | 1:L:283:THR:CG2 | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:399:LEU:HA | 1:K:402:TRP:HE3 | 1.76 | 0.51 |
| 1:M:42:LEU:HD22 | 1:M:447:TRP:HZ2 | 1.75 | 0.51 |
| 1:M:71:ARG:HB3 | 1:M:73:PHE:CE1 | 2.46 | 0.51 |
| 1:N:48:PRO:HG2 | 1:N:49:TYR:CD1 | 2.46 | 0.51 |
| 1:O:125:LYS:HD3 | 1:O:126:LEU:N | 2.26 | 0.51 |
| 1:A:61:LEU:O | 1:A:61:LEU:CD1 | 2.54 | 0.51 |
| 1:A:154:THR:O | 1:A:336:THR:HG23 | 2.10 | 0.51 |
| 1:A:343:SER:HB3 | 1:A:364:LEU:HD23 | 1.93 | 0.51 |
| 1:B:171:LYS:CD | 1:B:171:LYS:CB | 2.78 | 0.51 |
| 1:B:259:HIS:CE1 | 1:C:130:GLU:HG2 | 2.46 | 0.51 |
| 1:C:249:TYR:CD1 | 1:C:249:TYR:C | 2.83 | 0.51 |
| 1:D:185:CYS:SG | 1:D:186:PRO:HD2 | 2.50 | 0.51 |
| 1:D:358:THR:HA | 1:E:266:THR:HG21 | 1.90 | 0.51 |
| 1:F:213:LEU:CD1 | 1:J:344:LEU:HD13 | 2.41 | 0.51 |
| 1:F:341:ASN:HB3 | 1:F:366:HIS:HB2 | 1.92 | 0.51 |
| 1:H:155:GLN:HB3 | 1:H:252:ARG:HB3 | 1.91 | 0.51 |
| 1:I:363:TYR:CE2 | 1:J:185:CYS:HB2 | 2.46 | 0.51 |
| 1:I:398:ILE:HG22 | 1:I:402:TRP:CE3 | 2.46 | 0.51 |
| 1:J:90:PHE:CD1 | 1:J:91:TYR:HB3 | 2.47 | 0.51 |
| 1:J:280:SER:CA | 1:J:284:ALA:HB2 | 2.41 | 0.51 |
| 1:J:399:LEU:HA | 1:J:402:TRP:HE3 | 1.75 | 0.51 |
| 1:K:442:LYS:HB3 | 1:K:443:LYS:HD3 | 1.93 | 0.51 |
| 1:L:153:GLN:HE22 | 1:L:300:VAL:HA | 1.76 | 0.51 |
| 1:M:72:VAL:HG23 | 1:M:197:ASP:HA | 1.93 | 0.51 |
| 1:O:452:LYS:CD | 1:O:452:LYS:NZ | 2.73 | 0.51 |
| 1:B:54:LYS:CG | 1:B:56:ASN:OD1 | 2.59 | 0.50 |
| 1:D:315:ARG:O | 1:D:316:ALA:HB2 | 2.11 | 0.50 |
| 1:E:36:HIS:ND1 | 1:E:37:ALA:N | 2.59 | 0.50 |
| 1:E:306:ILE:O | 1:E:306:ILE:HG22 | 2.11 | 0.50 |
| 1:F:42:LEU:HB2 | 1:F:370:TYR:HB2 | 1.93 | 0.50 |
| 1:F:162:LYS:C | 1:F:330:PHE:HD1 | 2.13 | 0.50 |
| 1:G:27:TYR:CE2 | 1:G:390:TYR:CE2 | 3.00 | 0.50 |
| 1:G:79:ASP:OD2 | 1:G:81:ASN:HB2 | 2.11 | 0.50 |
| 1:G:99:VAL:HG11 | 1:G:323:ILE:CG2 | 2.41 | 0.50 |
| 1:G:252:ARG:HD2 | 1:G:306:ILE:HD11 | 1.93 | 0.50 |
| 1:G:323:ILE:HG21 | 1:G:325:TRP:CH2 | 2.46 | 0.50 |
| 1:I:79:ASP:OD1 | 1:I:80:PRO:HD2 | 2.12 | 0.50 |
| 1:I:117:ILE:HD11 | 1:J:260:LEU:HD23 | 1.92 | 0.50 |
| 1:J:320:ASN:ND2 | 1:J:323:ILE:HB | 2.26 | 0.50 |
| 1:K:53:LYS:HD3 | 1:K:58:ASN:HA | 1.93 | 0.50 |
| 1:L:27:TYR:CE2 | 1:L:390:TYR:CE2 | 2.99 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:54:LYS:HG3 | 1:L:55:PRO:CD | 2.40 | 0.50 |
| 1:L:152:LYS:O | 1:L:152:LYS:HG3 | 2.11 | 0.50 |
| 1:M:74:ARG:NH2 | 1:M:441:LEU:CD1 | 2.58 | 0.50 |
| 1:M:157:CYS:HB2 | 1:M:307:PHE:HE2 | 1.75 | 0.50 |
| 1:M:373:GLN:CB | 1:M:464:LEU:HD12 | 2.41 | 0.50 |
| 1:N:77:LEU:O | 1:N:327:ASN:HB3 | 2.11 | 0.50 |
| 1:N:102:CYS:SG | 1:N:313:LEU:HD12 | 2.51 | 0.50 |
| 1:N:109:ARG:NH1 | 1:N:370:TYR:CD1 | 2.80 | 0.50 |
| 1:A:461:GLN:NE2 | 1:B:21:VAL:HB | 2.20 | 0.50 |
| 1:B:176:THR:CG2 | 1:B:176:THR:CA | 2.85 | 0.50 |
| 1:B:193:THR:CG2 | 1:B:230:LYS:HD2 | 2.41 | 0.50 |
| 1:B:320:ASN:HD21 | 1:B:323:ILE:HB | 1.76 | 0.50 |
| 1:C:71:ARG:NH1 | 1:C:198:GLY:H | 2.06 | 0.50 |
| 1:C:280:SER:C | 1:C:284:ALA:HB2 | 2.32 | 0.50 |
| 1:D:81:ASN:ND2 | 1:D:402:TRP:CD1 | 2.80 | 0.50 |
| 1:D:87:ASP:O | 1:D:90:PHE:HE2 | 1.93 | 0.50 |
| 1:D:172:GLY:O | 1:D:173:SER:C | 2.50 | 0.50 |
| 1:F:375:ILE:HG21 | 1:F:468:PHE:CD2 | 2.45 | 0.50 |
| 1:G:231:TYR:CD1 | 1:G:232:PRO:HD2 | 2.46 | 0.50 |
| 1:H:153:GLN:NE2 | 1:H:300:VAL:HG12 | 2.26 | 0.50 |
| 1:H:200:MET:O | 1:H:229:CYS:HA | 2.11 | 0.50 |
| 1:H:400:GLU:O | 1:H:402:TRP:N | 2.44 | 0.50 |
| 1:K:471:GLN:O | 1:K:472:LEU:OXT | 2.29 | 0.50 |
| 1:L:139:ALA:CB | 1:L:143:ASN:HD21 | 2.24 | 0.50 |
| 1:L:255:MET:HG2 | 1:L:256:PHE:H | 1.70 | 0.50 |
| 1:L:353:THR:O | 1:N:278:LYS:HB2 | 2.11 | 0.50 |
| 1:M:151:TYR:CZ | 1:M:224:ILE:HD13 | 2.47 | 0.50 |
| 1:M:237:MET:HB3 | 1:M:246:LEU:HD22 | 1.93 | 0.50 |
| 1:N:147:ILE:HG23 | 1:O:129:THR:O | 2.10 | 0.50 |
| 1:N:163:PRO:CA | 1:N:330:PHE:CD1 | 2.94 | 0.50 |
| 1:N:223:ASP:OD1 | 1:N:224:ILE:N | 2.44 | 0.50 |
| 1:O:22:VAL:HG23 | 1:O:22:VAL:O | 2.12 | 0.50 |
| 1:A:80:PRO:HG2 | 1:A:98:LEU:O | 2.12 | 0.50 |
| 1:B:90:PHE:HD1 | 1:B:91:TYR:HB3 | 1.76 | 0.50 |
| 1:C:459:LEU:C | 1:C:461:GLN:H | 2.14 | 0.50 |
| 1:D:54:LYS:HE3 | 1:D:55:PRO:CD | 2.26 | 0.50 |
| 1:D:122:LEU:O | 1:D:218:SER:HB2 | 2.11 | 0.50 |
| 1:E:172:GLY:O | 1:E:173:SER:C | 2.50 | 0.50 |
| 1:F:42:LEU:HB2 | 1:F:370:TYR:CB | 2.41 | 0.50 |
| 1:F:172:GLY:O | 1:F:173:SER:C | 2.49 | 0.50 |
| 1:F:255:MET:O | 1:J:300:VAL:HG22 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:123:LEU:O | 1:G:125:LYS:N | 2.44 | 0.50 |
| 1:H:160:GLY:O | 1:H:329:LEU:HD23 | 2.11 | 0.50 |
| 1:J:71:ARG:NH1 | 1:J:71:ARG:HA | 2.23 | 0.50 |
| 1:J:320:ASN:HD22 | 1:J:325:TRP:HE1 | 1.57 | 0.50 |
| 1:J:444:TYR:HB2 | 1:J:446:PHE:CZ | 2.47 | 0.50 |
| 1:K:209:ASP:O | 1:K:213:LEU:HB2 | 2.11 | 0.50 |
| 1:K:440:PRO:HA | 1:K:443:LYS:HZ2 | 1.77 | 0.50 |
| 1:L:60:ILE:O | 1:L:60:ILE:HG13 | 2.10 | 0.50 |
| 1:L:220:VAL:O | 1:L:221:PRO:O | 2.30 | 0.50 |
| 1:M:139:ALA:HB1 | 1:M:143:ASN:OD1 | 2.12 | 0.50 |
| 1:N:142:ASP:OD1 | 1:O:283:THR:OG1 | 2.30 | 0.50 |
| 1:N:234:TYR:O | 1:N:235:ILE:C | 2.49 | 0.50 |
| 1:O:384:THR:HG23 | 1:O:387:VAL:HG21 | 1.93 | 0.50 |
| 1:A:92:ASN:ND2 | 1:A:94:ASP:H | 2.09 | 0.50 |
| 1:B:80:PRO:C | 1:B:82:LYS:N | 2.64 | 0.50 |
| 1:B:96:GLN:HB3 | 1:B:382:THR:HA | 1.92 | 0.50 |
| 1:B:142:ASP:CG | 1:C:283:THR:HG1 | 2.08 | 0.50 |
| 1:C:41:ARG:HG2 | 1:C:42:LEU:O | 2.11 | 0.50 |
| 1:C:70:TYR:OH | 1:C:232:PRO:HD3 | 2.10 | 0.50 |
| 1:C:119:GLY:HA3 | 1:C:148:SER:HB3 | 1.94 | 0.50 |
| 1:C:139:ALA:HB1 | 1:C:143:ASN:HD21 | 1.75 | 0.50 |
| 1:D:150:ASP:CG | 1:D:150:ASP:O | 2.48 | 0.50 |
| 1:E:33:ILE:HB | 1:E:378:LEU:HB3 | 1.93 | 0.50 |
| 1:E:159:ILE:HG22 | 1:E:247:PHE:HE1 | 1.77 | 0.50 |
| 1:E:242:TYR:HB3 | 1:E:244:ASP:OD1 | 2.11 | 0.50 |
| 1:G:52:ILE:O | 1:G:61:LEU:HB3 | 2.11 | 0.50 |
| 1:G:81:ASN:ND2 | 1:G:402:TRP:CD1 | 2.79 | 0.50 |
| 1:I:108:GLY:N | 1:I:371:ASP:O | 2.44 | 0.50 |
| 1:I:237:MET:HB3 | 1:I:246:LEU:CD2 | 2.42 | 0.50 |
| 1:J:372:LEU:HB3 | 1:J:374:PHE:CE1 | 2.45 | 0.50 |
| 1:K:355:TYR:CE1 | 1:L:144:ARG:HD3 | 2.47 | 0.50 |
| 1:L:107:VAL:O | 1:L:307:PHE:HB3 | 2.11 | 0.50 |
| 1:M:170:GLY:HA2 | 1:M:213:LEU:HD21 | 1.94 | 0.50 |
| 1:M:364:LEU:HD11 | 1:N:290:ASN:HA | 1.92 | 0.50 |
| 1:N:311:TYR:CD2 | 1:N:311:TYR:N | 2.75 | 0.50 |
| 1:N:397:THR:O | 1:N:398:ILE:C | 2.48 | 0.50 |
| 1:O:228:ILE:N | 1:O:228:ILE:CD1 | 2.64 | 0.50 |
| 1:A:120:HIS:ND1 | 1:A:121:PRO:HD2 | 2.25 | 0.50 |
| 1:A:150:ASP:CG | 1:A:150:ASP:O | 2.49 | 0.50 |
| 1:A:300:VAL:CG1 | 1:A:300:VAL:CA | 2.79 | 0.50 |
| 1:A:391:ILE:HG21 | 1:A:402:TRP:CZ3 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:109:ARG:NH1 | 1:B:370:TYR:CE1 | 2.80 | 0.50 |
| 1:C:214:GLN:CD | 1:C:219:GLU:HG3 | 2.32 | 0.50 |
| 1:D:92:ASN:C | 1:D:94:ASP:H | 2.15 | 0.50 |
| 1:E:71:ARG:HD2 | 1:E:447:TRP:CZ3 | 2.47 | 0.50 |
| 1:E:240:GLU:HG3 | 1:E:243:GLY:N | 2.27 | 0.50 |
| 1:E:384:THR:OG1 | 1:E:387:VAL:HG23 | 2.12 | 0.50 |
| 1:F:156:LEU:HD21 | 1:F:334:VAL:HG21 | 1.94 | 0.50 |
| 1:F:399:LEU:HA | 1:F:402:TRP:HE3 | 1.76 | 0.50 |
| 1:G:30:ARG:HH11 | 1:G:377:GLN:HE22 | 1.56 | 0.50 |
| 1:G:293:PRO:HG2 | 1:G:293:PRO:O | 2.11 | 0.50 |
| 1:G:463:PRO:HA | 1:G:466:ARG:NE | 2.25 | 0.50 |
| 1:H:53:LYS:HD3 | 1:H:58:ASN:HA | 1.93 | 0.50 |
| 1:H:68:LEU:CD2 | 1:H:203:THR:HG22 | 2.29 | 0.50 |
| 1:J:78:PRO:CD | 1:J:455:PHE:CE1 | 2.95 | 0.50 |
| 1:J:315:ARG:O | 1:J:316:ALA:HB2 | 2.11 | 0.50 |
| 1:K:24:THR:HA | 1:K:27:TYR:CE2 | 2.46 | 0.50 |
| 1:K:97:ARG:HG3 | 1:K:383:LEU:HD11 | 1.93 | 0.50 |
| 1:K:139:ALA:CB | 1:K:143:ASN:HD21 | 2.24 | 0.50 |
| 1:K:471:GLN:OE1 | 1:K:472:LEU:N | 2.45 | 0.50 |
| 1:L:54:LYS:HA | 1:L:54:LYS:NZ | 2.25 | 0.50 |
| 1:L:194:VAL:CG2 | 1:L:444:TYR:CE2 | 2.95 | 0.50 |
| 1:L:389:THR:OG1 | 1:L:390:TYR:N | 2.45 | 0.50 |
| 1:M:242:TYR:CE2 | 1:M:394:MET:HB2 | 2.46 | 0.50 |
| 1:M:383:LEU:CD2 | 1:M:388:MET:HE2 | 2.41 | 0.50 |
| 1:O:120:HIS:HE2 | 1:O:218:SER:HB3 | 1.72 | 0.50 |
| 1:A:115:VAL:H | 1:B:255:MET:HE3 | 1.75 | 0.50 |
| 1:C:98:LEU:HD13 | 1:C:378:LEU:HD11 | 1.93 | 0.50 |
| 1:D:81:ASN:ND2 | 1:D:402:TRP:HD1 | 2.09 | 0.50 |
| 1:D:109:ARG:HE | 1:D:338:ARG:HD2 | 1.77 | 0.50 |
| 1:D:200:MET:O | 1:D:229:CYS:HA | 2.11 | 0.50 |
| 1:D:384:THR:HG23 | 1:D:387:VAL:HG21 | 1.94 | 0.50 |
| 1:E:149:MET:CE | 1:E:205:PHE:HE1 | 2.25 | 0.50 |
| 1:E:152:LYS:HB2 | 1:E:255:MET:CB | 2.22 | 0.50 |
| 1:E:300:VAL:CG1 | 1:E:337:THR:HA | 2.39 | 0.50 |
| 1:F:255:MET:HE1 | 1:J:115:VAL:N | 2.11 | 0.50 |
| 1:F:257:VAL:O | 1:J:258:ARG:NH2 | 2.44 | 0.50 |
| 1:F:329:LEU:HD13 | 1:F:374:PHE:CE2 | 2.47 | 0.50 |
| 1:F:397:THR:O | 1:F:401:ASP:OD2 | 2.30 | 0.50 |
| 1:G:115:VAL:H | 1:H:255:MET:HE1 | 1.76 | 0.50 |
| 1:G:155:GLN:OE1 | 1:G:305:GLN:HA | 2.12 | 0.50 |
| 1:H:290:ASN:N | 1:H:290:ASN:HD22 | 2.08 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:75:ILE:HD13 | 1:J:329:LEU:HB3 | 1.94 | 0.50 |
| 1:J:75:ILE:HD12 | 1:J:75:ILE:N | 2.26 | 0.50 |
| 1:J:85:PHE:CZ | 1:J:378:LEU:HD22 | 2.46 | 0.50 |
| 1:J:101:ALA:O | 1:J:376:PHE:CA | 2.57 | 0.50 |
| 1:J:120:HIS:CE1 | 1:J:122:LEU:H | 2.27 | 0.50 |
| 1:K:28:VAL:HG12 | 1:K:29:ALA:N | 2.26 | 0.50 |
| 1:K:30:ARG:HH11 | 1:K:377:GLN:NE2 | 2.10 | 0.50 |
| 1:L:115:VAL:H | 1:M:255:MET:HE1 | 1.77 | 0.50 |
| 1:L:360:PHE:N | 1:L:360:PHE:CD1 | 2.80 | 0.50 |
| 1:M:387:VAL:HG13 | 1:M:391:ILE:HD11 | 1.94 | 0.50 |
| 1:N:163:PRO:HB3 | 1:N:330:PHE:CE1 | 2.46 | 0.50 |
| 1:O:96:GLN:HA | 1:O:382:THR:HA | 1.94 | 0.50 |
| 1:O:255:MET:HG2 | 1:O:256:PHE:N | 2.26 | 0.50 |
| 1:A:274:ASP:O | 1:E:217:LYS:HD3 | 2.11 | 0.50 |
| 1:B:292:PHE:C | 1:B:292:PHE:CD1 | 2.85 | 0.50 |
| 1:C:125:LYS:NZ | 1:D:132:ALA:O | 2.41 | 0.50 |
| 1:C:323:ILE:HG21 | 1:C:325:TRP:CH2 | 2.46 | 0.50 |
| 1:C:440:PRO:CA | 1:C:443:LYS:HZ1 | 2.24 | 0.50 |
| 1:D:307:PHE:C | 1:D:309:LYS:H | 2.15 | 0.50 |
| 1:D:312:TRP:CH2 | 1:D:468:PHE:HA | 2.46 | 0.50 |
| 1:E:103:VAL:HG22 | 1:E:375:ILE:O | 2.12 | 0.50 |
| 1:E:234:TYR:O | 1:E:235:ILE:C | 2.49 | 0.50 |
| 1:F:257:VAL:HG13 | 1:J:115:VAL:HG21 | 1.93 | 0.50 |
| 1:F:451:LEU:CD2 | 1:F:454:LYS:HG3 | 2.37 | 0.50 |
| 1:G:458:ASP:OD2 | 1:G:458:ASP:N | 2.44 | 0.50 |
| 1:H:170:GLY:HA2 | 1:H:213:LEU:HD21 | 1.94 | 0.50 |
| 1:H:361:LYS:CG | 1:H:361:LYS:CE | 2.87 | 0.50 |
| 1:K:149:MET:HA | 1:L:260:LEU:HD21 | 1.93 | 0.50 |
| 1:K:255:MET:SD | 1:O:115:VAL:HG22 | 2.52 | 0.50 |
| 1:L:373:GLN:HB2 | 1:L:464:LEU:HD12 | 1.94 | 0.50 |
| 1:M:360:PHE:O | 1:N:266:THR:HG23 | 2.12 | 0.50 |
| 1:N:155:GLN:OE1 | 1:N:305:GLN:HA | 2.12 | 0.50 |
| 1:N:214:GLN:OE1 | 1:N:219:GLU:HB2 | 2.12 | 0.50 |
| 1:N:443:LYS:HD3 | 1:N:443:LYS:N | 2.26 | 0.50 |
| 1:O:242:TYR:CE2 | 1:O:394:MET:CG | 2.85 | 0.50 |
| 1:B:103:VAL:CG2 | 1:B:104:GLY:N | 2.74 | 0.50 |
| 1:B:115:VAL:HG22 | 1:C:255:MET:SD | 2.52 | 0.50 |
| 1:C:68:LEU:HB3 | 1:C:201:VAL:HG22 | 1.94 | 0.50 |
| 1:D:21:VAL:HG12 | 1:D:390:TYR:OH | 2.12 | 0.50 |
| 1:E:92:ASN:ND2 | 1:E:95:THR:OG1 | 2.44 | 0.50 |
| 1:E:459:LEU:HB3 | 1:E:465:GLY:CA | 2.35 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:78:PRO:HD2 | 1:G:455:PHE:CE1 | 2.46 | 0.50 |
| 1:I:163:PRO:CA | 1:I:330:PHE:HD1 | 2.25 | 0.50 |
| 1:J:241:PRO:HG2 | 1:J:242:TYR:N | 2.27 | 0.50 |
| 1:K:54:LYS:HG3 | 1:K:55:PRO:CD | 2.41 | 0.50 |
| 1:K:134:ALA:O | 1:K:135:TYR:C | 2.50 | 0.50 |
| 1:L:400:GLU:O | 1:L:402:TRP:O | 2.29 | 0.50 |
| 1:L:459:LEU:HB3 | 1:L:465:GLY:CA | 2.42 | 0.50 |
| 1:M:276:TYR:CD1 | 1:M:277:ILE:N | 2.80 | 0.50 |
| 1:M:463:PRO:CB | 1:M:466:ARG:HH21 | 2.23 | 0.50 |
| 1:N:95:THR:O | 1:N:383:LEU:N | 2.38 | 0.50 |
| 1:N:221:PRO:HD2 | 1:N:224:ILE:HD11 | 1.93 | 0.50 |
| 1:O:77:LEU:HB2 | 1:O:327:ASN:HB3 | 1.94 | 0.50 |
| 1:O:267:VAL:HG12 | 1:O:269:GLU:O | 2.11 | 0.50 |
| 1:A:34:TYR:CZ | 1:A:377:GLN:HG3 | 2.41 | 0.50 |
| 1:A:176:THR:C | 1:A:177:GLN:HG3 | 2.32 | 0.50 |
| 1:A:357:ASN:H | 1:B:141:VAL:HG13 | 1.76 | 0.50 |
| 1:C:137:ALA:O | 1:C:138:ASN:O | 2.30 | 0.50 |
| 1:C:333:VAL:HG12 | 1:C:334:VAL:N | 2.27 | 0.50 |
| 1:D:167:GLU:HG2 | 1:D:231:TYR:O | 2.12 | 0.50 |
| 1:E:57:ASN:CG | 1:E:59:LYS:H | 2.14 | 0.50 |
| 1:E:66:SER:H | 1:E:69:GLN:HE21 | 1.59 | 0.50 |
| 1:E:120:HIS:HA | 1:E:222:LEU:HD13 | 1.93 | 0.50 |
| 1:E:167:GLU:HG2 | 1:E:233:ASP:HB2 | 1.94 | 0.50 |
| 1:F:152:LYS:HB2 | 1:F:255:MET:CB | 2.41 | 0.50 |
| 1:G:54:LYS:HA | 1:G:54:LYS:HZ2 | 1.77 | 0.50 |
| 1:G:242:TYR:CG | 1:G:394:MET:HG3 | 2.44 | 0.50 |
| 1:G:471:GLN:CD | 1:G:472:LEU:N | 2.65 | 0.50 |
| 1:H:68:LEU:HD22 | 1:H:203:THR:CG2 | 2.29 | 0.50 |
| 1:I:281:GLY:N | 1:I:284:ALA:HB3 | 2.26 | 0.50 |
| 1:J:395:ASN:O | 1:J:398:ILE:HG12 | 2.12 | 0.50 |
| 1:L:78:PRO:HD2 | 1:L:455:PHE:CE1 | 2.47 | 0.50 |
| 1:L:148:SER:HB3 | 1:M:291:TYR:CD2 | 2.47 | 0.50 |
| 1:M:248:PHE:CZ | 1:M:311:TYR:HB3 | 2.47 | 0.50 |
| 1:N:79:ASP:O | 1:N:83:PHE:N | 2.45 | 0.50 |
| 1:N:300:VAL:HG23 | 1:N:300:VAL:O | 2.12 | 0.50 |
| 1:A:194:VAL:HG12 | 1:A:195:ILE:N | 2.27 | 0.49 |
| 1:A:438:GLU:HG2 | 1:A:439:ASP:H | 1.76 | 0.49 |
| 1:E:223:ASP:OD1 | 1:E:224:ILE:HG23 | 2.12 | 0.49 |
| 1:F:255:MET:HE1 | 1:J:115:VAL:HG22 | 1.94 | 0.49 |
| 1:F:399:LEU:O | 1:F:402:TRP:HB2 | 2.12 | 0.49 |
| 1:F:463:PRO:HA | 1:F:466:ARG:HE | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:72:VAL:HG23 | 1:G:197:ASP:HA | 1.93 | 0.49 |
| 1:G:105:VAL:HG22 | 1:G:374:PHE:CD2 | 2.47 | 0.49 |
| 1:G:335:ASP:OD1 | 1:G:337:THR:OG1 | 2.30 | 0.49 |
| 1:I:231:TYR:CD1 | 1:I:232:PRO:HD2 | 2.48 | 0.49 |
| 1:K:77:LEU:HD22 | 1:K:455:PHE:HZ | 1.77 | 0.49 |
| 1:K:210:PHE:CE1 | 1:K:224:ILE:HB | 2.46 | 0.49 |
| 1:K:462:PHE:O | 1:K:466:ARG:HG3 | 2.12 | 0.49 |
| 1:L:48:PRO:HG2 | 1:L:49:TYR:CD1 | 2.46 | 0.49 |
| 1:L:205:PHE:CD1 | 1:L:220:VAL:HG12 | 2.47 | 0.49 |
| 1:M:71:ARG:HH12 | 1:M:198:GLY:N | 2.08 | 0.49 |
| 1:M:302:SER:HB2 | 1:N:253:GLU:H | 1.76 | 0.49 |
| 1:M:390:TYR:O | 1:M:392:HIS:N | 2.44 | 0.49 |
| 1:N:28:VAL:CG1 | 1:N:28:VAL:CA | 2.81 | 0.49 |
| 1:O:75:ILE:HB | 1:O:329:LEU:HB3 | 1.94 | 0.49 |
| 1:A:160:GLY:HA3 | 1:A:245:SER:O | 2.12 | 0.49 |
| 1:A:250:LEU:HD13 | 1:A:306:ILE:CG2 | 2.43 | 0.49 |
| 1:B:33:ILE:HA | 1:B:33:ILE:HD13 | 1.95 | 0.49 |
| 1:B:260:LEU:N | 1:B:260:LEU:HD12 | 2.26 | 0.49 |
| 1:C:155:GLN:HG2 | 1:C:307:PHE:CE1 | 2.48 | 0.49 |
| 1:D:162:LYS:HB3 | 1:D:163:PRO:HD2 | 1.94 | 0.49 |
| 1:D:237:MET:SD | 1:D:246:LEU:HD22 | 2.52 | 0.49 |
| 1:E:27:TYR:CE2 | 1:E:390:TYR:CE2 | 3.00 | 0.49 |
| 1:G:180:VAL:HG13 | 1:G:184:ASP:HB3 | 1.92 | 0.49 |
| 1:I:54:LYS:HA | 1:I:54:LYS:HZ1 | 1.77 | 0.49 |
| 1:I:69:GLN:HA | 1:I:199:ASP:O | 2.13 | 0.49 |
| 1:I:76:HIS:HB2 | 1:I:450:ASN:HA | 1.93 | 0.49 |
| 1:I:250:LEU:HD12 | 1:I:250:LEU:H | 1.76 | 0.49 |
| 1:J:184:ASP:O | 1:J:185:CYS:C | 2.51 | 0.49 |
| 1:L:220:VAL:O | 1:L:221:PRO:C | 2.48 | 0.49 |
| 1:M:180:VAL:HG12 | 1:M:181:GLN:H | 1.77 | 0.49 |
| 1:N:217:LYS:HD3 | 1:O:274:ASP:C | 2.30 | 0.49 |
| 1:O:119:GLY:HA3 | 1:O:148:SER:HB3 | 1.94 | 0.49 |
| 1:A:120:HIS:ND1 | 1:A:121:PRO:CD | 2.75 | 0.49 |
| 1:A:178:VAL:C | 1:A:180:VAL:H | 2.10 | 0.49 |
| 1:A:399:LEU:O | 1:A:402:TRP:HB2 | 2.12 | 0.49 |
| 1:E:170:GLY:O | 1:E:188:LEU:HA | 2.13 | 0.49 |
| 1:G:119:GLY:HA3 | 1:G:148:SER:HB3 | 1.94 | 0.49 |
| 1:G:248:PHE:CZ | 1:G:311:TYR:HB3 | 2.48 | 0.49 |
| 1:G:316:ALA:C | 1:G:318:GLY:N | 2.65 | 0.49 |
| 1:G:439:ASP:HB3 | 1:G:442:LYS:HE3 | 1.94 | 0.49 |
| 1:H:355:TYR:CD1 | 1:I:144:ARG:HD3 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:395:ASN:HB3 | 1:H:398:ILE:HG12 | 1.94 | 0.49 |
| 1:I:70:TYR:O | 1:I:71:ARG:NH1 | 2.45 | 0.49 |
| 1:I:122:LEU:O | 1:I:218:SER:HB2 | 2.12 | 0.49 |
| 1:I:216:ASN:OD1 | 1:I:218:SER:N | 2.45 | 0.49 |
| 1:I:236:LYS:CB | 1:I:236:LYS:CD | 2.82 | 0.49 |
| 1:J:193:THR:HG23 | 1:J:230:LYS:HD2 | 1.95 | 0.49 |
| 1:K:50:PHE:HB2 | 1:K:51:PRO:HD2 | 1.94 | 0.49 |
| 1:K:77:LEU:HD22 | 1:K:455:PHE:CZ | 2.47 | 0.49 |
| 1:K:150:ASP:CG | 1:L:257:VAL:HG21 | 2.32 | 0.49 |
| 1:K:260:LEU:O | 1:K:261:PHE:CD2 | 2.65 | 0.49 |
| 1:K:293:PRO:HD3 | 1:O:117:ILE:HG21 | 1.95 | 0.49 |
| 1:M:439:ASP:OD2 | 1:M:440:PRO:HD2 | 2.12 | 0.49 |
| 1:N:158:LEU:HD23 | 1:N:249:TYR:HB2 | 1.93 | 0.49 |
| 1:N:302:SER:CB | 1:O:253:GLU:H | 2.25 | 0.49 |
| 1:O:442:LYS:HG2 | 1:O:442:LYS:HZ3 | 1.76 | 0.49 |
| 1:B:65:VAL:HA | 1:B:69:GLN:NE2 | 2.24 | 0.49 |
| 1:B:124:ASN:OD1 | 1:B:264:ALA:N | 2.33 | 0.49 |
| 1:B:148:SER:HB3 | 1:C:291:TYR:CD2 | 2.48 | 0.49 |
| 1:B:153:GLN:NE2 | 1:B:300:VAL:HG12 | 2.28 | 0.49 |
| 1:B:163:PRO:N | 1:B:330:PHE:HD1 | 2.11 | 0.49 |
| 1:E:54:LYS:HB3 | 1:E:57:ASN:HD22 | 1.77 | 0.49 |
| 1:E:395:ASN:C | 1:E:395:ASN:HD22 | 2.15 | 0.49 |
| 1:F:439:ASP:O | 1:F:442:LYS:HB2 | 2.12 | 0.49 |
| 1:F:467:LYS:CD | 1:F:467:LYS:CB | 2.82 | 0.49 |
| 1:G:149:MET:HE1 | 1:G:205:PHE:CZ | 2.48 | 0.49 |
| 1:G:391:ILE:CG2 | 1:G:398:ILE:CG2 | 2.88 | 0.49 |
| 1:I:50:PHE:CD1 | 1:I:50:PHE:C | 2.85 | 0.49 |
| 1:I:101:ALA:O | 1:I:376:PHE:HA | 2.11 | 0.49 |
| 1:I:458:ASP:OD2 | 1:I:458:ASP:N | 2.45 | 0.49 |
| 1:J:91:TYR:CD1 | 1:J:92:ASN:N | 2.81 | 0.49 |
| 1:J:438:GLU:HG2 | 1:J:439:ASP:N | 2.27 | 0.49 |
| 1:K:54:LYS:HB2 | 1:K:57:ASN:HD22 | 1.77 | 0.49 |
| 1:K:77:LEU:O | 1:K:327:ASN:HB3 | 2.12 | 0.49 |
| 1:L:69:GLN:HA | 1:L:199:ASP:O | 2.13 | 0.49 |
| 1:L:159:ILE:CD1 | 1:L:159:ILE:HG21 | 2.41 | 0.49 |
| 1:M:355:TYR:CD1 | 1:N:144:ARG:HD3 | 2.48 | 0.49 |
| 1:N:216:ASN:HB3 | 1:N:219:GLU:HG3 | 1.94 | 0.49 |
| 1:O:54:LYS:CB | 1:O:57:ASN:HB3 | 2.42 | 0.49 |
| 1:O:167:GLU:HG3 | 1:O:231:TYR:O | 2.11 | 0.49 |
| 1:B:21:VAL:CG1 | 1:B:22:VAL:N | 2.75 | 0.49 |
| 1:C:70:TYR:CD2 | 1:C:195:ILE:HG21 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:281:GLY:O | 1:C:284:ALA:CB | 2.60 | 0.49 |
| 1:C:317:GLN:NE2 | 1:C:317:GLN:C | 2.65 | 0.49 |
| 1:E:316:ALA:O | 1:E:318:GLY:N | 2.45 | 0.49 |
| 1:F:24:THR:C | 1:F:26:GLU:N | 2.66 | 0.49 |
| 1:F:145:GLU:OE1 | 1:G:134:ALA:N | 2.46 | 0.49 |
| 1:F:145:GLU:OE1 | 1:G:134:ALA:HA | 2.11 | 0.49 |
| 1:I:74:ARG:CB | 1:I:330:PHE:HE2 | 2.25 | 0.49 |
| 1:K:66:SER:HA | 1:K:366:HIS:ND1 | 2.27 | 0.49 |
| 1:K:79:ASP:CG | 1:K:81:ASN:HB2 | 2.33 | 0.49 |
| 1:K:272:PRO:HD2 | 1:K:275:LEU:HD11 | 1.94 | 0.49 |
| 1:L:21:VAL:CG1 | 1:L:390:TYR:OH | 2.60 | 0.49 |
| 1:M:36:HIS:ND1 | 1:M:36:HIS:C | 2.66 | 0.49 |
| 1:M:326:GLY:O | 1:M:327:ASN:HB2 | 2.12 | 0.49 |
| 1:O:305:GLN:HE22 | 1:O:337:THR:HG21 | 1.77 | 0.49 |
| 1:A:471:GLN:CD | 1:A:472:LEU:N | 2.65 | 0.49 |
| 1:B:348:ILE:HD12 | 1:C:182:PRO:O | 2.12 | 0.49 |
| 1:D:27:TYR:CE2 | 1:D:390:TYR:CE2 | 3.01 | 0.49 |
| 1:D:137:ALA:CB | 1:D:137:ALA:N | 2.66 | 0.49 |
| 1:D:302:SER:C | 1:D:304:ALA:H | 2.16 | 0.49 |
| 1:E:98:LEU:CD2 | 1:E:379:CYS:O | 2.57 | 0.49 |
| 1:F:68:LEU:O | 1:F:201:VAL:HG22 | 2.12 | 0.49 |
| 1:F:149:MET:HE1 | 1:F:205:PHE:CE1 | 2.47 | 0.49 |
| 1:F:472:LEU:HD23 | 1:O:138:ASN:HD22 | 1.76 | 0.49 |
| 1:G:105:VAL:HG12 | 1:G:106:GLU:N | 2.24 | 0.49 |
| 1:H:119:GLY:N | 1:H:221:PRO:HB3 | 2.28 | 0.49 |
| 1:I:115:VAL:HG21 | 1:J:257:VAL:HG13 | 1.95 | 0.49 |
| 1:I:163:PRO:N | 1:I:330:PHE:CD1 | 2.79 | 0.49 |
| 1:I:163:PRO:HA | 1:I:330:PHE:CD1 | 2.47 | 0.49 |
| 1:I:168:HIS:HB2 | 1:I:208:MET:HA | 1.95 | 0.49 |
| 1:I:384:THR:H | 1:I:387:VAL:HB | 1.77 | 0.49 |
| 1:I:451:LEU:HA | 1:I:454:LYS:HG3 | 1.93 | 0.49 |
| 1:J:178:VAL:CG1 | 1:J:178:VAL:CG2 | 2.82 | 0.49 |
| 1:J:391:ILE:HD13 | 1:J:402:TRP:HH2 | 1.78 | 0.49 |
| 1:J:397:THR:O | 1:J:401:ASP:OD2 | 2.29 | 0.49 |
| 1:K:259:HIS:CE1 | 1:L:130:GLU:HG2 | 2.48 | 0.49 |
| 1:K:395:ASN:HB3 | 1:K:398:ILE:CG1 | 2.42 | 0.49 |
| 1:L:180:VAL:HG12 | 1:L:181:GLN:H | 1.76 | 0.49 |
| 1:M:126:LEU:HD13 | 1:M:264:ALA:HB2 | 1.95 | 0.49 |
| 1:M:167:GLU:HG3 | 1:M:167:GLU:O | 2.11 | 0.49 |
| 1:N:74:ARG:HG3 | 1:N:330:PHE:HE2 | 1.75 | 0.49 |
| 1:N:384:THR:OG1 | 1:N:385:ALA:N | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:60:ILE:HD13 | 1:C:60:ILE:CG2 | 2.36 | 0.49 |
| 1:C:258:ARG:HG3 | 1:C:259:HIS:ND1 | 2.28 | 0.49 |
| 1:D:176:THR:C | 1:D:177:GLN:CG | 2.81 | 0.49 |
| 1:D:472:LEU:HD23 | 1:I:138:ASN:ND2 | 2.19 | 0.49 |
| 1:E:105:VAL:HG12 | 1:E:106:GLU:N | 2.25 | 0.49 |
| 1:F:325:TRP:CZ2 | 1:F:394:MET:HE1 | 2.47 | 0.49 |
| 1:G:290:ASN:HD22 | 1:G:290:ASN:N | 2.10 | 0.49 |
| 1:H:306:ILE:N | 1:H:306:ILE:HD13 | 2.28 | 0.49 |
| 1:H:354:THR:O | 1:H:356:LYS:HG3 | 2.12 | 0.49 |
| 1:H:363:TYR:CE2 | 1:I:185:CYS:HB2 | 2.46 | 0.49 |
| 1:H:451:LEU:HA | 1:H:454:LYS:CG | 2.41 | 0.49 |
| 1:I:34:TYR:CE2 | 1:I:377:GLN:CB | 2.92 | 0.49 |
| 1:I:279:GLY:C | 1:I:284:ALA:HB2 | 2.33 | 0.49 |
| 1:J:153:GLN:NE2 | 1:J:298:SER:O | 2.45 | 0.49 |
| 1:J:180:VAL:CG2 | 1:J:180:VAL:CA | 2.81 | 0.49 |
| 1:K:49:TYR:CE2 | 1:K:118:SER:HA | 2.47 | 0.49 |
| 1:K:115:VAL:HG22 | 1:L:255:MET:SD | 2.53 | 0.49 |
| 1:K:260:LEU:O | 1:K:261:PHE:HD2 | 1.96 | 0.49 |
| 1:K:461:GLN:HE22 | 1:L:21:VAL:HB | 1.78 | 0.49 |
| 1:L:193:THR:CG2 | 1:L:230:LYS:HD2 | 2.42 | 0.49 |
| 1:L:255:MET:CG | 1:L:256:PHE:N | 2.68 | 0.49 |
| 1:L:463:PRO:HG2 | 1:L:464:LEU:N | 2.27 | 0.49 |
| 1:M:99:VAL:HG12 | 1:M:100:TRP:N | 2.27 | 0.49 |
| 1:M:149:MET:HE2 | 1:M:205:PHE:CE1 | 2.47 | 0.49 |
| 1:M:151:TYR:OH | 1:M:221:PRO:CB | 2.60 | 0.49 |
| 1:N:74:ARG:C | 1:N:75:ILE:HD12 | 2.26 | 0.49 |
| 1:N:250:LEU:HD12 | 1:N:250:LEU:H | 1.77 | 0.49 |
| 1:O:24:THR:HG23 | 1:O:320:ASN:HA | 1.92 | 0.49 |
| 1:O:108:GLY:N | 1:O:371:ASP:O | 2.44 | 0.49 |
| 1:A:68:LEU:CD2 | 1:A:201:VAL:HG21 | 2.37 | 0.49 |
| 1:A:246:LEU:CD2 | 1:A:246:LEU:N | 2.76 | 0.49 |
| 1:C:465:GLY:O | 1:C:468:PHE:N | 2.45 | 0.49 |
| 1:E:98:LEU:HA | 1:E:379:CYS:O | 2.12 | 0.49 |
| 1:G:378:LEU:HD12 | 1:G:379:CYS:H | 1.77 | 0.49 |
| 1:H:42:LEU:HB3 | 1:H:447:TRP:CZ2 | 2.48 | 0.49 |
| 1:J:465:GLY:O | 1:J:468:PHE:N | 2.45 | 0.49 |
| 1:L:166:GLY:H | 1:L:195:ILE:CD1 | 2.22 | 0.49 |
| 1:L:201:VAL:HG23 | 1:L:202:ASP:O | 2.13 | 0.49 |
| 1:L:226:THR:HG21 | 1:M:275:LEU:HD22 | 1.95 | 0.49 |
| 1:L:302:SER:C | 1:L:304:ALA:H | 2.15 | 0.49 |
| 1:M:96:GLN:NE2 | 1:M:382:THR:HG22 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:162:LYS:C | 1:M:330:PHE:CD1 | 2.83 | 0.49 |
| 1:O:219:GLU:HB3 | 1:O:263:ARG:CZ | 2.42 | 0.49 |
| 1:A:141:VAL:O | 1:A:142:ASP:HB3 | 2.13 | 0.49 |
| 1:A:355:TYR:CD2 | 1:A:356:LYS:N | 2.81 | 0.49 |
| 1:B:189:GLU:O | 1:B:191:ILE:HG13 | 2.13 | 0.49 |
| 1:C:115:VAL:N | 1:D:255:MET:SD | 2.84 | 0.49 |
| 1:E:72:VAL:HG22 | 1:E:332:THR:HG23 | 1.94 | 0.49 |
| 1:E:463:PRO:HA | 1:E:466:ARG:HE | 1.77 | 0.49 |
| 1:F:24:THR:C | 1:F:26:GLU:H | 2.15 | 0.49 |
| 1:F:121:PRO:HD3 | 1:F:222:LEU:CD2 | 2.42 | 0.49 |
| 1:G:259:HIS:HE1 | 1:H:130:GLU:CG | 2.26 | 0.49 |
| 1:H:120:HIS:HA | 1:H:222:LEU:HD13 | 1.94 | 0.49 |
| 1:H:459:LEU:HB3 | 1:H:465:GLY:HA3 | 1.94 | 0.49 |
| 1:J:24:THR:HA | 1:J:27:TYR:CE2 | 2.46 | 0.49 |
| 1:J:75:ILE:CD1 | 1:J:331:VAL:HG23 | 2.42 | 0.49 |
| 1:J:201:VAL:HG23 | 1:J:202:ASP:O | 2.12 | 0.49 |
| 1:K:106:GLU:HG3 | 1:K:309:LYS:C | 2.33 | 0.49 |
| 1:K:262:ASN:HD22 | 1:K:263:ARG:N | 2.11 | 0.49 |
| 1:L:147:ILE:HG22 | 1:L:148:SER:N | 2.26 | 0.49 |
| 1:M:71:ARG:HA | 1:M:71:ARG:NH1 | 2.15 | 0.49 |
| 1:N:54:LYS:HE3 | 1:N:55:PRO:HD2 | 1.95 | 0.49 |
| 1:O:163:PRO:HD3 | 1:O:330:PHE:HE1 | 1.78 | 0.49 |
| 1:A:21:VAL:C | 1:A:22:VAL:HG13 | 2.33 | 0.49 |
| 1:A:216:ASN:CB | 1:E:345:CYS:SG | 3.01 | 0.49 |
| 1:A:231:TYR:CD2 | 1:E:112:PRO:CD | 2.92 | 0.49 |
| 1:A:438:GLU:HG2 | 1:A:439:ASP:N | 2.27 | 0.49 |
| 1:A:471:GLN:O | 1:F:140:GLY:HA2 | 2.13 | 0.49 |
| 1:B:96:GLN:CB | 1:B:382:THR:HA | 2.43 | 0.49 |
| 1:B:196:GLN:HA | 1:B:446:PHE:CE2 | 2.47 | 0.49 |
| 1:C:92:ASN:N | 1:C:96:GLN:OE1 | 2.41 | 0.49 |
| 1:D:21:VAL:O | 1:D:22:VAL:CG1 | 2.61 | 0.49 |
| 1:D:216:ASN:OD1 | 1:D:218:SER:N | 2.45 | 0.49 |
| 1:E:91:TYR:HA | 1:E:96:GLN:OE1 | 2.13 | 0.49 |
| 1:F:41:ARG:O | 1:F:41:ARG:HG2 | 2.10 | 0.49 |
| 1:F:54:LYS:HB3 | 1:F:57:ASN:HD22 | 1.77 | 0.49 |
| 1:F:240:GLU:HG3 | 1:F:243:GLY:CA | 2.42 | 0.49 |
| 1:G:97:ARG:HG3 | 1:G:383:LEU:HD13 | 1.94 | 0.49 |
| 1:G:97:ARG:HG3 | 1:G:383:LEU:CD1 | 2.43 | 0.49 |
| 1:G:242:TYR:CD2 | 1:G:394:MET:CG | 2.86 | 0.49 |
| 1:H:281:GLY:O | 1:H:284:ALA:N | 2.42 | 0.49 |
| 1:H:325:TRP:CZ2 | 1:H:394:MET:HE1 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:57:ASN:HD21 | 1:I:59:LYS:N | 2.09 | 0.49 |
| 1:I:367:GLY:C | 1:I:368:GLU:HG2 | 2.33 | 0.49 |
| 1:I:440:PRO:HA | 1:I:443:LYS:NZ | 2.28 | 0.49 |
| 1:J:240:GLU:HG3 | 1:J:243:GLY:H | 1.77 | 0.49 |
| 1:K:71:ARG:HH11 | 1:K:71:ARG:CA | 2.24 | 0.49 |
| 1:K:178:VAL:CG1 | 1:K:178:VAL:CA | 2.84 | 0.49 |
| 1:M:113:LEU:H | 1:M:113:LEU:HD13 | 1.77 | 0.49 |
| 1:M:167:GLU:N | 1:M:231:TYR:O | 2.46 | 0.49 |
| 1:A:355:TYR:O | 1:A:356:LYS:HG2 | 2.12 | 0.48 |
| 1:B:22:VAL:O | 1:B:22:VAL:HG23 | 2.13 | 0.48 |
| 1:B:363:TYR:CD2 | 1:C:185:CYS:HB2 | 2.48 | 0.48 |
| 1:B:391:ILE:HG22 | 1:B:399:LEU:CG | 2.42 | 0.48 |
| 1:B:439:ASP:HB3 | 1:B:442:LYS:HD3 | 1.95 | 0.48 |
| 1:C:343:SER:HB3 | 1:C:364:LEU:CD2 | 2.43 | 0.48 |
| 1:D:149:MET:CE | 1:D:205:PHE:CE1 | 2.96 | 0.48 |
| 1:D:260:LEU:O | 1:D:261:PHE:CD2 | 2.65 | 0.48 |
| 1:D:280:SER:O | 1:D:280:SER:OG | 2.25 | 0.48 |
| 1:D:400:GLU:C | 1:D:402:TRP:N | 2.66 | 0.48 |
| 1:E:246:LEU:N | 1:E:246:LEU:CD2 | 2.71 | 0.48 |
| 1:F:181:GLN:OE1 | 1:F:182:PRO:O | 2.31 | 0.48 |
| 1:F:193:THR:CG2 | 1:F:230:LYS:HD3 | 2.43 | 0.48 |
| 1:G:130:GLU:CB | 1:G:260:LEU:HD13 | 2.43 | 0.48 |
| 1:G:149:MET:CE | 1:G:295:PRO:HD2 | 2.42 | 0.48 |
| 1:G:440:PRO:HA | 1:G:443:LYS:NZ | 2.27 | 0.48 |
| 1:H:139:ALA:CB | 1:H:139:ALA:N | 2.67 | 0.48 |
| 1:H:300:VAL:HG12 | 1:H:337:THR:HG22 | 1.95 | 0.48 |
| 1:H:303:ASP:N | 1:H:303:ASP:OD1 | 2.46 | 0.48 |
| 1:I:158:LEU:O | 1:I:332:THR:N | 2.44 | 0.48 |
| 1:J:122:LEU:O | 1:J:218:SER:HB2 | 2.12 | 0.48 |
| 1:J:152:LYS:CB | 1:J:255:MET:HB2 | 2.42 | 0.48 |
| 1:J:185:CYS:HA | 1:J:186:PRO:HD3 | 1.64 | 0.48 |
| 1:K:151:TYR:CG | 1:K:203:THR:HB | 2.47 | 0.48 |
| 1:K:240:GLU:HG3 | 1:K:243:GLY:H | 1.77 | 0.48 |
| 1:K:348:ILE:CG2 | 1:K:359:ASN:OD1 | 2.59 | 0.48 |
| 1:L:216:ASN:C | 1:L:216:ASN:OD1 | 2.52 | 0.48 |
| 1:L:341:ASN:HB3 | 1:L:366:HIS:HB2 | 1.94 | 0.48 |
| 1:M:201:VAL:CG2 | 1:M:202:ASP:O | 2.61 | 0.48 |
| 1:M:300:VAL:H | 1:M:300:VAL:HG22 | 1.40 | 0.48 |
| 1:N:31:THR:HG23 | 1:N:378:LEU:O | 2.13 | 0.48 |
| 1:N:219:GLU:O | 1:N:220:VAL:HG13 | 2.13 | 0.48 |
| 1:O:172:GLY:O | 1:O:173:SER:O | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:390:TYR:O | 1:A:392:HIS:N | 2.45 | 0.48 |
| 1:B:184:ASP:O | 1:B:185:CYS:O | 2.30 | 0.48 |
| 1:B:280:SER:CA | 1:B:284:ALA:HB2 | 2.43 | 0.48 |
| 1:B:280:SER:N | 1:B:284:ALA:HB2 | 2.28 | 0.48 |
| 1:B:372:LEU:HB3 | 1:B:374:PHE:CE1 | 2.48 | 0.48 |
| 1:B:463:PRO:CG | 1:B:464:LEU:N | 2.75 | 0.48 |
| 1:D:49:TYR:HE1 | 1:D:364:LEU:CD1 | 2.25 | 0.48 |
| 1:D:68:LEU:C | 1:D:201:VAL:HG22 | 2.23 | 0.48 |
| 1:E:114:GLY:N | 1:E:337:THR:O | 2.43 | 0.48 |
| 1:E:152:LYS:HB3 | 1:E:255:MET:HG3 | 1.94 | 0.48 |
| 1:E:333:VAL:CG1 | 1:E:334:VAL:N | 2.76 | 0.48 |
| 1:F:260:LEU:HD22 | 1:J:148:SER:O | 2.12 | 0.48 |
| 1:G:80:PRO:CG | 1:G:98:LEU:O | 2.60 | 0.48 |
| 1:G:171:LYS:HG3 | 1:G:187:PRO:HD2 | 1.95 | 0.48 |
| 1:G:359:ASN:OD1 | 1:G:359:ASN:O | 2.31 | 0.48 |
| 1:H:262:ASN:ND2 | 1:H:288:SER:HB3 | 2.28 | 0.48 |
| 1:I:149:MET:CE | 1:I:205:PHE:HE1 | 2.26 | 0.48 |
| 1:I:162:LYS:C | 1:I:330:PHE:HD1 | 2.17 | 0.48 |
| 1:I:344:LEU:CD1 | 1:J:185:CYS:SG | 3.01 | 0.48 |
| 1:J:46:GLY:HA3 | 1:J:63:PRO:O | 2.13 | 0.48 |
| 1:J:378:LEU:HD12 | 1:J:379:CYS:N | 2.28 | 0.48 |
| 1:J:463:PRO:CB | 1:J:466:ARG:HH21 | 2.26 | 0.48 |
| 1:K:74:ARG:CB | 1:K:330:PHE:HE2 | 2.27 | 0.48 |
| 1:K:160:GLY:HA3 | 1:K:245:SER:O | 2.13 | 0.48 |
| 1:K:242:TYR:CD2 | 1:K:394:MET:CG | 2.93 | 0.48 |
| 1:K:451:LEU:HD23 | 1:K:454:LYS:HG3 | 1.95 | 0.48 |
| 1:L:135:TYR:HE2 | 1:L:287:ALA:HB2 | 1.78 | 0.48 |
| 1:L:241:PRO:CG | 1:L:242:TYR:N | 2.76 | 0.48 |
| 1:M:366:HIS:CD2 | 1:M:367:GLY:H | 2.32 | 0.48 |
| 1:N:74:ARG:HB2 | 1:N:330:PHE:HE2 | 1.78 | 0.48 |
| 1:O:24:THR:C | 1:O:26:GLU:N | 2.65 | 0.48 |
| 1:B:66:SER:OG | 1:B:67:GLY:N | 2.46 | 0.48 |
| 1:B:250:LEU:HD22 | 1:B:306:ILE:HG23 | 1.95 | 0.48 |
| 1:C:106:GLU:HB3 | 1:C:373:GLN:HB2 | 1.95 | 0.48 |
| 1:C:143:ASN:O | 1:C:145:GLU:HG2 | 2.13 | 0.48 |
| 1:C:184:ASP:O | 1:C:185:CYS:C | 2.49 | 0.48 |
| 1:D:232:PRO:HB2 | 1:D:234:TYR:CE2 | 2.47 | 0.48 |
| 1:E:157:CYS:HA | 1:E:332:THR:O | 2.13 | 0.48 |
| 1:E:183:GLY:O | 1:E:184:ASP:C | 2.51 | 0.48 |
| 1:F:65:VAL:O | 1:F:65:VAL:HG12 | 2.13 | 0.48 |
| 1:F:180:VAL:HG12 | 1:F:181:GLN:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:216:ASN:N | 1:J:345:CYS:SG | 2.79 | 0.48 |
| 1:F:365:ARG:HD3 | 1:F:365:ARG:CA | 2.39 | 0.48 |
| 1:G:52:ILE:HB | 1:G:62:VAL:HB | 1.94 | 0.48 |
| 1:G:120:HIS:HB3 | 1:G:123:LEU:HB2 | 1.95 | 0.48 |
| 1:G:163:PRO:HA | 1:G:330:PHE:CD1 | 2.47 | 0.48 |
| 1:G:178:VAL:CG1 | 1:G:178:VAL:HB | 2.21 | 0.48 |
| 1:H:96:GLN:HA | 1:H:382:THR:HA | 1.95 | 0.48 |
| 1:H:216:ASN:C | 1:H:216:ASN:OD1 | 2.51 | 0.48 |
| 1:I:463:PRO:HA | 1:I:466:ARG:HE | 1.78 | 0.48 |
| 1:J:104:GLY:O | 1:J:374:PHE:HA | 2.13 | 0.48 |
| 1:K:92:ASN:C | 1:K:94:ASP:H | 2.16 | 0.48 |
| 1:K:234:TYR:O | 1:K:237:MET:N | 2.46 | 0.48 |
| 1:L:92:ASN:HD22 | 1:L:95:THR:HG1 | 1.58 | 0.48 |
| 1:M:90:PHE:CD1 | 1:M:90:PHE:C | 2.86 | 0.48 |
| 1:M:141:VAL:CG1 | 1:M:142:ASP:N | 2.76 | 0.48 |
| 1:M:280:SER:N | 1:M:284:ALA:HB2 | 2.28 | 0.48 |
| 1:N:76:HIS:HB2 | 1:N:450:ASN:HA | 1.95 | 0.48 |
| 1:O:120:HIS:ND1 | 1:O:121:PRO:CD | 2.76 | 0.48 |
| 1:O:463:PRO:HA | 1:O:466:ARG:HE | 1.78 | 0.48 |
| 1:B:33:ILE:HB | 1:B:378:LEU:HB3 | 1.95 | 0.48 |
| 1:B:54:LYS:HE3 | 1:B:55:PRO:CD | 2.21 | 0.48 |
| 1:B:188:LEU:HD11 | 1:B:213:LEU:HD11 | 1.96 | 0.48 |
| 1:B:298:SER:OG | 1:B:299:MET:N | 2.47 | 0.48 |
| 1:B:459:LEU:C | 1:B:461:GLN:H | 2.16 | 0.48 |
| 1:C:249:TYR:O | 1:C:249:TYR:CD1 | 2.66 | 0.48 |
| 1:D:77:LEU:HD11 | 1:D:376:PHE:CE2 | 2.49 | 0.48 |
| 1:D:159:ILE:HD12 | 1:D:248:PHE:CD2 | 2.46 | 0.48 |
| 1:E:344:LEU:HD21 | 1:E:365:ARG:HG2 | 1.94 | 0.48 |
| 1:F:48:PRO:HG2 | 1:F:49:TYR:CD1 | 2.48 | 0.48 |
| 1:F:67:GLY:C | 1:F:68:LEU:HG | 2.34 | 0.48 |
| 1:F:457:ALA:O | 1:F:459:LEU:CD2 | 2.59 | 0.48 |
| 1:H:52:ILE:HB | 1:H:62:VAL:HB | 1.94 | 0.48 |
| 1:H:70:TYR:CZ | 1:H:230:LYS:O | 2.66 | 0.48 |
| 1:H:459:LEU:O | 1:H:461:GLN:N | 2.46 | 0.48 |
| 1:I:217:LYS:HG2 | 1:J:276:TYR:N | 2.29 | 0.48 |
| 1:I:222:LEU:HD21 | 1:J:271:VAL:CG1 | 2.43 | 0.48 |
| 1:J:367:GLY:O | 1:J:368:GLU:HG2 | 2.13 | 0.48 |
| 1:J:438:GLU:HG2 | 1:J:439:ASP:H | 1.78 | 0.48 |
| 1:K:33:ILE:O | 1:K:377:GLN:HA | 2.13 | 0.48 |
| 1:K:112:PRO:HB3 | 1:L:231:TYR:CG | 2.48 | 0.48 |
| 1:K:293:PRO:O | 1:K:293:PRO:CD | 2.60 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:391:ILE:HD13 | 1:K:402:TRP:HH2 | 1.79 | 0.48 |
| 1:L:42:LEU:HB2 | 1:L:370:TYR:HB2 | 1.95 | 0.48 |
| 1:L:43:LEU:HD12 | 1:L:369:GLU:HA | 1.95 | 0.48 |
| 1:L:176:THR:O | 1:L:177:GLN:HG3 | 2.14 | 0.48 |
| 1:L:223:ASP:OD1 | 1:L:224:ILE:N | 2.47 | 0.48 |
| 1:M:176:THR:O | 1:M:177:GLN:HG3 | 2.13 | 0.48 |
| 1:N:54:LYS:O | 1:N:57:ASN:O | 2.31 | 0.48 |
| 1:N:183:GLY:O | 1:N:185:CYS:N | 2.46 | 0.48 |
| 1:N:262:ASN:CG | 1:N:288:SER:HB3 | 2.32 | 0.48 |
| 1:N:342:MET:HB2 | 1:O:208:MET:HE1 | 1.93 | 0.48 |
| 1:B:162:LYS:NZ | 1:B:395:ASN:OD1 | 2.44 | 0.48 |
| 1:C:75:ILE:HG22 | 1:C:76:HIS:N | 2.21 | 0.48 |
| 1:C:228:ILE:N | 1:C:228:ILE:CD1 | 2.77 | 0.48 |
| 1:C:317:GLN:H | 1:C:317:GLN:HG3 | 1.38 | 0.48 |
| 1:D:105:VAL:CG1 | 1:D:106:GLU:N | 2.76 | 0.48 |
| 1:E:152:LYS:HE2 | 1:E:202:ASP:CB | 2.42 | 0.48 |
| 1:E:383:LEU:HA | 1:E:387:VAL:CG1 | 2.43 | 0.48 |
| 1:F:168:HIS:HB2 | 1:F:208:MET:CA | 2.40 | 0.48 |
| 1:F:234:TYR:CD1 | 1:F:251:ARG:NH2 | 2.81 | 0.48 |
| 1:F:365:ARG:HG3 | 1:F:365:ARG:HH11 | 1.78 | 0.48 |
| 1:F:399:LEU:HD23 | 1:F:402:TRP:CZ3 | 2.48 | 0.48 |
| 1:G:153:GLN:CD | 1:G:300:VAL:HG12 | 2.33 | 0.48 |
| 1:G:300:VAL:O | 1:H:254:GLN:HA | 2.12 | 0.48 |
| 1:G:355:TYR:CD1 | 1:H:144:ARG:HD3 | 2.48 | 0.48 |
| 1:H:27:TYR:CE2 | 1:H:390:TYR:CE2 | 3.01 | 0.48 |
| 1:H:255:MET:CG | 1:H:256:PHE:N | 2.77 | 0.48 |
| 1:I:75:ILE:HG22 | 1:I:451:LEU:HD12 | 1.94 | 0.48 |
| 1:I:345:CYS:SG | 1:J:216:ASN:CB | 2.95 | 0.48 |
| 1:I:347:ALA:H | 1:J:215:ALA:CB | 2.26 | 0.48 |
| 1:I:391:ILE:HG21 | 1:I:402:TRP:HZ3 | 1.77 | 0.48 |
| 1:J:391:ILE:HD13 | 1:J:402:TRP:CH2 | 2.49 | 0.48 |
| 1:K:166:GLY:H | 1:K:195:ILE:HG13 | 1.77 | 0.48 |
| 1:K:185:CYS:SG | 1:O:365:ARG:NH1 | 2.86 | 0.48 |
| 1:M:117:ILE:CD1 | 1:N:260:LEU:HD23 | 2.39 | 0.48 |
| 1:M:192:ASN:C | 1:M:193:THR:HG22 | 2.32 | 0.48 |
| 1:O:125:LYS:HG3 | 1:O:147:ILE:CD1 | 2.44 | 0.48 |
| 1:A:307:PHE:O | 1:A:308:ASN:CB | 2.61 | 0.48 |
| 1:A:444:TYR:HB3 | 1:A:446:PHE:CZ | 2.49 | 0.48 |
| 1:B:54:LYS:HG2 | 1:B:56:ASN:OD1 | 2.14 | 0.48 |
| 1:B:272:PRO:HD2 | 1:B:275:LEU:HD11 | 1.94 | 0.48 |
| 1:B:363:TYR:CE1 | 1:C:185:CYS:HB2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:441:LEU:CD2 | 1:B:441:LEU:CB | 2.82 | 0.48 |
| 1:C:71:ARG:NH1 | 1:C:197:ASP:OD1 | 2.47 | 0.48 |
| 1:D:78:PRO:HD3 | 1:D:452:LYS:CA | 2.37 | 0.48 |
| 1:E:96:GLN:HA | 1:E:382:THR:HA | 1.95 | 0.48 |
| 1:F:266:THR:OG1 | 1:F:266:THR:O | 2.25 | 0.48 |
| 1:F:317:GLN:NE2 | 1:F:317:GLN:C | 2.66 | 0.48 |
| 1:F:373:GLN:HB3 | 1:F:464:LEU:HD12 | 1.96 | 0.48 |
| 1:G:118:SER:CB | 1:G:151:TYR:CE1 | 2.95 | 0.48 |
| 1:G:170:GLY:O | 1:G:188:LEU:HA | 2.14 | 0.48 |
| 1:I:70:TYR:CE1 | 1:I:201:VAL:HG12 | 2.49 | 0.48 |
| 1:I:395:ASN:HB3 | 1:I:398:ILE:HG12 | 1.96 | 0.48 |
| 1:J:90:PHE:HD1 | 1:J:91:TYR:HB3 | 1.77 | 0.48 |
| 1:J:383:LEU:HD22 | 1:J:388:MET:CE | 2.44 | 0.48 |
| 1:K:170:GLY:O | 1:K:188:LEU:HA | 2.14 | 0.48 |
| 1:L:193:THR:HG23 | 1:L:230:LYS:HD2 | 1.95 | 0.48 |
| 1:L:363:TYR:CZ | 1:M:185:CYS:HB2 | 2.48 | 0.48 |
| 1:M:66:SER:H | 1:M:69:GLN:HE21 | 1.54 | 0.48 |
| 1:M:125:LYS:HG3 | 1:M:147:ILE:CD1 | 2.43 | 0.48 |
| 1:M:289:SER:O | 1:M:291:TYR:CE1 | 2.66 | 0.48 |
| 1:M:329:LEU:HD13 | 1:M:374:PHE:CE2 | 2.48 | 0.48 |
| 1:N:142:ASP:CG | 1:O:283:THR:OG1 | 2.52 | 0.48 |
| 1:N:180:VAL:HG13 | 1:N:184:ASP:CB | 2.32 | 0.48 |
| 1:O:36:HIS:CG | 1:O:462:PHE:HD1 | 2.28 | 0.48 |
| 1:O:46:GLY:HA3 | 1:O:63:PRO:O | 2.13 | 0.48 |
| 1:O:70:TYR:OH | 1:O:232:PRO:CD | 2.35 | 0.48 |
| 1:A:61:LEU:O | 1:A:62:VAL:HG23 | 2.13 | 0.48 |
| 1:B:217:LYS:C | 1:B:218:SER:OG | 2.51 | 0.48 |
| 1:C:122:LEU:O | 1:C:218:SER:HB2 | 2.14 | 0.48 |
| 1:D:105:VAL:HG12 | 1:D:106:GLU:N | 2.28 | 0.48 |
| 1:D:345:CYS:SG | 1:D:345:CYS:O | 2.72 | 0.48 |
| 1:D:399:LEU:HA | 1:D:402:TRP:HE3 | 1.79 | 0.48 |
| 1:E:54:LYS:HG2 | 1:E:56:ASN:OD1 | 2.12 | 0.48 |
| 1:F:75:ILE:HG23 | 1:F:451:LEU:CD1 | 2.44 | 0.48 |
| 1:G:70:TYR:CE1 | 1:G:201:VAL:HA | 2.47 | 0.48 |
| 1:G:470:LEU:CD1 | 1:G:470:LEU:CD2 | 2.85 | 0.48 |
| 1:H:226:THR:HG21 | 1:I:275:LEU:CD2 | 2.43 | 0.48 |
| 1:I:42:LEU:HD13 | 1:I:447:TRP:CZ2 | 2.49 | 0.48 |
| 1:I:70:TYR:OH | 1:I:230:LYS:O | 2.16 | 0.48 |
| 1:I:333:VAL:HG12 | 1:I:334:VAL:N | 2.28 | 0.48 |
| 1:J:163:PRO:CA | 1:J:330:PHE:CD1 | 2.96 | 0.48 |
| 1:K:121:PRO:CG | 1:L:289:SER:HB2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:185:CYS:HB2 | 1:O:363:TYR:CD2 | 2.49 | 0.48 |
| 1:L:344:LEU:CD1 | 1:M:186:PRO:HG2 | 2.38 | 0.48 |
| 1:M:150:ASP:O | 1:M:296:SER:HA | 2.13 | 0.48 |
| 1:M:166:GLY:HA2 | 1:M:195:ILE:HD11 | 1.92 | 0.48 |
| 1:M:399:LEU:HD23 | 1:M:402:TRP:CZ3 | 2.48 | 0.48 |
| 1:N:383:LEU:HD22 | 1:N:388:MET:HE3 | 1.96 | 0.48 |
| 1:N:458:ASP:OD2 | 1:N:458:ASP:N | 2.47 | 0.48 |
| 1:O:155:GLN:HG2 | 1:O:307:PHE:HE1 | 1.78 | 0.48 |
| 1:A:49:TYR:HA | 1:A:223:ASP:HB3 | 1.96 | 0.48 |
| 1:A:112:PRO:HB3 | 1:B:231:TYR:CD1 | 2.48 | 0.48 |
| 1:A:298:SER:OG | 1:A:299:MET:N | 2.45 | 0.48 |
| 1:B:53:LYS:HD3 | 1:B:58:ASN:HA | 1.95 | 0.48 |
| 1:B:272:PRO:HD2 | 1:B:275:LEU:CD1 | 2.43 | 0.48 |
| 1:D:214:GLN:NE2 | 1:D:219:GLU:HB2 | 2.28 | 0.48 |
| 1:F:23:SER:HG | 1:F:25:ASP:HB2 | 1.71 | 0.48 |
| 1:G:372:LEU:HA | 1:G:372:LEU:HD23 | 1.54 | 0.48 |
| 1:G:451:LEU:CD2 | 1:G:454:LYS:HG3 | 2.41 | 0.48 |
| 1:H:259:HIS:CE1 | 1:I:130:GLU:CG | 2.97 | 0.48 |
| 1:H:439:ASP:OD2 | 1:H:440:PRO:HD2 | 2.14 | 0.48 |
| 1:I:27:TYR:O | 1:I:381:ILE:HG23 | 2.13 | 0.48 |
| 1:I:151:TYR:OH | 1:I:221:PRO:HG2 | 2.13 | 0.48 |
| 1:I:205:PHE:CD1 | 1:I:220:VAL:HG12 | 2.48 | 0.48 |
| 1:I:259:HIS:HE1 | 1:J:130:GLU:CG | 2.27 | 0.48 |
| 1:J:92:ASN:N | 1:J:96:GLN:OE1 | 2.47 | 0.48 |
| 1:J:335:ASP:OD1 | 1:J:337:THR:OG1 | 2.32 | 0.48 |
| 1:J:451:LEU:HA | 1:J:454:LYS:CG | 2.44 | 0.48 |
| 1:K:75:ILE:HB | 1:K:329:LEU:CB | 2.43 | 0.48 |
| 1:K:101:ALA:HB3 | 1:K:377:GLN:O | 2.14 | 0.48 |
| 1:K:166:GLY:H | 1:K:195:ILE:CG1 | 2.27 | 0.48 |
| 1:K:210:PHE:HD1 | 1:K:224:ILE:O | 1.97 | 0.48 |
| 1:M:121:PRO:HD3 | 1:M:222:LEU:HD13 | 1.94 | 0.48 |
| 1:M:144:ARG:CG | 1:M:144:ARG:H | 2.27 | 0.48 |
| 1:M:317:GLN:HE21 | 1:M:317:GLN:HB2 | 1.34 | 0.48 |
| 1:M:323:ILE:CD1 | 1:M:323:ILE:HG23 | 2.44 | 0.48 |
| 1:O:36:HIS:ND1 | 1:O:462:PHE:CD1 | 2.82 | 0.48 |
| 1:B:217:LYS:HG2 | 1:C:276:TYR:HA | 1.96 | 0.48 |
| 1:B:386:ASP:OD2 | 1:B:386:ASP:N | 2.47 | 0.48 |
| 1:B:451:LEU:HA | 1:B:454:LYS:CG | 2.44 | 0.48 |
| 1:C:263:ARG:HG2 | 1:C:292:PHE:HD2 | 1.79 | 0.48 |
| 1:D:342:MET:CE | 1:D:342:MET:CG | 2.91 | 0.48 |
| 1:D:383:LEU:HD23 | 1:D:388:MET:HE2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:248:PHE:CZ | 1:E:311:TYR:HB3 | 2.48 | 0.48 |
| 1:E:472:LEU:CD2 | 1:J:138:ASN:ND2 | 2.52 | 0.48 |
| 1:G:119:GLY:HA3 | 1:H:291:TYR:CZ | 2.49 | 0.48 |
| 1:G:147:ILE:HG23 | 1:H:129:THR:O | 2.13 | 0.48 |
| 1:G:323:ILE:HG21 | 1:G:325:TRP:CZ2 | 2.48 | 0.48 |
| 1:G:365:ARG:NH2 | 1:H:269:GLU:OE1 | 2.47 | 0.48 |
| 1:I:49:TYR:N | 1:I:49:TYR:CD1 | 2.82 | 0.48 |
| 1:I:107:VAL:HG23 | 1:I:311:TYR:HE1 | 1.78 | 0.48 |
| 1:I:158:LEU:HD23 | 1:I:249:TYR:HB2 | 1.96 | 0.48 |
| 1:I:391:ILE:HB | 1:I:399:LEU:HD21 | 1.96 | 0.48 |
| 1:K:276:TYR:CD2 | 1:K:276:TYR:N | 2.82 | 0.48 |
| 1:K:299:MET:CA | 1:L:256:PHE:HB3 | 2.41 | 0.48 |
| 1:L:54:LYS:CE | 1:L:55:PRO:HD2 | 2.44 | 0.48 |
| 1:L:71:ARG:NH1 | 1:L:197:ASP:CG | 2.68 | 0.48 |
| 1:L:278:LYS:HB2 | 1:O:354:THR:HG22 | 1.94 | 0.48 |
| 1:M:110:GLY:O | 1:M:111:GLN:NE2 | 2.45 | 0.48 |
| 1:N:159:ILE:HD12 | 1:N:248:PHE:HD2 | 1.77 | 0.48 |
| 1:N:391:ILE:HG21 | 1:N:402:TRP:HZ3 | 1.78 | 0.48 |
| 1:A:54:LYS:HB3 | 1:A:57:ASN:HB3 | 1.95 | 0.48 |
| 1:A:123:LEU:O | 1:A:125:LYS:N | 2.47 | 0.48 |
| 1:A:180:VAL:CG1 | 1:A:184:ASP:HB3 | 2.40 | 0.48 |
| 1:A:231:TYR:CD1 | 1:E:112:PRO:HB3 | 2.49 | 0.48 |
| 1:B:348:ILE:CG2 | 1:B:359:ASN:OD1 | 2.46 | 0.48 |
| 1:B:463:PRO:HA | 1:B:466:ARG:NE | 2.26 | 0.48 |
| 1:C:75:ILE:HB | 1:C:329:LEU:CB | 2.44 | 0.48 |
| 1:F:112:PRO:HB2 | 1:G:202:ASP:OD2 | 2.14 | 0.48 |
| 1:F:300:VAL:HG12 | 1:F:337:THR:HG22 | 1.95 | 0.48 |
| 1:G:50:PHE:CB | 1:G:51:PRO:HD2 | 2.41 | 0.48 |
| 1:G:259:HIS:HE1 | 1:H:130:GLU:HG3 | 1.79 | 0.48 |
| 1:G:390:TYR:C | 1:G:392:HIS:N | 2.67 | 0.48 |
| 1:H:71:ARG:HA | 1:H:71:ARG:NH1 | 2.10 | 0.48 |
| 1:I:122:LEU:HD21 | 1:J:286:LEU:CD1 | 2.44 | 0.48 |
| 1:I:369:GLU:OE1 | 1:J:167:GLU:OE1 | 2.32 | 0.48 |
| 1:I:400:GLU:O | 1:I:401:ASP:C | 2.51 | 0.48 |
| 1:J:246:LEU:HD23 | 1:J:246:LEU:N | 2.12 | 0.48 |
| 1:K:190:LEU:HD21 | 1:O:369:GLU:OE1 | 2.14 | 0.48 |
| 1:L:49:TYR:CD1 | 1:L:49:TYR:N | 2.81 | 0.48 |
| 1:L:223:ASP:OD1 | 1:L:224:ILE:HG12 | 2.14 | 0.48 |
| 1:L:438:GLU:HG2 | 1:L:439:ASP:N | 2.29 | 0.48 |
| 1:M:390:TYR:C | 1:M:392:HIS:N | 2.68 | 0.48 |
| 1:N:97:ARG:HG3 | 1:N:383:LEU:HD11 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:196:GLN:OE1 | 1:O:445:THR:N | 2.43 | 0.48 |
| 1:O:356:LYS:O | 1:O:357:ASN:C | 2.52 | 0.48 |
| 1:A:124:ASN:HB3 | 1:A:263:ARG:HH11 | 1.79 | 0.47 |
| 1:A:299:MET:CA | 1:B:256:PHE:HB3 | 2.37 | 0.47 |
| 1:B:61:LEU:CD1 | 1:B:61:LEU:CD2 | 2.82 | 0.47 |
| 1:B:149:MET:HE2 | 1:B:205:PHE:CE1 | 2.49 | 0.47 |
| 1:D:103:VAL:HG21 | 1:D:468:PHE:CE1 | 2.49 | 0.47 |
| 1:D:163:PRO:O | 1:D:163:PRO:HG2 | 2.13 | 0.47 |
| 1:E:329:LEU:HD23 | 1:E:329:LEU:HA | 1.70 | 0.47 |
| 1:G:237:MET:HB3 | 1:G:246:LEU:CD2 | 2.42 | 0.47 |
| 1:H:232:PRO:HB2 | 1:H:234:TYR:CZ | 2.49 | 0.47 |
| 1:I:115:VAL:HG22 | 1:J:255:MET:SD | 2.53 | 0.47 |
| 1:I:344:LEU:HD21 | 1:I:365:ARG:HB2 | 1.96 | 0.47 |
| 1:I:459:LEU:C | 1:I:461:GLN:H | 2.18 | 0.47 |
| 1:J:208:MET:CG | 1:J:210:PHE:CE2 | 2.96 | 0.47 |
| 1:J:250:LEU:HD12 | 1:J:250:LEU:N | 2.28 | 0.47 |
| 1:K:22:VAL:O | 1:K:23:SER:C | 2.52 | 0.47 |
| 1:K:185:CYS:HB2 | 1:O:363:TYR:CE2 | 2.49 | 0.47 |
| 1:K:209:ASP:CG | 1:K:212:THR:HG23 | 2.35 | 0.47 |
| 1:L:139:ALA:CB | 1:L:143:ASN:ND2 | 2.76 | 0.47 |
| 1:L:155:GLN:HB3 | 1:L:252:ARG:HB3 | 1.96 | 0.47 |
| 1:L:163:PRO:CA | 1:L:330:PHE:CD1 | 2.97 | 0.47 |
| 1:M:217:LYS:HG2 | 1:N:276:TYR:HA | 1.96 | 0.47 |
| 1:N:464:LEU:O | 1:N:464:LEU:CD2 | 2.62 | 0.47 |
| 1:O:345:CYS:SG | 1:O:345:CYS:O | 2.72 | 0.47 |
| 1:O:355:TYR:CD2 | 1:O:356:LYS:N | 2.82 | 0.47 |
| 1:A:356:LYS:NZ | 1:A:356:LYS:CD | 2.68 | 0.47 |
| 1:A:443:LYS:NZ | 1:A:443:LYS:CD | 2.70 | 0.47 |
| 1:B:219:GLU:O | 1:B:220:VAL:HG13 | 2.14 | 0.47 |
| 1:B:237:MET:HB3 | 1:B:246:LEU:HD22 | 1.95 | 0.47 |
| 1:D:185:CYS:HA | 1:D:186:PRO:HD3 | 1.76 | 0.47 |
| 1:E:80:PRO:O | 1:E:85:PHE:HE1 | 1.97 | 0.47 |
| 1:E:231:TYR:OH | 1:E:253:GLU:OE2 | 2.25 | 0.47 |
| 1:E:261:PHE:HB3 | 1:E:292:PHE:CE2 | 2.48 | 0.47 |
| 1:E:451:LEU:O | 1:E:454:LYS:HB2 | 2.13 | 0.47 |
| 1:F:70:TYR:CE1 | 1:F:201:VAL:HA | 2.49 | 0.47 |
| 1:F:92:ASN:C | 1:F:94:ASP:H | 2.16 | 0.47 |
| 1:F:97:ARG:CB | 1:F:383:LEU:HD11 | 2.44 | 0.47 |
| 1:G:97:ARG:HB2 | 1:G:383:LEU:HD11 | 1.96 | 0.47 |
| 1:G:250:LEU:HD12 | 1:G:250:LEU:O | 2.14 | 0.47 |
| 1:H:42:LEU:HD13 | 1:H:447:TRP:CE2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:105:VAL:CG1 | 1:I:106:GLU:N | 2.76 | 0.47 |
| 1:I:105:VAL:HA | 1:I:373:GLN:O | 2.14 | 0.47 |
| 1:J:111:GLN:HG2 | 1:J:369:GLU:HB3 | 1.96 | 0.47 |
| 1:J:390:TYR:C | 1:J:392:HIS:N | 2.66 | 0.47 |
| 1:K:142:ASP:OD2 | 1:K:144:ARG:NE | 2.47 | 0.47 |
| 1:K:248:PHE:CE2 | 1:K:311:TYR:HB3 | 2.49 | 0.47 |
| 1:L:230:LYS:CD | 1:L:230:LYS:HZ2 | 2.23 | 0.47 |
| 1:M:66:SER:N | 1:M:69:GLN:NE2 | 2.53 | 0.47 |
| 1:M:72:VAL:HG22 | 1:M:332:THR:HG23 | 1.95 | 0.47 |
| 1:N:152:LYS:HB2 | 1:N:255:MET:CB | 2.32 | 0.47 |
| 1:O:391:ILE:HG22 | 1:O:398:ILE:HB | 1.97 | 0.47 |
| 1:A:275:LEU:HD23 | 1:E:226:THR:HG21 | 1.97 | 0.47 |
| 1:A:279:GLY:HA3 | 1:A:283:THR:C | 2.34 | 0.47 |
| 1:B:252:ARG:CD | 1:B:306:ILE:HD11 | 2.40 | 0.47 |
| 1:C:147:ILE:HG23 | 1:D:129:THR:O | 2.15 | 0.47 |
| 1:D:153:GLN:NE2 | 1:D:300:VAL:HA | 2.29 | 0.47 |
| 1:F:67:GLY:N | 1:F:366:HIS:HE1 | 2.11 | 0.47 |
| 1:F:92:ASN:HA | 1:F:93:PRO:HD2 | 1.75 | 0.47 |
| 1:F:126:LEU:HB2 | 1:F:262:ASN:HB3 | 1.93 | 0.47 |
| 1:F:259:HIS:CE1 | 1:G:130:GLU:HG2 | 2.49 | 0.47 |
| 1:G:217:LYS:O | 1:G:218:SER:CB | 2.61 | 0.47 |
| 1:H:222:LEU:HA | 1:H:225:CYS:SG | 2.54 | 0.47 |
| 1:H:307:PHE:C | 1:H:309:LYS:N | 2.64 | 0.47 |
| 1:H:380:LYS:CE | 1:H:380:LYS:CG | 2.83 | 0.47 |
| 1:H:461:GLN:HE22 | 1:I:21:VAL:HG23 | 1.79 | 0.47 |
| 1:I:141:VAL:O | 1:I:142:ASP:CB | 2.62 | 0.47 |
| 1:I:312:TRP:CE3 | 1:I:312:TRP:HA | 2.48 | 0.47 |
| 1:J:36:HIS:HB2 | 1:J:459:LEU:HD22 | 1.95 | 0.47 |
| 1:J:375:ILE:HG21 | 1:J:468:PHE:CD2 | 2.49 | 0.47 |
| 1:L:361:LYS:HD2 | 1:M:183:GLY:CA | 2.44 | 0.47 |
| 1:M:302:SER:O | 1:M:305:GLN:HG2 | 2.15 | 0.47 |
| 1:N:255:MET:CG | 1:N:256:PHE:N | 2.76 | 0.47 |
| 1:N:384:THR:O | 1:N:388:MET:HB2 | 2.14 | 0.47 |
| 1:O:75:ILE:HG21 | 1:O:451:LEU:HD12 | 1.95 | 0.47 |
| 1:A:115:VAL:HG22 | 1:B:255:MET:CE | 2.43 | 0.47 |
| 1:D:28:VAL:HA | 1:D:381:ILE:HG12 | 1.96 | 0.47 |
| 1:D:80:PRO:HG2 | 1:D:98:LEU:O | 2.14 | 0.47 |
| 1:D:122:LEU:CD1 | 1:E:286:LEU:HD11 | 2.41 | 0.47 |
| 1:F:459:LEU:O | 1:F:461:GLN:N | 2.48 | 0.47 |
| 1:G:259:HIS:CE1 | 1:H:130:GLU:CG | 2.98 | 0.47 |
| 1:H:31:THR:HG23 | 1:H:378:LEU:O | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:373:GLN:C | 1:J:374:PHE:CD1 | 2.87 | 0.47 |
| 1:K:162:LYS:CD | 1:K:162:LYS:NZ | 2.69 | 0.47 |
| 1:K:176:THR:O | 1:K:177:GLN:HG3 | 2.14 | 0.47 |
| 1:K:241:PRO:HG2 | 1:K:242:TYR:H | 1.80 | 0.47 |
| 1:K:461:GLN:NE2 | 1:L:21:VAL:H | 2.11 | 0.47 |
| 1:M:79:ASP:CG | 1:M:81:ASN:HB2 | 2.27 | 0.47 |
| 1:M:116:GLY:N | 1:M:339:SER:OG | 2.47 | 0.47 |
| 1:M:459:LEU:HB3 | 1:M:465:GLY:HA3 | 1.95 | 0.47 |
| 1:N:75:ILE:CG2 | 1:N:451:LEU:HD12 | 2.42 | 0.47 |
| 1:N:151:TYR:CD2 | 1:N:203:THR:O | 2.64 | 0.47 |
| 1:N:189:GLU:O | 1:N:191:ILE:HG13 | 2.13 | 0.47 |
| 1:O:168:HIS:CE1 | 1:O:191:ILE:HB | 2.49 | 0.47 |
| 1:A:149:MET:HE2 | 1:A:205:PHE:CE1 | 2.50 | 0.47 |
| 1:A:185:CYS:HB2 | 1:E:363:TYR:CG | 2.50 | 0.47 |
| 1:A:202:ASP:OD2 | 1:E:112:PRO:HB2 | 2.14 | 0.47 |
| 1:B:190:LEU:HA | 1:B:190:LEU:HD12 | 1.52 | 0.47 |
| 1:B:247:PHE:HD1 | 1:B:248:PHE:N | 2.12 | 0.47 |
| 1:C:57:ASN:ND2 | 1:C:59:LYS:H | 2.12 | 0.47 |
| 1:D:114:GLY:N | 1:D:337:THR:O | 2.46 | 0.47 |
| 1:E:96:GLN:HE21 | 1:E:382:THR:HG23 | 1.78 | 0.47 |
| 1:F:96:GLN:NE2 | 1:F:380:LYS:HD2 | 2.29 | 0.47 |
| 1:F:246:LEU:HD23 | 1:F:246:LEU:N | 2.09 | 0.47 |
| 1:G:113:LEU:N | 1:G:113:LEU:HD12 | 2.30 | 0.47 |
| 1:G:142:ASP:OD1 | 1:H:283:THR:OG1 | 2.25 | 0.47 |
| 1:G:169:TRP:HB3 | 1:G:188:LEU:HD12 | 1.97 | 0.47 |
| 1:H:320:ASN:OD1 | 1:H:322:GLY:N | 2.39 | 0.47 |
| 1:H:380:LYS:CD | 1:H:380:LYS:HZ2 | 2.27 | 0.47 |
| 1:I:240:GLU:HG3 | 1:I:243:GLY:H | 1.78 | 0.47 |
| 1:L:36:HIS:ND1 | 1:L:36:HIS:C | 2.66 | 0.47 |
| 1:L:292:PHE:CD1 | 1:L:292:PHE:C | 2.88 | 0.47 |
| 1:O:149:MET:HE3 | 1:O:294:THR:CG2 | 2.36 | 0.47 |
| 1:O:255:MET:HG2 | 1:O:256:PHE:H | 1.80 | 0.47 |
| 1:A:169:TRP:N | 1:A:208:MET:HA | 2.29 | 0.47 |
| 1:A:217:LYS:O | 1:A:218:SER:CB | 2.61 | 0.47 |
| 1:A:238:VAL:C | 1:A:240:GLU:H | 2.18 | 0.47 |
| 1:B:28:VAL:CG2 | 1:B:381:ILE:HD11 | 2.35 | 0.47 |
| 1:D:68:LEU:HD22 | 1:D:203:THR:HG22 | 1.96 | 0.47 |
| 1:D:372:LEU:HB3 | 1:D:374:PHE:CE1 | 2.50 | 0.47 |
| 1:E:30:ARG:NH1 | 1:E:377:GLN:NE2 | 2.56 | 0.47 |
| 1:E:83:PHE:HB3 | 1:E:85:PHE:CE1 | 2.49 | 0.47 |
| 1:E:231:TYR:CD1 | 1:E:232:PRO:HD2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:200:MET:O | 1:F:229:CYS:HA | 2.14 | 0.47 |
| 1:G:173:SER:HA | 1:G:174:PRO:HD3 | 1.63 | 0.47 |
| 1:G:307:PHE:C | 1:G:309:LYS:H | 2.17 | 0.47 |
| 1:H:54:LYS:CB | 1:H:57:ASN:HD22 | 2.27 | 0.47 |
| 1:H:162:LYS:HG3 | 1:H:244:ASP:HB3 | 1.97 | 0.47 |
| 1:I:111:GLN:HG2 | 1:I:369:GLU:HB2 | 1.96 | 0.47 |
| 1:I:151:TYR:OH | 1:I:221:PRO:CB | 2.63 | 0.47 |
| 1:I:363:TYR:CZ | 1:J:185:CYS:HB2 | 2.49 | 0.47 |
| 1:J:34:TYR:HE2 | 1:J:377:GLN:HB2 | 1.77 | 0.47 |
| 1:J:169:TRP:H | 1:J:208:MET:HA | 1.80 | 0.47 |
| 1:K:107:VAL:O | 1:K:107:VAL:HG12 | 2.13 | 0.47 |
| 1:K:279:GLY:HA3 | 1:K:283:THR:C | 2.34 | 0.47 |
| 1:N:49:TYR:HA | 1:N:223:ASP:HB3 | 1.96 | 0.47 |
| 1:N:215:ALA:O | 1:N:217:LYS:N | 2.48 | 0.47 |
| 1:N:325:TRP:HB3 | 1:N:398:ILE:HD11 | 1.97 | 0.47 |
| 1:O:442:LYS:HB3 | 1:O:443:LYS:HD3 | 1.96 | 0.47 |
| 1:A:65:VAL:CA | 1:A:69:GLN:HE22 | 1.99 | 0.47 |
| 1:A:72:VAL:HG23 | 1:A:197:ASP:HA | 1.97 | 0.47 |
| 1:A:121:PRO:C | 1:A:122:LEU:HD23 | 2.34 | 0.47 |
| 1:A:163:PRO:CA | 1:A:330:PHE:CD1 | 2.98 | 0.47 |
| 1:A:257:VAL:HG13 | 1:E:115:VAL:HG21 | 1.96 | 0.47 |
| 1:A:443:LYS:HZ3 | 1:A:443:LYS:CG | 2.28 | 0.47 |
| 1:B:36:HIS:ND1 | 1:B:36:HIS:C | 2.68 | 0.47 |
| 1:B:77:LEU:HD11 | 1:B:376:PHE:CE2 | 2.50 | 0.47 |
| 1:B:325:TRP:CZ2 | 1:B:394:MET:HE1 | 2.49 | 0.47 |
| 1:C:53:LYS:HD3 | 1:C:58:ASN:HA | 1.96 | 0.47 |
| 1:C:66:SER:OG | 1:C:67:GLY:N | 2.46 | 0.47 |
| 1:C:71:ARG:HH12 | 1:C:198:GLY:N | 2.08 | 0.47 |
| 1:C:83:PHE:HD2 | 1:C:85:PHE:CE2 | 2.33 | 0.47 |
| 1:C:189:GLU:O | 1:C:191:ILE:HG13 | 2.15 | 0.47 |
| 1:C:217:LYS:CD | 1:C:217:LYS:NZ | 2.70 | 0.47 |
| 1:D:66:SER:HA | 1:D:366:HIS:ND1 | 2.29 | 0.47 |
| 1:D:219:GLU:HB3 | 1:D:263:ARG:CZ | 2.44 | 0.47 |
| 1:D:355:TYR:CD2 | 1:D:356:LYS:N | 2.82 | 0.47 |
| 1:E:54:LYS:HG3 | 1:E:55:PRO:HD2 | 1.95 | 0.47 |
| 1:F:185:CYS:SG | 1:F:186:PRO:N | 2.87 | 0.47 |
| 1:F:188:LEU:HA | 1:F:188:LEU:HD13 | 1.70 | 0.47 |
| 1:F:356:LYS:O | 1:F:358:THR:N | 2.48 | 0.47 |
| 1:G:168:HIS:H | 1:G:190:LEU:CD1 | 2.27 | 0.47 |
| 1:H:159:ILE:O | 1:H:246:LEU:HA | 2.15 | 0.47 |
| 1:H:164:PRO:HG3 | 1:H:332:THR:HG21 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:166:GLY:CA | 1:H:195:ILE:CD1 | 2.82 | 0.47 |
| 1:H:216:ASN:OD1 | 1:H:218:SER:N | 2.48 | 0.47 |
| 1:H:247:PHE:CD1 | 1:H:248:PHE:N | 2.76 | 0.47 |
| 1:H:387:VAL:O | 1:H:391:ILE:HG13 | 2.14 | 0.47 |
| 1:H:459:LEU:C | 1:H:461:GLN:H | 2.18 | 0.47 |
| 1:I:27:TYR:CZ | 1:I:390:TYR:HE2 | 2.33 | 0.47 |
| 1:I:97:ARG:HA | 1:I:97:ARG:NH1 | 2.28 | 0.47 |
| 1:I:386:ASP:OD2 | 1:I:386:ASP:N | 2.48 | 0.47 |
| 1:J:46:GLY:N | 1:J:65:VAL:HB | 2.28 | 0.47 |
| 1:J:49:TYR:HA | 1:J:223:ASP:HB3 | 1.97 | 0.47 |
| 1:J:72:VAL:HG21 | 1:J:195:ILE:O | 2.15 | 0.47 |
| 1:J:74:ARG:CG | 1:J:74:ARG:NE | 2.69 | 0.47 |
| 1:J:85:PHE:CE2 | 1:J:378:LEU:HD22 | 2.50 | 0.47 |
| 1:J:154:THR:O | 1:J:336:THR:HG23 | 2.15 | 0.47 |
| 1:K:185:CYS:HB2 | 1:O:363:TYR:CZ | 2.50 | 0.47 |
| 1:K:213:LEU:HD13 | 1:K:213:LEU:HA | 1.55 | 0.47 |
| 1:K:219:GLU:O | 1:K:220:VAL:CG1 | 2.60 | 0.47 |
| 1:K:240:GLU:HG3 | 1:K:243:GLY:N | 2.30 | 0.47 |
| 1:K:311:TYR:CD2 | 1:K:311:TYR:N | 2.81 | 0.47 |
| 1:L:98:LEU:N | 1:L:98:LEU:HD23 | 2.29 | 0.47 |
| 1:L:105:VAL:HA | 1:L:373:GLN:O | 2.14 | 0.47 |
| 1:L:208:MET:HG2 | 1:L:210:PHE:CE2 | 2.50 | 0.47 |
| 1:L:356:LYS:O | 1:L:357:ASN:C | 2.53 | 0.47 |
| 1:M:317:GLN:H | 1:M:317:GLN:HG3 | 1.55 | 0.47 |
| 1:N:33:ILE:HD12 | 1:N:33:ILE:HG23 | 1.52 | 0.47 |
| 1:N:115:VAL:H | 1:O:255:MET:CE | 2.23 | 0.47 |
| 1:N:121:PRO:HG3 | 1:O:289:SER:CB | 2.42 | 0.47 |
| 1:N:290:ASN:N | 1:N:290:ASN:HD22 | 2.13 | 0.47 |
| 1:N:313:LEU:CD2 | 1:N:313:LEU:HG | 2.20 | 0.47 |
| 1:N:463:PRO:O | 1:N:466:ARG:HB2 | 2.15 | 0.47 |
| 1:O:67:GLY:C | 1:O:68:LEU:HG | 2.34 | 0.47 |
| 1:O:96:GLN:HB3 | 1:O:382:THR:HG22 | 1.96 | 0.47 |
| 1:O:307:PHE:C | 1:O:309:LYS:H | 2.18 | 0.47 |
| 1:A:234:TYR:CD1 | 1:A:251:ARG:NH2 | 2.83 | 0.47 |
| 1:A:463:PRO:HB3 | 1:A:466:ARG:HH21 | 1.79 | 0.47 |
| 1:B:67:GLY:C | 1:B:68:LEU:HG | 2.35 | 0.47 |
| 1:B:463:PRO:HB3 | 1:B:466:ARG:NH2 | 2.22 | 0.47 |
| 1:C:472:LEU:HD23 | 1:H:138:ASN:HD22 | 1.80 | 0.47 |
| 1:D:176:THR:CA | 1:D:176:THR:HB | 2.21 | 0.47 |
| 1:F:67:GLY:N | 1:F:366:HIS:CE1 | 2.83 | 0.47 |
| 1:F:188:LEU:HD21 | 1:J:344:LEU:CD1 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:205:PHE:CE1 | 1:F:220:VAL:HG12 | 2.50 | 0.47 |
| 1:F:396:SER:O | 1:F:397:THR:C | 2.52 | 0.47 |
| 1:G:109:ARG:N | 1:G:308:ASN:OD1 | 2.48 | 0.47 |
| 1:G:180:VAL:HG13 | 1:G:184:ASP:CB | 2.39 | 0.47 |
| 1:G:354:THR:HG22 | 1:I:278:LYS:CB | 2.44 | 0.47 |
| 1:H:80:PRO:O | 1:H:98:LEU:HD12 | 2.15 | 0.47 |
| 1:H:149:MET:CE | 1:H:205:PHE:CE1 | 2.98 | 0.47 |
| 1:H:179:ALA:O | 1:H:180:VAL:O | 2.33 | 0.47 |
| 1:H:312:TRP:CH2 | 1:H:468:PHE:HA | 2.49 | 0.47 |
| 1:I:153:GLN:NE2 | 1:I:300:VAL:HA | 2.30 | 0.47 |
| 1:K:92:ASN:HA | 1:K:93:PRO:HD2 | 1.87 | 0.47 |
| 1:K:97:ARG:HG3 | 1:K:383:LEU:HD13 | 1.97 | 0.47 |
| 1:K:372:LEU:HB3 | 1:K:374:PHE:HE1 | 1.80 | 0.47 |
| 1:L:54:LYS:HB3 | 1:L:57:ASN:HD22 | 1.79 | 0.47 |
| 1:L:80:PRO:HG3 | 1:L:98:LEU:O | 2.15 | 0.47 |
| 1:M:124:ASN:OD1 | 1:M:264:ALA:N | 2.47 | 0.47 |
| 1:M:152:LYS:HE3 | 1:M:154:THR:OG1 | 2.15 | 0.47 |
| 1:N:54:LYS:HB3 | 1:N:57:ASN:ND2 | 2.26 | 0.47 |
| 1:O:381:ILE:O | 1:O:383:LEU:HD12 | 2.14 | 0.47 |
| 1:A:151:TYR:CD2 | 1:A:203:THR:CB | 2.92 | 0.47 |
| 1:B:336:THR:C | 1:B:338:ARG:H | 2.18 | 0.47 |
| 1:D:73:PHE:HD1 | 1:D:73:PHE:H | 1.62 | 0.47 |
| 1:D:99:VAL:HG21 | 1:D:325:TRP:HZ3 | 1.80 | 0.47 |
| 1:D:107:VAL:HG11 | 1:D:333:VAL:HG21 | 1.97 | 0.47 |
| 1:D:323:ILE:HG21 | 1:D:325:TRP:CH2 | 2.50 | 0.47 |
| 1:E:209:ASP:O | 1:E:213:LEU:HB2 | 2.14 | 0.47 |
| 1:E:307:PHE:O | 1:E:308:ASN:HB2 | 2.15 | 0.47 |
| 1:F:149:MET:CE | 1:F:205:PHE:CZ | 2.98 | 0.47 |
| 1:F:163:PRO:CA | 1:F:330:PHE:CD1 | 2.98 | 0.47 |
| 1:G:149:MET:HE2 | 1:G:205:PHE:CE1 | 2.50 | 0.47 |
| 1:H:119:GLY:C | 1:H:221:PRO:HA | 2.34 | 0.47 |
| 1:H:178:VAL:O | 1:H:180:VAL:N | 2.41 | 0.47 |
| 1:H:344:LEU:HB3 | 1:I:213:LEU:HB3 | 1.96 | 0.47 |
| 1:H:374:PHE:CB | 1:H:376:PHE:CE1 | 2.97 | 0.47 |
| 1:I:155:GLN:OE1 | 1:I:305:GLN:HA | 2.15 | 0.47 |
| 1:I:471:GLN:OE1 | 1:I:472:LEU:N | 2.48 | 0.47 |
| 1:J:463:PRO:CA | 1:J:466:ARG:HH21 | 2.27 | 0.47 |
| 1:K:148:SER:HB3 | 1:L:291:TYR:CD2 | 2.50 | 0.47 |
| 1:L:57:ASN:HD21 | 1:L:59:LYS:CB | 2.27 | 0.47 |
| 1:L:163:PRO:HA | 1:L:330:PHE:CD1 | 2.50 | 0.47 |
| 1:L:281:GLY:N | 1:L:284:ALA:HB3 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:361:LYS:HD3 | 1:N:268:GLY:HA2 | 1.97 | 0.47 |
| 1:M:391:ILE:CG2 | 1:M:398:ILE:HG21 | 2.44 | 0.47 |
| 1:M:461:GLN:HE22 | 1:N:21:VAL:H | 1.63 | 0.47 |
| 1:O:164:PRO:CG | 1:O:332:THR:HG21 | 2.45 | 0.47 |
| 1:O:210:PHE:CE1 | 1:O:224:ILE:HB | 2.50 | 0.47 |
| 1:B:92:ASN:C | 1:B:94:ASP:H | 2.19 | 0.47 |
| 1:B:165:ILE:CD1 | 1:B:165:ILE:HB | 2.45 | 0.47 |
| 1:C:49:TYR:HA | 1:C:223:ASP:HB3 | 1.96 | 0.47 |
| 1:D:49:TYR:HE1 | 1:D:364:LEU:HD12 | 1.80 | 0.47 |
| 1:D:299:MET:HA | 1:E:256:PHE:HB3 | 1.97 | 0.47 |
| 1:E:21:VAL:CG1 | 1:E:390:TYR:OH | 2.63 | 0.47 |
| 1:E:24:THR:C | 1:E:26:GLU:H | 2.17 | 0.47 |
| 1:F:60:ILE:HD12 | 1:F:63:PRO:HB3 | 1.96 | 0.47 |
| 1:F:96:GLN:CB | 1:F:382:THR:HA | 2.45 | 0.47 |
| 1:G:242:TYR:CE2 | 1:G:394:MET:CG | 2.91 | 0.47 |
| 1:G:399:LEU:O | 1:G:402:TRP:CB | 2.59 | 0.47 |
| 1:H:33:ILE:O | 1:H:377:GLN:HA | 2.13 | 0.47 |
| 1:H:113:LEU:HD12 | 1:H:113:LEU:N | 2.30 | 0.47 |
| 1:H:219:GLU:O | 1:H:220:VAL:CG1 | 2.57 | 0.47 |
| 1:H:302:SER:O | 1:H:304:ALA:N | 2.47 | 0.47 |
| 1:I:149:MET:HE1 | 1:I:205:PHE:CE1 | 2.50 | 0.47 |
| 1:I:299:MET:HA | 1:J:256:PHE:HB3 | 1.96 | 0.47 |
| 1:I:357:ASN:HB2 | 1:J:141:VAL:HG13 | 1.97 | 0.47 |
| 1:J:176:THR:O | 1:J:177:GLN:HG3 | 2.15 | 0.47 |
| 1:K:153:GLN:NE2 | 1:K:300:VAL:HA | 2.28 | 0.47 |
| 1:L:133:SER:O | 1:L:134:ALA:HB2 | 2.13 | 0.47 |
| 1:L:219:GLU:O | 1:L:220:VAL:HG13 | 2.14 | 0.47 |
| 1:L:281:GLY:N | 1:L:284:ALA:CB | 2.78 | 0.47 |
| 1:L:360:PHE:CE2 | 1:M:216:ASN:HA | 2.50 | 0.47 |
| 1:M:81:ASN:O | 1:M:82:LYS:HG3 | 2.15 | 0.47 |
| 1:N:49:TYR:HE1 | 1:N:364:LEU:CD1 | 2.27 | 0.47 |
| 1:N:163:PRO:HA | 1:N:330:PHE:CD1 | 2.50 | 0.47 |
| 1:O:113:LEU:N | 1:O:113:LEU:CD1 | 2.78 | 0.47 |
| 1:O:155:GLN:OE1 | 1:O:305:GLN:HA | 2.15 | 0.47 |
| 1:O:230:LYS:NZ | 1:O:230:LYS:HD3 | 2.28 | 0.47 |
| 1:O:333:VAL:CG1 | 1:O:334:VAL:N | 2.77 | 0.47 |
| 1:A:134:ALA:O | 1:A:135:TYR:C | 2.53 | 0.46 |
| 1:A:171:LYS:HG3 | 1:A:187:PRO:HD2 | 1.97 | 0.46 |
| 1:B:123:LEU:HD12 | 1:B:124:ASN:N | 2.30 | 0.46 |
| 1:C:22:VAL:O | 1:C:23:SER:C | 2.54 | 0.46 |
| 1:C:234:TYR:CE1 | 1:C:251:ARG:NE | 2.83 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:246:LEU:HD12 | 1:C:249:TYR:HB3 | 1.96 | 0.46 |
| 1:E:153:GLN:NE2 | 1:E:300:VAL:HA | 2.29 | 0.46 |
| 1:F:121:PRO:HG3 | 1:G:289:SER:CB | 2.43 | 0.46 |
| 1:F:133:SER:O | 1:F:134:ALA:HB2 | 2.14 | 0.46 |
| 1:G:344:LEU:HB2 | 1:H:213:LEU:O | 2.15 | 0.46 |
| 1:G:470:LEU:O | 1:G:470:LEU:CD2 | 2.63 | 0.46 |
| 1:I:36:HIS:CG | 1:I:37:ALA:N | 2.83 | 0.46 |
| 1:K:42:LEU:HD13 | 1:K:447:TRP:CZ2 | 2.50 | 0.46 |
| 1:K:185:CYS:HB2 | 1:O:363:TYR:CG | 2.49 | 0.46 |
| 1:K:210:PHE:CE1 | 1:K:224:ILE:HG13 | 2.50 | 0.46 |
| 1:K:275:LEU:HD23 | 1:O:226:THR:HG21 | 1.97 | 0.46 |
| 1:L:54:LYS:HG2 | 1:L:57:ASN:HB3 | 1.95 | 0.46 |
| 1:L:139:ALA:O | 1:L:140:GLY:O | 2.33 | 0.46 |
| 1:L:361:LYS:NZ | 1:L:361:LYS:HD3 | 2.27 | 0.46 |
| 1:L:384:THR:OG1 | 1:L:385:ALA:N | 2.45 | 0.46 |
| 1:M:101:ALA:HA | 1:M:322:GLY:O | 2.16 | 0.46 |
| 1:M:345:CYS:SG | 1:M:345:CYS:O | 2.74 | 0.46 |
| 1:O:33:ILE:HB | 1:O:378:LEU:HB3 | 1.96 | 0.46 |
| 1:O:158:LEU:HB2 | 1:O:332:THR:CB | 2.45 | 0.46 |
| 1:O:316:ALA:C | 1:O:318:GLY:H | 2.18 | 0.46 |
| 1:A:147:ILE:HG22 | 1:A:148:SER:N | 2.29 | 0.46 |
| 1:B:154:THR:H | 1:B:336:THR:HG21 | 1.80 | 0.46 |
| 1:C:66:SER:H | 1:C:69:GLN:NE2 | 2.12 | 0.46 |
| 1:C:167:GLU:OE1 | 1:C:190:LEU:HD21 | 2.15 | 0.46 |
| 1:C:180:VAL:HG13 | 1:C:184:ASP:HB3 | 1.96 | 0.46 |
| 1:C:391:ILE:HG21 | 1:C:402:TRP:CZ3 | 2.49 | 0.46 |
| 1:D:85:PHE:CE2 | 1:D:378:LEU:HD22 | 2.49 | 0.46 |
| 1:D:166:GLY:N | 1:D:195:ILE:HG13 | 2.31 | 0.46 |
| 1:E:66:SER:N | 1:E:69:GLN:HE21 | 2.13 | 0.46 |
| 1:F:54:LYS:CB | 1:F:57:ASN:HD22 | 2.27 | 0.46 |
| 1:G:105:VAL:CG1 | 1:G:106:GLU:N | 2.78 | 0.46 |
| 1:H:46:GLY:HA3 | 1:H:65:VAL:HB | 1.96 | 0.46 |
| 1:I:276:TYR:C | 1:I:277:ILE:HG12 | 2.35 | 0.46 |
| 1:J:101:ALA:O | 1:J:377:GLN:N | 2.47 | 0.46 |
| 1:L:159:ILE:CD1 | 1:L:159:ILE:CG2 | 2.93 | 0.46 |
| 1:L:240:GLU:OE1 | 1:L:241:PRO:HG2 | 2.14 | 0.46 |
| 1:O:24:THR:HA | 1:O:27:TYR:CE2 | 2.50 | 0.46 |
| 1:O:210:PHE:HD1 | 1:O:224:ILE:O | 1.99 | 0.46 |
| 1:O:217:LYS:HG2 | 1:O:217:LYS:O | 2.15 | 0.46 |
| 1:A:85:PHE:CE2 | 1:A:378:LEU:HD22 | 2.51 | 0.46 |
| 1:A:318:GLY:HA2 | 1:E:466:ARG:NH1 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:96:GLN:HE21 | 1:B:382:THR:CG2 | 2.27 | 0.46 |
| 1:B:365:ARG:HH11 | 1:B:365:ARG:HG3 | 1.80 | 0.46 |
| 1:B:438:GLU:OE1 | 1:B:443:LYS:HE3 | 2.15 | 0.46 |
| 1:C:355:TYR:CE1 | 1:D:144:ARG:HD3 | 2.50 | 0.46 |
| 1:C:441:LEU:HA | 1:C:444:TYR:HD1 | 1.80 | 0.46 |
| 1:D:23:SER:HG | 1:D:25:ASP:HB2 | 1.80 | 0.46 |
| 1:F:42:LEU:HA | 1:F:42:LEU:HD23 | 1.21 | 0.46 |
| 1:F:99:VAL:HG12 | 1:F:100:TRP:N | 2.31 | 0.46 |
| 1:F:320:ASN:OD1 | 1:F:320:ASN:C | 2.54 | 0.46 |
| 1:G:72:VAL:HG22 | 1:G:332:THR:HG23 | 1.96 | 0.46 |
| 1:G:96:GLN:HA | 1:G:381:ILE:O | 2.16 | 0.46 |
| 1:G:247:PHE:HD1 | 1:G:248:PHE:H | 1.63 | 0.46 |
| 1:G:451:LEU:HA | 1:G:454:LYS:CG | 2.44 | 0.46 |
| 1:H:49:TYR:HE1 | 1:H:364:LEU:CD1 | 2.28 | 0.46 |
| 1:H:122:LEU:CD1 | 1:I:286:LEU:HD11 | 2.41 | 0.46 |
| 1:I:162:LYS:HG2 | 1:I:244:ASP:HB3 | 1.98 | 0.46 |
| 1:I:240:GLU:HG3 | 1:I:243:GLY:N | 2.31 | 0.46 |
| 1:I:307:PHE:O | 1:I:308:ASN:HB2 | 2.14 | 0.46 |
| 1:J:209:ASP:O | 1:J:213:LEU:HD23 | 2.14 | 0.46 |
| 1:L:106:GLU:HG3 | 1:L:309:LYS:O | 2.15 | 0.46 |
| 1:M:68:LEU:HD13 | 1:M:151:TYR:HD1 | 1.79 | 0.46 |
| 1:M:271:VAL:H | 1:M:271:VAL:HG23 | 1.36 | 0.46 |
| 1:N:384:THR:HG23 | 1:N:387:VAL:CG2 | 2.46 | 0.46 |
| 1:O:281:GLY:O | 1:O:284:ALA:HB3 | 2.16 | 0.46 |
| 1:O:333:VAL:HG12 | 1:O:334:VAL:N | 2.30 | 0.46 |
| 1:B:180:VAL:HG12 | 1:B:181:GLN:C | 2.34 | 0.46 |
| 1:B:325:TRP:NE1 | 1:B:394:MET:CE | 2.79 | 0.46 |
| 1:B:391:ILE:HG21 | 1:B:402:TRP:HZ3 | 1.80 | 0.46 |
| 1:B:458:ASP:OD2 | 1:B:458:ASP:N | 2.47 | 0.46 |
| 1:C:139:ALA:HB1 | 1:C:143:ASN:ND2 | 2.30 | 0.46 |
| 1:C:217:LYS:O | 1:C:218:SER:HB3 | 2.16 | 0.46 |
| 1:C:323:ILE:HG21 | 1:C:325:TRP:CD2 | 2.51 | 0.46 |
| 1:C:456:SER:OG | 1:C:458:ASP:OD2 | 2.32 | 0.46 |
| 1:D:57:ASN:ND2 | 1:D:59:LYS:H | 2.13 | 0.46 |
| 1:E:441:LEU:HA | 1:E:444:TYR:HD1 | 1.80 | 0.46 |
| 1:F:104:GLY:O | 1:F:374:PHE:HA | 2.16 | 0.46 |
| 1:F:152:LYS:O | 1:F:152:LYS:HG3 | 2.15 | 0.46 |
| 1:G:80:PRO:HD3 | 1:G:100:TRP:CD1 | 2.50 | 0.46 |
| 1:G:463:PRO:CA | 1:G:466:ARG:NH2 | 2.67 | 0.46 |
| 1:H:77:LEU:HB2 | 1:H:327:ASN:HB3 | 1.97 | 0.46 |
| 1:I:107:VAL:O | 1:I:307:PHE:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:178:VAL:C | 1:I:180:VAL:H | 2.18 | 0.46 |
| 1:L:74:ARG:HA | 1:L:330:PHE:CD2 | 2.51 | 0.46 |
| 1:L:307:PHE:C | 1:L:309:LYS:H | 2.16 | 0.46 |
| 1:M:21:VAL:O | 1:M:22:VAL:CG1 | 2.62 | 0.46 |
| 1:M:148:SER:OG | 1:N:129:THR:HB | 2.16 | 0.46 |
| 1:N:120:HIS:HB2 | 1:N:221:PRO:HA | 1.97 | 0.46 |
| 1:O:47:HIS:HB3 | 1:O:50:PHE:O | 2.16 | 0.46 |
| 1:O:52:ILE:O | 1:O:61:LEU:N | 2.47 | 0.46 |
| 1:O:164:PRO:HG3 | 1:O:332:THR:OG1 | 2.14 | 0.46 |
| 1:O:242:TYR:CD2 | 1:O:394:MET:CG | 2.93 | 0.46 |
| 1:A:75:ILE:HB | 1:A:329:LEU:HB2 | 1.96 | 0.46 |
| 1:A:77:LEU:O | 1:A:327:ASN:HB3 | 2.15 | 0.46 |
| 1:A:147:ILE:CG2 | 1:A:148:SER:N | 2.78 | 0.46 |
| 1:A:248:PHE:O | 1:A:249:TYR:HB3 | 2.14 | 0.46 |
| 1:A:256:PHE:HB3 | 1:E:299:MET:HA | 1.96 | 0.46 |
| 1:B:21:VAL:CG1 | 1:B:390:TYR:OH | 2.63 | 0.46 |
| 1:B:75:ILE:HB | 1:B:329:LEU:CB | 2.45 | 0.46 |
| 1:C:42:LEU:HB2 | 1:C:370:TYR:HB2 | 1.96 | 0.46 |
| 1:C:106:GLU:HB3 | 1:C:373:GLN:HG3 | 1.96 | 0.46 |
| 1:D:99:VAL:HG21 | 1:D:325:TRP:CZ3 | 2.51 | 0.46 |
| 1:D:172:GLY:O | 1:D:173:SER:O | 2.33 | 0.46 |
| 1:D:214:GLN:HE22 | 1:D:219:GLU:HB2 | 1.81 | 0.46 |
| 1:E:66:SER:N | 1:E:69:GLN:NE2 | 2.61 | 0.46 |
| 1:F:125:LYS:HE3 | 1:F:261:PHE:CE2 | 2.51 | 0.46 |
| 1:F:126:LEU:HG | 1:F:127:ASP:CG | 2.36 | 0.46 |
| 1:F:293:PRO:HD3 | 1:J:117:ILE:CG2 | 2.45 | 0.46 |
| 1:G:193:THR:HG23 | 1:G:230:LYS:HD3 | 1.97 | 0.46 |
| 1:I:105:VAL:HG12 | 1:I:106:GLU:N | 2.25 | 0.46 |
| 1:I:150:ASP:OD1 | 1:I:296:SER:CA | 2.61 | 0.46 |
| 1:I:259:HIS:HB2 | 1:I:294:THR:OG1 | 2.16 | 0.46 |
| 1:J:384:THR:H | 1:J:387:VAL:HB | 1.80 | 0.46 |
| 1:K:451:LEU:HA | 1:K:454:LYS:CG | 2.45 | 0.46 |
| 1:L:201:VAL:HG11 | 1:L:334:VAL:HG13 | 1.97 | 0.46 |
| 1:N:399:LEU:O | 1:N:402:TRP:HB2 | 2.16 | 0.46 |
| 1:O:98:LEU:CD2 | 1:O:379:CYS:O | 2.63 | 0.46 |
| 1:O:351:SER:O | 1:O:352:GLU:O | 2.34 | 0.46 |
| 1:A:387:VAL:O | 1:A:390:TYR:N | 2.48 | 0.46 |
| 1:A:390:TYR:C | 1:A:392:HIS:N | 2.67 | 0.46 |
| 1:B:143:ASN:O | 1:B:144:ARG:C | 2.54 | 0.46 |
| 1:B:262:ASN:CG | 1:B:288:SER:HB3 | 2.35 | 0.46 |
| 1:B:375:ILE:HG21 | 1:B:468:PHE:CE2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:150:ASP:CB | 1:D:257:VAL:HG21 | 2.46 | 0.46 |
| 1:D:48:PRO:HG2 | 1:D:49:TYR:CD1 | 2.50 | 0.46 |
| 1:E:43:LEU:CD1 | 1:E:369:GLU:HA | 2.40 | 0.46 |
| 1:F:122:LEU:O | 1:F:218:SER:HB2 | 2.15 | 0.46 |
| 1:G:81:ASN:ND2 | 1:G:402:TRP:HD1 | 2.14 | 0.46 |
| 1:G:96:GLN:NE2 | 1:G:382:THR:CG2 | 2.79 | 0.46 |
| 1:G:125:LYS:HE2 | 1:G:261:PHE:CD2 | 2.50 | 0.46 |
| 1:H:64:LYS:HZ2 | 1:H:200:MET:CE | 2.28 | 0.46 |
| 1:J:241:PRO:HG2 | 1:J:242:TYR:H | 1.79 | 0.46 |
| 1:K:54:LYS:CE | 1:K:55:PRO:HD2 | 2.32 | 0.46 |
| 1:K:96:GLN:HE21 | 1:K:382:THR:CG2 | 2.29 | 0.46 |
| 1:K:257:VAL:HG13 | 1:O:115:VAL:HG21 | 1.98 | 0.46 |
| 1:K:302:SER:C | 1:K:304:ALA:H | 2.19 | 0.46 |
| 1:M:263:ARG:HD3 | 1:M:292:PHE:CE2 | 2.51 | 0.46 |
| 1:M:391:ILE:HB | 1:M:399:LEU:HD21 | 1.98 | 0.46 |
| 1:N:157:CYS:HB2 | 1:N:307:PHE:HE2 | 1.80 | 0.46 |
| 1:N:391:ILE:O | 1:N:391:ILE:CG2 | 2.61 | 0.46 |
| 1:A:256:PHE:CD1 | 1:A:257:VAL:O | 2.69 | 0.46 |
| 1:B:91:TYR:HA | 1:B:96:GLN:OE1 | 2.15 | 0.46 |
| 1:B:463:PRO:CA | 1:B:466:ARG:HE | 2.25 | 0.46 |
| 1:C:96:GLN:NE2 | 1:C:382:THR:HG22 | 2.31 | 0.46 |
| 1:D:260:LEU:HD12 | 1:D:260:LEU:N | 2.30 | 0.46 |
| 1:E:30:ARG:HD3 | 1:E:377:GLN:NE2 | 2.31 | 0.46 |
| 1:E:65:VAL:CA | 1:E:69:GLN:NE2 | 2.76 | 0.46 |
| 1:E:105:VAL:CG1 | 1:E:106:GLU:N | 2.76 | 0.46 |
| 1:E:323:ILE:HD13 | 1:E:323:ILE:N | 2.31 | 0.46 |
| 1:F:254:GLN:HE22 | 1:F:298:SER:HB3 | 1.80 | 0.46 |
| 1:F:396:SER:O | 1:F:398:ILE:N | 2.49 | 0.46 |
| 1:G:119:GLY:HA2 | 1:G:148:SER:HA | 1.98 | 0.46 |
| 1:H:65:VAL:HA | 1:H:69:GLN:HE22 | 1.80 | 0.46 |
| 1:H:148:SER:HB3 | 1:I:291:TYR:CD2 | 2.50 | 0.46 |
| 1:H:362:GLU:OE2 | 1:I:219:GLU:OE2 | 2.34 | 0.46 |
| 1:H:469:LEU:CD2 | 1:H:469:LEU:HB3 | 2.45 | 0.46 |
| 1:I:120:HIS:CD2 | 1:I:222:LEU:HD12 | 2.50 | 0.46 |
| 1:J:258:ARG:HB2 | 1:J:296:SER:HB2 | 1.98 | 0.46 |
| 1:K:106:GLU:HG3 | 1:K:309:LYS:O | 2.15 | 0.46 |
| 1:K:122:LEU:HD11 | 1:L:286:LEU:CD1 | 2.46 | 0.46 |
| 1:K:162:LYS:HG2 | 1:K:162:LYS:HE2 | 1.98 | 0.46 |
| 1:K:283:THR:OG1 | 1:O:142:ASP:OD1 | 2.29 | 0.46 |
| 1:K:391:ILE:O | 1:K:391:ILE:HG22 | 2.16 | 0.46 |
| 1:L:154:THR:H | 1:L:336:THR:HG21 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:126:LEU:HD12 | 1:M:264:ALA:HB2 | 1.97 | 0.46 |
| 1:N:348:ILE:HD11 | 1:O:181:GLN:HE22 | 1.80 | 0.46 |
| 1:O:119:GLY:N | 1:O:221:PRO:HB3 | 2.31 | 0.46 |
| 1:O:124:ASN:HD22 | 1:O:216:ASN:ND2 | 2.14 | 0.46 |
| 1:O:180:VAL:HG12 | 1:O:184:ASP:HB2 | 1.91 | 0.46 |
| 1:O:227:SER:C | 1:O:228:ILE:HD12 | 2.35 | 0.46 |
| 1:A:34:TYR:HE2 | 1:A:377:GLN:CG | 2.20 | 0.46 |
| 1:A:120:HIS:CE1 | 1:A:122:LEU:H | 2.31 | 0.46 |
| 1:A:189:GLU:O | 1:A:191:ILE:HG13 | 2.16 | 0.46 |
| 1:B:62:VAL:HG12 | 1:B:63:PRO:N | 2.27 | 0.46 |
| 1:C:242:TYR:HE2 | 1:C:394:MET:HB2 | 1.78 | 0.46 |
| 1:C:302:SER:C | 1:C:304:ALA:N | 2.64 | 0.46 |
| 1:D:35:TYR:CD2 | 1:D:456:SER:C | 2.89 | 0.46 |
| 1:D:163:PRO:N | 1:D:330:PHE:HD1 | 2.09 | 0.46 |
| 1:E:188:LEU:HA | 1:E:188:LEU:HD13 | 1.59 | 0.46 |
| 1:F:22:VAL:HG23 | 1:F:22:VAL:O | 2.16 | 0.46 |
| 1:F:39:THR:HG23 | 1:F:372:LEU:HB2 | 1.97 | 0.46 |
| 1:F:175:CYS:SG | 1:F:175:CYS:HA | 2.55 | 0.46 |
| 1:G:297:GLY:C | 1:G:298:SER:O | 2.54 | 0.46 |
| 1:H:32:ASN:CB | 1:H:32:ASN:ND2 | 2.66 | 0.46 |
| 1:H:180:VAL:CG1 | 1:H:184:ASP:CB | 2.88 | 0.46 |
| 1:H:384:THR:O | 1:H:388:MET:HB2 | 2.16 | 0.46 |
| 1:H:398:ILE:HG22 | 1:H:402:TRP:CE3 | 2.50 | 0.46 |
| 1:I:193:THR:N | 1:I:193:THR:HG22 | 2.29 | 0.46 |
| 1:I:320:ASN:OD1 | 1:I:323:ILE:HG12 | 2.16 | 0.46 |
| 1:K:149:MET:HE1 | 1:K:205:PHE:CZ | 2.51 | 0.46 |
| 1:K:210:PHE:CD1 | 1:K:224:ILE:HB | 2.51 | 0.46 |
| 1:L:49:TYR:HE2 | 1:L:118:SER:CA | 2.29 | 0.46 |
| 1:L:113:LEU:HD12 | 1:L:113:LEU:N | 2.31 | 0.46 |
| 1:L:233:ASP:OD2 | 1:L:236:LYS:HB2 | 2.15 | 0.46 |
| 1:L:258:ARG:HB2 | 1:L:296:SER:HB2 | 1.96 | 0.46 |
| 1:M:33:ILE:O | 1:M:377:GLN:HA | 2.16 | 0.46 |
| 1:M:60:ILE:O | 1:M:60:ILE:HG13 | 2.15 | 0.46 |
| 1:M:247:PHE:CD1 | 1:M:248:PHE:N | 2.84 | 0.46 |
| 1:N:36:HIS:ND1 | 1:N:37:ALA:N | 2.64 | 0.46 |
| 1:N:119:GLY:O | 1:N:221:PRO:HA | 2.16 | 0.46 |
| 1:O:33:ILE:HD12 | 1:O:33:ILE:HG23 | 1.37 | 0.46 |
| 1:A:241:PRO:CG | 1:A:242:TYR:H | 2.28 | 0.46 |
| 1:A:320:ASN:HD21 | 1:A:323:ILE:HB | 1.80 | 0.46 |
| 1:A:440:PRO:HA | 1:A:443:LYS:NZ | 2.31 | 0.46 |
| 1:A:465:GLY:O | 1:A:468:PHE:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:163:PRO:CD | 1:B:330:PHE:CE1 | 2.96 | 0.46 |
| 1:B:209:ASP:OD2 | 1:B:228:ILE:HG13 | 2.16 | 0.46 |
| 1:B:217:LYS:HG2 | 1:B:217:LYS:O | 2.16 | 0.46 |
| 1:B:345:CYS:HA | 1:B:361:LYS:O | 2.15 | 0.46 |
| 1:B:392:HIS:CA | 1:B:399:LEU:HD11 | 2.46 | 0.46 |
| 1:B:471:GLN:O | 1:B:472:LEU:OXT | 2.33 | 0.46 |
| 1:C:282:SER:C | 1:C:284:ALA:H | 2.20 | 0.46 |
| 1:D:471:GLN:CD | 1:D:472:LEU:N | 2.69 | 0.46 |
| 1:E:53:LYS:HD3 | 1:E:58:ASN:HA | 1.96 | 0.46 |
| 1:F:125:LYS:HE2 | 1:F:127:ASP:C | 2.35 | 0.46 |
| 1:G:200:MET:O | 1:G:229:CYS:HA | 2.15 | 0.46 |
| 1:G:280:SER:O | 1:G:281:GLY:C | 2.55 | 0.46 |
| 1:H:122:LEU:O | 1:H:218:SER:HB2 | 2.16 | 0.46 |
| 1:H:342:MET:HB2 | 1:I:208:MET:CE | 2.34 | 0.46 |
| 1:I:46:GLY:HA3 | 1:I:63:PRO:O | 2.16 | 0.46 |
| 1:J:99:VAL:HG12 | 1:J:100:TRP:O | 2.15 | 0.46 |
| 1:K:42:LEU:HD13 | 1:K:447:TRP:CE2 | 2.51 | 0.46 |
| 1:K:115:VAL:CG2 | 1:L:257:VAL:HG13 | 2.45 | 0.46 |
| 1:K:178:VAL:O | 1:K:180:VAL:N | 2.40 | 0.46 |
| 1:K:355:TYR:CD2 | 1:K:356:LYS:N | 2.83 | 0.46 |
| 1:L:92:ASN:C | 1:L:94:ASP:N | 2.64 | 0.46 |
| 1:M:329:LEU:HA | 1:M:329:LEU:HD23 | 1.57 | 0.46 |
| 1:M:363:TYR:CZ | 1:N:185:CYS:HB2 | 2.51 | 0.46 |
| 1:O:105:VAL:HA | 1:O:373:GLN:O | 2.16 | 0.46 |
| 1:O:180:VAL:HG12 | 1:O:181:GLN:N | 2.31 | 0.46 |
| 1:A:365:ARG:NH2 | 1:B:269:GLU:OE1 | 2.47 | 0.46 |
| 1:B:234:TYR:O | 1:B:235:ILE:C | 2.54 | 0.46 |
| 1:D:80:PRO:HG2 | 1:D:98:LEU:C | 2.37 | 0.46 |
| 1:E:184:ASP:O | 1:E:185:CYS:C | 2.54 | 0.46 |
| 1:F:241:PRO:C | 1:F:243:GLY:H | 2.19 | 0.46 |
| 1:F:247:PHE:CD1 | 1:F:247:PHE:N | 2.84 | 0.46 |
| 1:F:281:GLY:O | 1:F:282:SER:C | 2.54 | 0.46 |
| 1:G:71:ARG:HG3 | 1:G:370:TYR:CE1 | 2.51 | 0.46 |
| 1:G:72:VAL:HG22 | 1:G:332:THR:HG22 | 1.96 | 0.46 |
| 1:G:248:PHE:CE2 | 1:G:311:TYR:CD1 | 2.96 | 0.46 |
| 1:H:301:THR:HG23 | 1:H:304:ALA:HB3 | 1.98 | 0.46 |
| 1:I:271:VAL:HA | 1:I:272:PRO:HD3 | 1.63 | 0.46 |
| 1:J:54:LYS:HB3 | 1:J:57:ASN:ND2 | 2.30 | 0.46 |
| 1:J:96:GLN:HA | 1:J:381:ILE:C | 2.34 | 0.46 |
| 1:J:196:GLN:HA | 1:J:446:PHE:CE2 | 2.51 | 0.46 |
| 1:J:280:SER:O | 1:J:281:GLY:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:307:PHE:O | 1:J:308:ASN:CB | 2.64 | 0.46 |
| 1:K:92:ASN:O | 1:K:94:ASP:N | 2.49 | 0.46 |
| 1:K:216:ASN:HA | 1:O:360:PHE:CE2 | 2.51 | 0.46 |
| 1:K:361:LYS:HB3 | 1:K:363:TYR:CE1 | 2.50 | 0.46 |
| 1:K:463:PRO:HA | 1:K:466:ARG:HE | 1.81 | 0.46 |
| 1:M:299:MET:HE2 | 1:N:298:SER:CB | 2.46 | 0.46 |
| 1:N:91:TYR:CE2 | 1:N:93:PRO:HD3 | 2.51 | 0.46 |
| 1:O:216:ASN:CG | 1:O:219:GLU:OE2 | 2.54 | 0.46 |
| 1:A:61:LEU:HG | 1:A:62:VAL:HG23 | 1.97 | 0.45 |
| 1:A:140:GLY:O | 1:A:141:VAL:HB | 2.16 | 0.45 |
| 1:B:27:TYR:CE2 | 1:B:390:TYR:CE2 | 3.05 | 0.45 |
| 1:B:101:ALA:O | 1:B:376:PHE:HA | 2.15 | 0.45 |
| 1:D:126:LEU:CB | 1:D:262:ASN:HB3 | 2.38 | 0.45 |
| 1:D:210:PHE:O | 1:D:214:GLN:HB2 | 2.16 | 0.45 |
| 1:D:439:ASP:HB3 | 1:D:442:LYS:HE3 | 1.97 | 0.45 |
| 1:E:70:TYR:OH | 1:E:230:LYS:O | 2.29 | 0.45 |
| 1:E:158:LEU:O | 1:E:331:VAL:HA | 2.15 | 0.45 |
| 1:E:241:PRO:HG2 | 1:E:242:TYR:H | 1.81 | 0.45 |
| 1:G:42:LEU:HD12 | 1:G:73:PHE:HE2 | 1.82 | 0.45 |
| 1:G:210:PHE:CD1 | 1:G:224:ILE:HB | 2.50 | 0.45 |
| 1:G:399:LEU:HA | 1:G:402:TRP:CE3 | 2.49 | 0.45 |
| 1:H:80:PRO:O | 1:H:85:PHE:HE1 | 1.99 | 0.45 |
| 1:J:220:VAL:O | 1:J:220:VAL:HG23 | 2.15 | 0.45 |
| 1:K:81:ASN:OD1 | 1:K:98:LEU:N | 2.47 | 0.45 |
| 1:K:458:ASP:OD2 | 1:K:458:ASP:N | 2.49 | 0.45 |
| 1:L:49:TYR:CE2 | 1:L:118:SER:HA | 2.49 | 0.45 |
| 1:L:147:ILE:CG2 | 1:L:148:SER:N | 2.80 | 0.45 |
| 1:L:164:PRO:O | 1:L:164:PRO:HG2 | 2.17 | 0.45 |
| 1:L:262:ASN:HD22 | 1:L:262:ASN:C | 2.20 | 0.45 |
| 1:O:164:PRO:HG3 | 1:O:332:THR:CG2 | 2.46 | 0.45 |
| 1:O:251:ARG:O | 1:O:252:ARG:HB2 | 2.16 | 0.45 |
| 1:A:155:GLN:HG3 | 1:A:307:PHE:HE1 | 1.81 | 0.45 |
| 1:A:269:GLU:HG3 | 1:E:363:TYR:CD2 | 2.51 | 0.45 |
| 1:A:375:ILE:CG1 | 1:A:464:LEU:HD13 | 2.40 | 0.45 |
| 1:B:75:ILE:HG12 | 1:B:374:PHE:CZ | 2.51 | 0.45 |
| 1:C:217:LYS:CE | 1:C:217:LYS:HB2 | 2.46 | 0.45 |
| 1:C:325:TRP:CZ2 | 1:C:394:MET:HE1 | 2.51 | 0.45 |
| 1:C:391:ILE:O | 1:C:391:ILE:CG2 | 2.63 | 0.45 |
| 1:D:22:VAL:O | 1:D:22:VAL:HG23 | 2.17 | 0.45 |
| 1:E:107:VAL:O | 1:E:307:PHE:HB3 | 2.16 | 0.45 |
| 1:E:307:PHE:C | 1:E:309:LYS:H | 2.19 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:235:ILE:HG23 | 1:F:235:ILE:HD12 | 1.68 | 0.45 |
| 1:G:34:TYR:HE2 | 1:G:377:GLN:HB2 | 1.76 | 0.45 |
| 1:G:85:PHE:CE2 | 1:G:378:LEU:HD22 | 2.51 | 0.45 |
| 1:G:112:PRO:HB3 | 1:H:231:TYR:CD1 | 2.52 | 0.45 |
| 1:G:205:PHE:CD1 | 1:G:220:VAL:HG12 | 2.51 | 0.45 |
| 1:H:76:HIS:HB2 | 1:H:450:ASN:HA | 1.98 | 0.45 |
| 1:H:105:VAL:HG22 | 1:H:374:PHE:CE2 | 2.52 | 0.45 |
| 1:J:29:ALA:HB3 | 1:J:380:LYS:HG3 | 1.98 | 0.45 |
| 1:J:29:ALA:HB3 | 1:J:380:LYS:O | 2.16 | 0.45 |
| 1:J:471:GLN:OE1 | 1:J:472:LEU:N | 2.49 | 0.45 |
| 1:K:439:ASP:C | 1:K:441:LEU:H | 2.19 | 0.45 |
| 1:N:49:TYR:CE1 | 1:N:364:LEU:CD1 | 3.00 | 0.45 |
| 1:N:113:LEU:HA | 1:N:337:THR:O | 2.17 | 0.45 |
| 1:O:176:THR:CG2 | 1:O:176:THR:HB | 2.21 | 0.45 |
| 1:O:180:VAL:HG12 | 1:O:181:GLN:O | 2.16 | 0.45 |
| 1:O:234:TYR:CD1 | 1:O:251:ARG:NH2 | 2.84 | 0.45 |
| 1:A:188:LEU:HA | 1:A:188:LEU:HD13 | 1.63 | 0.45 |
| 1:A:242:TYR:CE2 | 1:A:394:MET:HB2 | 2.51 | 0.45 |
| 1:B:157:CYS:HA | 1:B:332:THR:O | 2.16 | 0.45 |
| 1:C:54:LYS:HZ2 | 1:C:55:PRO:CD | 2.26 | 0.45 |
| 1:C:217:LYS:CE | 1:C:217:LYS:CB | 2.93 | 0.45 |
| 1:D:307:PHE:O | 1:D:308:ASN:HB2 | 2.16 | 0.45 |
| 1:E:365:ARG:HA | 1:E:365:ARG:HD3 | 1.81 | 0.45 |
| 1:E:394:MET:HB3 | 1:E:395:ASN:H | 1.51 | 0.45 |
| 1:E:397:THR:O | 1:E:401:ASP:N | 2.47 | 0.45 |
| 1:E:440:PRO:HA | 1:E:443:LYS:NZ | 2.30 | 0.45 |
| 1:F:33:ILE:HB | 1:F:378:LEU:HB3 | 1.97 | 0.45 |
| 1:F:293:PRO:HD3 | 1:J:117:ILE:HG21 | 1.97 | 0.45 |
| 1:G:65:VAL:O | 1:G:65:VAL:HG12 | 2.17 | 0.45 |
| 1:G:156:LEU:C | 1:G:156:LEU:HD12 | 2.36 | 0.45 |
| 1:H:374:PHE:O | 1:H:375:ILE:HD13 | 2.16 | 0.45 |
| 1:I:82:LYS:HZ3 | 1:I:403:ASN:HD22 | 1.64 | 0.45 |
| 1:I:108:GLY:CA | 1:I:371:ASP:O | 2.65 | 0.45 |
| 1:I:248:PHE:CE2 | 1:I:311:TYR:HB3 | 2.51 | 0.45 |
| 1:J:312:TRP:CH2 | 1:J:468:PHE:HB2 | 2.51 | 0.45 |
| 1:K:105:VAL:HG22 | 1:K:374:PHE:CD2 | 2.52 | 0.45 |
| 1:K:139:ALA:HA | 1:K:143:ASN:HD21 | 1.82 | 0.45 |
| 1:L:47:HIS:CG | 1:L:48:PRO:HD2 | 2.52 | 0.45 |
| 1:L:361:LYS:HD2 | 1:M:183:GLY:HA3 | 1.98 | 0.45 |
| 1:L:363:TYR:CD1 | 1:M:185:CYS:HB2 | 2.52 | 0.45 |
| 1:L:441:LEU:HA | 1:L:444:TYR:HD1 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:280:SER:CA | 1:M:284:ALA:HB2 | 2.46 | 0.45 |
| 1:M:307:PHE:O | 1:M:308:ASN:CB | 2.56 | 0.45 |
| 1:M:458:ASP:O | 1:M:458:ASP:OD2 | 2.35 | 0.45 |
| 1:N:149:MET:HA | 1:O:260:LEU:CD2 | 2.47 | 0.45 |
| 1:N:234:TYR:O | 1:N:236:LYS:N | 2.49 | 0.45 |
| 1:C:39:THR:HG22 | 1:C:449:VAL:HG11 | 1.98 | 0.45 |
| 1:C:47:HIS:HB2 | 1:C:52:ILE:CD1 | 2.45 | 0.45 |
| 1:C:139:ALA:CB | 1:C:143:ASN:HD21 | 2.30 | 0.45 |
| 1:C:237:MET:CB | 1:C:246:LEU:CD2 | 2.94 | 0.45 |
| 1:D:181:GLN:CG | 1:D:181:GLN:NE2 | 2.69 | 0.45 |
| 1:E:96:GLN:HB3 | 1:E:382:THR:HA | 1.98 | 0.45 |
| 1:E:155:GLN:HE21 | 1:E:155:GLN:HB2 | 1.52 | 0.45 |
| 1:E:316:ALA:C | 1:E:318:GLY:N | 2.69 | 0.45 |
| 1:F:54:LYS:HG3 | 1:F:55:PRO:HD2 | 1.97 | 0.45 |
| 1:F:107:VAL:HB | 1:F:307:PHE:HD2 | 1.82 | 0.45 |
| 1:F:180:VAL:HG13 | 1:F:184:ASP:CB | 2.47 | 0.45 |
| 1:F:180:VAL:HG13 | 1:F:184:ASP:HB2 | 1.91 | 0.45 |
| 1:G:110:GLY:O | 1:G:111:GLN:NE2 | 2.46 | 0.45 |
| 1:H:247:PHE:CE2 | 1:H:322:GLY:HA2 | 2.51 | 0.45 |
| 1:I:149:MET:HE3 | 1:I:294:THR:HG22 | 1.99 | 0.45 |
| 1:J:247:PHE:HD1 | 1:J:248:PHE:N | 2.14 | 0.45 |
| 1:J:329:LEU:HD13 | 1:J:374:PHE:HE2 | 1.79 | 0.45 |
| 1:K:74:ARG:NH2 | 1:K:441:LEU:HD12 | 2.31 | 0.45 |
| 1:K:166:GLY:N | 1:K:195:ILE:HD11 | 2.31 | 0.45 |
| 1:K:213:LEU:HD12 | 1:O:344:LEU:CB | 2.46 | 0.45 |
| 1:K:253:GLU:H | 1:O:302:SER:HB2 | 1.81 | 0.45 |
| 1:K:269:GLU:HG3 | 1:O:363:TYR:CE2 | 2.51 | 0.45 |
| 1:L:27:TYR:CZ | 1:L:390:TYR:HE2 | 2.34 | 0.45 |
| 1:L:249:TYR:O | 1:L:249:TYR:CD1 | 2.69 | 0.45 |
| 1:L:275:LEU:CD2 | 1:L:275:LEU:CB | 2.86 | 0.45 |
| 1:M:97:ARG:HG3 | 1:M:383:LEU:HD11 | 1.97 | 0.45 |
| 1:M:246:LEU:HD23 | 1:M:246:LEU:H | 1.81 | 0.45 |
| 1:M:364:LEU:HA | 1:M:364:LEU:HD23 | 1.50 | 0.45 |
| 1:N:68:LEU:C | 1:N:201:VAL:HG22 | 2.33 | 0.45 |
| 1:N:159:ILE:HD13 | 1:N:159:ILE:HG21 | 1.63 | 0.45 |
| 1:N:185:CYS:SG | 1:N:186:PRO:HD2 | 2.56 | 0.45 |
| 1:O:27:TYR:O | 1:O:381:ILE:HG23 | 2.17 | 0.45 |
| 1:O:98:LEU:HD22 | 1:O:379:CYS:O | 2.16 | 0.45 |
| 1:O:133:SER:O | 1:O:134:ALA:HB2 | 2.17 | 0.45 |
| 1:O:152:LYS:O | 1:O:152:LYS:CG | 2.65 | 0.45 |
| 1:A:188:LEU:HD11 | 1:A:213:LEU:HD11 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:147:ILE:CG2 | 1:B:148:SER:N | 2.79 | 0.45 |
| 1:B:399:LEU:HA | 1:B:402:TRP:HE3 | 1.81 | 0.45 |
| 1:C:46:GLY:CA | 1:C:65:VAL:HB | 2.47 | 0.45 |
| 1:C:163:PRO:CD | 1:C:330:PHE:HE1 | 2.27 | 0.45 |
| 1:C:240:GLU:HG3 | 1:C:243:GLY:N | 2.30 | 0.45 |
| 1:C:300:VAL:O | 1:D:254:GLN:HA | 2.17 | 0.45 |
| 1:C:335:ASP:OD1 | 1:C:337:THR:OG1 | 2.34 | 0.45 |
| 1:D:49:TYR:CE2 | 1:D:118:SER:HA | 2.51 | 0.45 |
| 1:D:70:TYR:CE1 | 1:D:201:VAL:HA | 2.52 | 0.45 |
| 1:E:372:LEU:HD23 | 1:E:372:LEU:HA | 1.70 | 0.45 |
| 1:G:150:ASP:HB3 | 1:H:257:VAL:HG21 | 1.99 | 0.45 |
| 1:H:64:LYS:NZ | 1:H:200:MET:HE2 | 2.31 | 0.45 |
| 1:H:461:GLN:HE22 | 1:I:21:VAL:H | 1.64 | 0.45 |
| 1:I:96:GLN:HA | 1:I:382:THR:HA | 1.98 | 0.45 |
| 1:I:114:GLY:N | 1:I:337:THR:O | 2.50 | 0.45 |
| 1:J:57:ASN:HD21 | 1:J:59:LYS:CB | 2.30 | 0.45 |
| 1:J:77:LEU:HD22 | 1:J:455:PHE:HZ | 1.82 | 0.45 |
| 1:K:52:ILE:N | 1:K:52:ILE:CD1 | 2.70 | 0.45 |
| 1:M:451:LEU:HD23 | 1:M:451:LEU:HA | 1.88 | 0.45 |
| 1:N:126:LEU:HD12 | 1:N:126:LEU:HA | 1.45 | 0.45 |
| 1:N:188:LEU:HD11 | 1:N:213:LEU:CD1 | 2.44 | 0.45 |
| 1:A:123:LEU:HD23 | 1:A:147:ILE:CG2 | 2.47 | 0.45 |
| 1:A:190:LEU:HD12 | 1:A:191:ILE:H | 1.79 | 0.45 |
| 1:A:260:LEU:HD23 | 1:E:117:ILE:HD11 | 1.98 | 0.45 |
| 1:A:439:ASP:HA | 1:A:440:PRO:HD3 | 1.86 | 0.45 |
| 1:B:325:TRP:HB3 | 1:B:398:ILE:HD11 | 1.99 | 0.45 |
| 1:C:141:VAL:CG1 | 1:C:142:ASP:N | 2.80 | 0.45 |
| 1:D:46:GLY:HA3 | 1:D:63:PRO:O | 2.16 | 0.45 |
| 1:D:57:ASN:HD21 | 1:D:59:LYS:HB2 | 1.82 | 0.45 |
| 1:D:176:THR:CB | 1:D:176:THR:C | 2.79 | 0.45 |
| 1:E:166:GLY:CA | 1:E:195:ILE:HD11 | 2.47 | 0.45 |
| 1:E:242:TYR:CE2 | 1:E:394:MET:HG3 | 2.51 | 0.45 |
| 1:F:77:LEU:HD22 | 1:F:455:PHE:HZ | 1.80 | 0.45 |
| 1:F:155:GLN:HG2 | 1:F:306:ILE:HG12 | 1.99 | 0.45 |
| 1:F:260:LEU:HD12 | 1:F:260:LEU:H | 1.75 | 0.45 |
| 1:F:262:ASN:ND2 | 1:F:288:SER:HB3 | 2.31 | 0.45 |
| 1:G:155:GLN:CD | 1:G:306:ILE:HG12 | 2.36 | 0.45 |
| 1:G:262:ASN:HD21 | 1:G:288:SER:HB3 | 1.81 | 0.45 |
| 1:G:390:TYR:C | 1:G:392:HIS:H | 2.20 | 0.45 |
| 1:H:72:VAL:HG23 | 1:H:197:ASP:HA | 1.99 | 0.45 |
| 1:I:246:LEU:N | 1:I:246:LEU:CD2 | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:344:LEU:HD13 | 1:J:213:LEU:HD12 | 1.98 | 0.45 |
| 1:J:44:ALA:HB3 | 1:J:368:GLU:HB2 | 1.98 | 0.45 |
| 1:J:66:SER:N | 1:J:69:GLN:NE2 | 2.54 | 0.45 |
| 1:J:272:PRO:O | 1:J:275:LEU:HG | 2.15 | 0.45 |
| 1:K:345:CYS:SG | 1:K:345:CYS:O | 2.74 | 0.45 |
| 1:M:47:HIS:HB3 | 1:M:50:PHE:O | 2.17 | 0.45 |
| 1:M:121:PRO:CG | 1:N:289:SER:HB2 | 2.47 | 0.45 |
| 1:M:323:ILE:HG23 | 1:M:323:ILE:HD12 | 1.97 | 0.45 |
| 1:M:459:LEU:C | 1:M:461:GLN:N | 2.69 | 0.45 |
| 1:N:83:PHE:O | 1:N:85:PHE:N | 2.49 | 0.45 |
| 1:N:208:MET:SD | 1:N:210:PHE:HE2 | 2.40 | 0.45 |
| 1:O:150:ASP:O | 1:O:296:SER:HA | 2.15 | 0.45 |
| 1:A:21:VAL:C | 1:A:22:VAL:CG1 | 2.85 | 0.45 |
| 1:A:57:ASN:ND2 | 1:A:59:LYS:CB | 2.62 | 0.45 |
| 1:A:112:PRO:HD3 | 1:B:231:TYR:CG | 2.52 | 0.45 |
| 1:A:117:ILE:HD11 | 1:B:260:LEU:HD23 | 1.99 | 0.45 |
| 1:A:150:ASP:O | 1:A:296:SER:HA | 2.16 | 0.45 |
| 1:A:185:CYS:HB2 | 1:E:363:TYR:CZ | 2.52 | 0.45 |
| 1:A:257:VAL:HG12 | 1:A:293:PRO:CB | 2.44 | 0.45 |
| 1:B:196:GLN:HA | 1:B:446:PHE:HE2 | 1.81 | 0.45 |
| 1:B:344:LEU:HD12 | 1:C:186:PRO:HG2 | 1.98 | 0.45 |
| 1:B:344:LEU:N | 1:B:344:LEU:CD2 | 2.72 | 0.45 |
| 1:C:97:ARG:HA | 1:C:97:ARG:NH1 | 2.32 | 0.45 |
| 1:C:463:PRO:HB3 | 1:C:466:ARG:NH2 | 2.30 | 0.45 |
| 1:D:79:ASP:OD2 | 1:D:82:LYS:HG3 | 2.17 | 0.45 |
| 1:D:193:THR:OG1 | 1:D:194:VAL:N | 2.50 | 0.45 |
| 1:D:348:ILE:CD1 | 1:E:182:PRO:O | 2.65 | 0.45 |
| 1:D:375:ILE:CG1 | 1:D:464:LEU:HD13 | 2.37 | 0.45 |
| 1:F:451:LEU:HA | 1:F:454:LYS:CG | 2.46 | 0.45 |
| 1:G:71:ARG:HB3 | 1:G:73:PHE:HE1 | 1.77 | 0.45 |
| 1:G:85:PHE:HB3 | 1:G:87:ASP:O | 2.16 | 0.45 |
| 1:G:210:PHE:HD1 | 1:G:224:ILE:HB | 1.82 | 0.45 |
| 1:G:439:ASP:O | 1:G:442:LYS:HB2 | 2.16 | 0.45 |
| 1:H:36:HIS:CG | 1:H:37:ALA:N | 2.84 | 0.45 |
| 1:I:50:PHE:CD1 | 1:I:50:PHE:O | 2.70 | 0.45 |
| 1:I:112:PRO:HB3 | 1:J:231:TYR:CG | 2.51 | 0.45 |
| 1:I:149:MET:HE3 | 1:I:295:PRO:HD2 | 1.99 | 0.45 |
| 1:I:300:VAL:O | 1:I:300:VAL:HG23 | 2.16 | 0.45 |
| 1:J:81:ASN:C | 1:J:82:LYS:HG3 | 2.37 | 0.45 |
| 1:K:391:ILE:HD13 | 1:K:402:TRP:CZ3 | 2.52 | 0.45 |
| 1:K:395:ASN:HB3 | 1:K:398:ILE:HG12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:74:ARG:HB2 | 1:L:330:PHE:HE2 | 1.82 | 0.45 |
| 1:L:96:GLN:NE2 | 1:L:382:THR:CG2 | 2.79 | 0.45 |
| 1:L:155:GLN:HE21 | 1:L:155:GLN:HB2 | 1.50 | 0.45 |
| 1:L:461:GLN:HE22 | 1:M:21:VAL:CG2 | 2.30 | 0.45 |
| 1:M:54:LYS:CB | 1:M:57:ASN:HD22 | 2.30 | 0.45 |
| 1:M:201:VAL:O | 1:M:229:CYS:SG | 2.74 | 0.45 |
| 1:N:280:SER:O | 1:N:281:GLY:C | 2.53 | 0.45 |
| 1:O:155:GLN:HG2 | 1:O:307:PHE:CE1 | 2.52 | 0.45 |
| 1:O:156:LEU:C | 1:O:156:LEU:HD12 | 2.37 | 0.45 |
| 1:O:211:THR:O | 1:O:211:THR:HG22 | 2.16 | 0.45 |
| 1:O:373:GLN:HB3 | 1:O:464:LEU:HD12 | 1.99 | 0.45 |
| 1:O:380:LYS:C | 1:O:381:ILE:HG13 | 2.37 | 0.45 |
| 1:A:30:ARG:HB3 | 1:A:377:GLN:NE2 | 2.32 | 0.45 |
| 1:A:42:LEU:HD12 | 1:A:73:PHE:CE2 | 2.51 | 0.45 |
| 1:A:207:ALA:CB | 1:A:229:CYS:O | 2.61 | 0.45 |
| 1:B:46:GLY:HA3 | 1:B:63:PRO:O | 2.17 | 0.45 |
| 1:B:97:ARG:HA | 1:B:97:ARG:NH1 | 2.29 | 0.45 |
| 1:C:52:ILE:HD12 | 1:C:52:ILE:N | 2.32 | 0.45 |
| 1:C:52:ILE:CG1 | 1:D:269:GLU:OE2 | 2.65 | 0.45 |
| 1:C:344:LEU:HB2 | 1:D:213:LEU:O | 2.16 | 0.45 |
| 1:C:348:ILE:HD12 | 1:D:182:PRO:O | 2.17 | 0.45 |
| 1:F:30:ARG:HD3 | 1:F:377:GLN:HE22 | 1.82 | 0.45 |
| 1:F:46:GLY:O | 1:F:365:ARG:HD2 | 2.17 | 0.45 |
| 1:F:54:LYS:CG | 1:F:56:ASN:OD1 | 2.62 | 0.45 |
| 1:F:202:ASP:OD2 | 1:J:112:PRO:CB | 2.60 | 0.45 |
| 1:F:344:LEU:N | 1:F:344:LEU:CD2 | 2.79 | 0.45 |
| 1:G:68:LEU:HD23 | 1:G:201:VAL:CG2 | 2.47 | 0.45 |
| 1:G:216:ASN:CB | 1:G:219:GLU:OE2 | 2.65 | 0.45 |
| 1:G:456:SER:HB3 | 1:G:462:PHE:HE1 | 1.81 | 0.45 |
| 1:H:60:ILE:HG13 | 1:H:60:ILE:O | 2.15 | 0.45 |
| 1:H:166:GLY:N | 1:H:195:ILE:HG13 | 2.25 | 0.45 |
| 1:I:231:TYR:HA | 1:I:232:PRO:HD3 | 1.77 | 0.45 |
| 1:I:307:PHE:CD1 | 1:I:307:PHE:N | 2.84 | 0.45 |
| 1:J:196:GLN:N | 1:J:199:ASP:OD2 | 2.49 | 0.45 |
| 1:J:207:ALA:CB | 1:J:229:CYS:O | 2.58 | 0.45 |
| 1:J:300:VAL:O | 1:J:300:VAL:HG23 | 2.17 | 0.45 |
| 1:J:451:LEU:HA | 1:J:454:LYS:HG2 | 1.99 | 0.45 |
| 1:K:307:PHE:C | 1:K:309:LYS:N | 2.67 | 0.45 |
| 1:L:27:TYR:CE2 | 1:L:390:TYR:HE2 | 2.34 | 0.45 |
| 1:L:107:VAL:HG13 | 1:L:372:LEU:HD21 | 1.99 | 0.45 |
| 1:M:80:PRO:HG2 | 1:M:81:ASN:N | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:263:ARG:CD | 1:M:292:PHE:CD2 | 2.99 | 0.45 |
| 1:N:338:ARG:CD | 1:N:338:ARG:HB2 | 2.44 | 0.45 |
| 1:O:183:GLY:O | 1:O:184:ASP:C | 2.55 | 0.45 |
| 1:O:228:ILE:HD12 | 1:O:228:ILE:H | 1.79 | 0.45 |
| 1:A:70:TYR:CE1 | 1:A:201:VAL:HA | 2.52 | 0.45 |
| 1:A:254:GLN:HG3 | 1:A:254:GLN:O | 2.17 | 0.45 |
| 1:A:255:MET:O | 1:E:300:VAL:HG22 | 2.17 | 0.45 |
| 1:A:272:PRO:HD2 | 1:A:275:LEU:HD11 | 1.98 | 0.45 |
| 1:A:281:GLY:O | 1:A:284:ALA:N | 2.36 | 0.45 |
| 1:A:465:GLY:O | 1:A:467:LYS:N | 2.50 | 0.45 |
| 1:A:467:LYS:O | 1:A:468:PHE:C | 2.52 | 0.45 |
| 1:C:214:GLN:CD | 1:C:219:GLU:HB2 | 2.37 | 0.45 |
| 1:D:62:VAL:CG1 | 1:D:63:PRO:HD2 | 2.47 | 0.45 |
| 1:D:82:LYS:HZ3 | 1:D:403:ASN:HD22 | 1.60 | 0.45 |
| 1:D:167:GLU:CB | 1:D:190:LEU:HD11 | 2.27 | 0.45 |
| 1:E:150:ASP:CG | 1:E:150:ASP:O | 2.53 | 0.45 |
| 1:F:67:GLY:H | 1:F:366:HIS:CE1 | 2.35 | 0.45 |
| 1:F:178:VAL:CG1 | 1:F:178:VAL:CG2 | 2.86 | 0.45 |
| 1:G:150:ASP:CG | 1:G:150:ASP:O | 2.54 | 0.45 |
| 1:G:180:VAL:HG11 | 1:G:184:ASP:CB | 2.40 | 0.45 |
| 1:G:279:GLY:C | 1:G:284:ALA:HB2 | 2.37 | 0.45 |
| 1:G:354:THR:HG22 | 1:I:278:LYS:HB3 | 1.99 | 0.45 |
| 1:G:438:GLU:OE1 | 1:G:443:LYS:HE3 | 2.17 | 0.45 |
| 1:I:342:MET:SD | 1:J:208:MET:HE3 | 2.57 | 0.45 |
| 1:I:399:LEU:HA | 1:I:402:TRP:CE3 | 2.51 | 0.45 |
| 1:J:89:SER:O | 1:J:91:TYR:N | 2.50 | 0.45 |
| 1:J:458:ASP:O | 1:J:458:ASP:OD2 | 2.35 | 0.45 |
| 1:K:30:ARG:CG | 1:K:30:ARG:NE | 2.66 | 0.45 |
| 1:K:81:ASN:HD21 | 1:K:402:TRP:HE1 | 1.64 | 0.45 |
| 1:K:439:ASP:C | 1:K:441:LEU:N | 2.70 | 0.45 |
| 1:K:465:GLY:O | 1:K:466:ARG:C | 2.54 | 0.45 |
| 1:N:162:LYS:HB3 | 1:N:163:PRO:CD | 2.42 | 0.45 |
| 1:N:272:PRO:C | 1:N:274:ASP:H | 2.19 | 0.45 |
| 1:O:51:PRO:C | 1:O:52:ILE:HD12 | 2.37 | 0.45 |
| 1:A:72:VAL:H | 1:A:197:ASP:HB2 | 1.82 | 0.45 |
| 1:A:92:ASN:C | 1:A:94:ASP:H | 2.20 | 0.45 |
| 1:A:228:ILE:CD1 | 1:A:228:ILE:CB | 2.81 | 0.45 |
| 1:B:82:LYS:CB | 1:B:82:LYS:HD2 | 2.41 | 0.45 |
| 1:B:123:LEU:O | 1:B:125:LYS:N | 2.50 | 0.45 |
| 1:C:354:THR:HG22 | 1:E:278:LYS:HB3 | 1.99 | 0.45 |
| 1:C:471:GLN:CD | 1:C:471:GLN:C | 2.75 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:398:ILE:HG22 | 1:D:402:TRP:CE3 | 2.51 | 0.45 |
| 1:E:42:LEU:HB2 | 1:E:370:TYR:CB | 2.47 | 0.45 |
| 1:F:163:PRO:HD3 | 1:F:330:PHE:HE1 | 1.80 | 0.45 |
| 1:F:336:THR:C | 1:F:338:ARG:H | 2.20 | 0.45 |
| 1:H:28:VAL:HA | 1:H:381:ILE:HG12 | 1.98 | 0.45 |
| 1:H:108:GLY:N | 1:H:371:ASP:O | 2.43 | 0.45 |
| 1:H:158:LEU:HD23 | 1:H:249:TYR:HB2 | 1.99 | 0.45 |
| 1:I:75:ILE:CD1 | 1:I:75:ILE:N | 2.72 | 0.45 |
| 1:I:104:GLY:O | 1:I:374:PHE:HA | 2.18 | 0.45 |
| 1:I:166:GLY:H | 1:I:195:ILE:CG1 | 2.29 | 0.45 |
| 1:I:384:THR:OG1 | 1:I:385:ALA:N | 2.49 | 0.45 |
| 1:J:149:MET:CE | 1:J:294:THR:HG22 | 2.47 | 0.45 |
| 1:J:323:ILE:HG21 | 1:J:325:TRP:CE2 | 2.51 | 0.45 |
| 1:K:141:VAL:O | 1:K:142:ASP:CB | 2.64 | 0.45 |
| 1:L:280:SER:CA | 1:L:284:ALA:HB2 | 2.47 | 0.45 |
| 1:M:30:ARG:NH2 | 1:M:321:ASN:HD22 | 2.15 | 0.45 |
| 1:M:35:TYR:CE2 | 1:M:457:ALA:N | 2.85 | 0.45 |
| 1:M:70:TYR:CD2 | 1:M:195:ILE:HG21 | 2.51 | 0.45 |
| 1:M:106:GLU:HG3 | 1:M:309:LYS:O | 2.17 | 0.45 |
| 1:M:109:ARG:HD3 | 1:M:370:TYR:CE2 | 2.52 | 0.45 |
| 1:M:126:LEU:HB2 | 1:M:264:ALA:HB2 | 1.98 | 0.45 |
| 1:M:166:GLY:O | 1:M:192:ASN:HA | 2.17 | 0.45 |
| 1:N:107:VAL:O | 1:N:107:VAL:HG12 | 2.16 | 0.45 |
| 1:N:173:SER:HA | 1:N:174:PRO:HD3 | 1.64 | 0.45 |
| 1:O:391:ILE:CG2 | 1:O:398:ILE:HB | 2.46 | 0.45 |
| 1:B:110:GLY:O | 1:B:111:GLN:NE2 | 2.50 | 0.44 |
| 1:B:451:LEU:HD23 | 1:B:454:LYS:HG3 | 2.00 | 0.44 |
| 1:D:442:LYS:HB3 | 1:D:443:LYS:HD3 | 1.98 | 0.44 |
| 1:E:60:ILE:HG13 | 1:E:60:ILE:O | 2.16 | 0.44 |
| 1:E:184:ASP:O | 1:E:185:CYS:O | 2.35 | 0.44 |
| 1:E:360:PHE:CD1 | 1:E:360:PHE:N | 2.85 | 0.44 |
| 1:F:22:VAL:O | 1:F:23:SER:C | 2.55 | 0.44 |
| 1:F:363:TYR:CZ | 1:G:185:CYS:HB2 | 2.52 | 0.44 |
| 1:F:395:ASN:HB3 | 1:F:398:ILE:HG12 | 1.99 | 0.44 |
| 1:G:75:ILE:HB | 1:G:329:LEU:HB3 | 1.99 | 0.44 |
| 1:G:163:PRO:HB2 | 1:G:194:VAL:HG13 | 1.99 | 0.44 |
| 1:G:363:TYR:CG | 1:H:185:CYS:HB2 | 2.52 | 0.44 |
| 1:G:391:ILE:HG22 | 1:G:398:ILE:HB | 1.99 | 0.44 |
| 1:H:48:PRO:HG2 | 1:H:49:TYR:CD1 | 2.52 | 0.44 |
| 1:I:152:LYS:HB3 | 1:I:255:MET:HG3 | 1.99 | 0.44 |
| 1:I:471:GLN:CD | 1:I:472:LEU:N | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:42:LEU:HD13 | 1:J:447:TRP:CE2 | 2.52 | 0.44 |
| 1:J:300:VAL:CG1 | 1:J:300:VAL:CA | 2.84 | 0.44 |
| 1:J:317:GLN:H | 1:J:317:GLN:HG3 | 1.56 | 0.44 |
| 1:K:42:LEU:CD1 | 1:K:73:PHE:CE2 | 2.96 | 0.44 |
| 1:K:300:VAL:O | 1:K:300:VAL:CG2 | 2.64 | 0.44 |
| 1:K:461:GLN:HE22 | 1:L:21:VAL:CB | 2.30 | 0.44 |
| 1:M:70:TYR:O | 1:M:71:ARG:NH1 | 2.50 | 0.44 |
| 1:N:33:ILE:O | 1:N:377:GLN:HA | 2.17 | 0.44 |
| 1:N:85:PHE:CZ | 1:N:378:LEU:HD22 | 2.52 | 0.44 |
| 1:N:112:PRO:HB2 | 1:O:202:ASP:OD2 | 2.17 | 0.44 |
| 1:N:235:ILE:HD12 | 1:N:235:ILE:HG23 | 1.76 | 0.44 |
| 1:O:355:TYR:CD2 | 1:O:355:TYR:C | 2.91 | 0.44 |
| 1:A:49:TYR:CE2 | 1:A:118:SER:HA | 2.50 | 0.44 |
| 1:A:242:TYR:CE2 | 1:A:394:MET:CB | 3.00 | 0.44 |
| 1:A:385:ALA:O | 1:A:389:THR:HG23 | 2.17 | 0.44 |
| 1:B:28:VAL:HG22 | 1:B:381:ILE:CG1 | 2.47 | 0.44 |
| 1:B:96:GLN:HB3 | 1:B:382:THR:CA | 2.47 | 0.44 |
| 1:B:219:GLU:HA | 1:B:263:ARG:NH1 | 2.32 | 0.44 |
| 1:C:91:TYR:HA | 1:C:96:GLN:OE1 | 2.16 | 0.44 |
| 1:C:323:ILE:CG2 | 1:C:325:TRP:CD2 | 3.00 | 0.44 |
| 1:D:71:ARG:HH11 | 1:D:71:ARG:CG | 2.31 | 0.44 |
| 1:D:210:PHE:HE1 | 1:D:224:ILE:HB | 1.76 | 0.44 |
| 1:E:440:PRO:HG2 | 1:E:441:LEU:HG | 1.99 | 0.44 |
| 1:F:23:SER:N | 1:F:319:HIS:HD2 | 2.14 | 0.44 |
| 1:F:24:THR:OG1 | 1:F:25:ASP:N | 2.50 | 0.44 |
| 1:F:97:ARG:HH11 | 1:F:97:ARG:CA | 2.22 | 0.44 |
| 1:F:97:ARG:N | 1:F:383:LEU:CD1 | 2.80 | 0.44 |
| 1:F:178:VAL:O | 1:F:180:VAL:N | 2.34 | 0.44 |
| 1:G:74:ARG:NH2 | 1:G:441:LEU:HD12 | 2.31 | 0.44 |
| 1:G:307:PHE:C | 1:G:309:LYS:N | 2.70 | 0.44 |
| 1:G:367:GLY:O | 1:G:368:GLU:HG2 | 2.17 | 0.44 |
| 1:H:87:ASP:O | 1:H:90:PHE:CE2 | 2.70 | 0.44 |
| 1:H:307:PHE:O | 1:H:308:ASN:HB2 | 2.17 | 0.44 |
| 1:H:389:THR:OG1 | 1:H:390:TYR:N | 2.50 | 0.44 |
| 1:H:471:GLN:O | 1:H:472:LEU:OXT | 2.35 | 0.44 |
| 1:I:42:LEU:HB2 | 1:I:370:TYR:HB2 | 1.99 | 0.44 |
| 1:I:72:VAL:HG23 | 1:I:197:ASP:HA | 2.00 | 0.44 |
| 1:K:117:ILE:HG23 | 1:K:117:ILE:O | 2.18 | 0.44 |
| 1:L:153:GLN:NE2 | 1:L:300:VAL:HG12 | 2.32 | 0.44 |
| 1:L:157:CYS:HA | 1:L:332:THR:O | 2.17 | 0.44 |
| 1:L:374:PHE:HB3 | 1:L:376:PHE:CE1 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:92:ASN:HD21 | 1:N:94:ASP:HB2 | 1.80 | 0.44 |
| 1:N:262:ASN:HD22 | 1:N:263:ARG:H | 1.61 | 0.44 |
| 1:A:121:PRO:CG | 1:B:289:SER:HB2 | 2.47 | 0.44 |
| 1:A:129:THR:HG21 | 1:A:291:TYR:CD2 | 2.53 | 0.44 |
| 1:A:135:TYR:HE2 | 1:A:287:ALA:CB | 2.17 | 0.44 |
| 1:A:290:ASN:HD22 | 1:A:290:ASN:N | 2.14 | 0.44 |
| 1:B:392:HIS:HB2 | 1:B:399:LEU:HD11 | 1.98 | 0.44 |
| 1:C:155:GLN:HG2 | 1:C:307:PHE:HE1 | 1.81 | 0.44 |
| 1:C:440:PRO:C | 1:C:443:LYS:HZ1 | 2.21 | 0.44 |
| 1:E:92:ASN:HD21 | 1:E:94:ASP:HB2 | 1.82 | 0.44 |
| 1:E:213:LEU:CD1 | 1:E:213:LEU:CD2 | 2.85 | 0.44 |
| 1:F:97:ARG:HG3 | 1:F:383:LEU:HD21 | 1.99 | 0.44 |
| 1:F:257:VAL:CG2 | 1:J:150:ASP:OD1 | 2.65 | 0.44 |
| 1:F:278:LYS:CB | 1:I:354:THR:HG22 | 2.47 | 0.44 |
| 1:G:30:ARG:NH1 | 1:G:377:GLN:NE2 | 2.58 | 0.44 |
| 1:G:152:LYS:HE3 | 1:G:154:THR:OG1 | 2.18 | 0.44 |
| 1:G:442:LYS:HB3 | 1:G:443:LYS:HD3 | 2.00 | 0.44 |
| 1:H:80:PRO:C | 1:H:82:LYS:H | 2.20 | 0.44 |
| 1:H:189:GLU:O | 1:H:191:ILE:HG13 | 2.16 | 0.44 |
| 1:I:57:ASN:CG | 1:I:59:LYS:H | 2.21 | 0.44 |
| 1:I:125:LYS:HD3 | 1:I:125:LYS:C | 2.38 | 0.44 |
| 1:J:246:LEU:HD23 | 1:J:246:LEU:O | 2.18 | 0.44 |
| 1:K:57:ASN:ND2 | 1:K:59:LYS:H | 2.16 | 0.44 |
| 1:K:70:TYR:CE1 | 1:K:201:VAL:HA | 2.52 | 0.44 |
| 1:K:150:ASP:OD2 | 1:K:150:ASP:N | 2.49 | 0.44 |
| 1:L:185:CYS:SG | 1:L:186:PRO:CD | 3.06 | 0.44 |
| 1:L:275:LEU:CD2 | 1:L:275:LEU:CD1 | 2.79 | 0.44 |
| 1:M:114:GLY:CA | 1:N:255:MET:SD | 3.05 | 0.44 |
| 1:M:126:LEU:HD12 | 1:M:126:LEU:HA | 1.86 | 0.44 |
| 1:M:247:PHE:HD1 | 1:M:248:PHE:H | 1.64 | 0.44 |
| 1:M:363:TYR:CE1 | 1:N:185:CYS:HB2 | 2.51 | 0.44 |
| 1:N:361:LYS:HD2 | 1:O:183:GLY:HA3 | 1.99 | 0.44 |
| 1:O:149:MET:CE | 1:O:205:PHE:CZ | 3.00 | 0.44 |
| 1:O:373:GLN:HB2 | 1:O:464:LEU:HD12 | 1.99 | 0.44 |
| 1:A:302:SER:C | 1:A:304:ALA:H | 2.21 | 0.44 |
| 1:B:98:LEU:HA | 1:B:379:CYS:O | 2.17 | 0.44 |
| 1:B:240:GLU:HG3 | 1:B:243:GLY:CA | 2.47 | 0.44 |
| 1:C:24:THR:O | 1:C:28:VAL:HG23 | 2.17 | 0.44 |
| 1:C:115:VAL:H | 1:D:255:MET:HE1 | 1.83 | 0.44 |
| 1:D:360:PHE:CE2 | 1:E:216:ASN:HA | 2.52 | 0.44 |
| 1:E:75:ILE:CD1 | 1:E:331:VAL:HG23 | 2.39 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:106:GLU:HB3 | 1:E:373:GLN:HB2 | 1.99 | 0.44 |
| 1:E:293:PRO:O | 1:E:293:PRO:CD | 2.65 | 0.44 |
| 1:E:323:ILE:O | 1:E:325:TRP:N | 2.49 | 0.44 |
| 1:E:390:TYR:O | 1:E:394:MET:N | 2.51 | 0.44 |
| 1:F:399:LEU:HD23 | 1:F:402:TRP:CE3 | 2.52 | 0.44 |
| 1:G:66:SER:O | 1:G:69:GLN:HG3 | 2.18 | 0.44 |
| 1:H:325:TRP:HB3 | 1:H:398:ILE:HD11 | 2.00 | 0.44 |
| 1:H:399:LEU:HA | 1:H:402:TRP:CE3 | 2.44 | 0.44 |
| 1:J:54:LYS:HG2 | 1:J:57:ASN:HB3 | 1.99 | 0.44 |
| 1:J:172:GLY:O | 1:J:173:SER:C | 2.55 | 0.44 |
| 1:K:124:ASN:HD22 | 1:K:216:ASN:ND2 | 2.15 | 0.44 |
| 1:K:141:VAL:O | 1:K:142:ASP:HB3 | 2.17 | 0.44 |
| 1:K:240:GLU:HG2 | 1:K:245:SER:OG | 2.16 | 0.44 |
| 1:L:254:GLN:O | 1:L:254:GLN:HG3 | 2.15 | 0.44 |
| 1:L:364:LEU:CD1 | 1:M:290:ASN:HA | 2.44 | 0.44 |
| 1:M:441:LEU:CD2 | 1:M:441:LEU:CB | 2.81 | 0.44 |
| 1:N:290:ASN:N | 1:N:290:ASN:ND2 | 2.64 | 0.44 |
| 1:N:382:THR:CG2 | 1:N:382:THR:CA | 2.84 | 0.44 |
| 1:A:231:TYR:CD2 | 1:E:112:PRO:HB3 | 2.53 | 0.44 |
| 1:A:283:THR:HG21 | 1:E:142:ASP:O | 2.17 | 0.44 |
| 1:B:54:LYS:HB3 | 1:B:57:ASN:HD22 | 1.82 | 0.44 |
| 1:C:153:GLN:NE2 | 1:C:300:VAL:HA | 2.32 | 0.44 |
| 1:C:276:TYR:CD2 | 1:C:276:TYR:N | 2.85 | 0.44 |
| 1:C:329:LEU:HA | 1:C:329:LEU:HD23 | 1.77 | 0.44 |
| 1:D:51:PRO:C | 1:D:52:ILE:HD12 | 2.38 | 0.44 |
| 1:D:242:TYR:CE2 | 1:D:394:MET:CB | 2.95 | 0.44 |
| 1:E:261:PHE:CB | 1:E:292:PHE:CE2 | 2.99 | 0.44 |
| 1:F:149:MET:HE1 | 1:F:205:PHE:CZ | 2.53 | 0.44 |
| 1:F:240:GLU:OE2 | 1:F:241:PRO:HD2 | 2.17 | 0.44 |
| 1:G:208:MET:CG | 1:G:210:PHE:CE2 | 3.00 | 0.44 |
| 1:H:153:GLN:NE2 | 1:H:300:VAL:CG1 | 2.80 | 0.44 |
| 1:H:159:ILE:HG21 | 1:H:159:ILE:HD13 | 1.85 | 0.44 |
| 1:I:148:SER:OG | 1:J:129:THR:HB | 2.17 | 0.44 |
| 1:I:355:TYR:CE1 | 1:J:144:ARG:HD3 | 2.53 | 0.44 |
| 1:J:47:HIS:HE1 | 1:J:49:TYR:HD1 | 1.63 | 0.44 |
| 1:J:70:TYR:O | 1:J:71:ARG:NH1 | 2.50 | 0.44 |
| 1:J:125:LYS:HE2 | 1:J:261:PHE:CD2 | 2.52 | 0.44 |
| 1:J:254:GLN:NE2 | 1:J:298:SER:HB3 | 2.32 | 0.44 |
| 1:K:253:GLU:HG3 | 1:O:113:LEU:HD22 | 2.00 | 0.44 |
| 1:L:210:PHE:O | 1:L:214:GLN:HB2 | 2.18 | 0.44 |
| 1:M:78:PRO:HD2 | 1:M:455:PHE:CE1 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:92:ASN:HA | 1:M:93:PRO:HD2 | 1.72 | 0.44 |
| 1:N:217:LYS:HG2 | 1:O:276:TYR:CA | 2.46 | 0.44 |
| 1:O:33:ILE:HA | 1:O:33:ILE:HD13 | 1.74 | 0.44 |
| 1:O:144:ARG:C | 1:O:145:GLU:HG2 | 2.37 | 0.44 |
| 1:A:185:CYS:HB2 | 1:E:363:TYR:CD2 | 2.53 | 0.44 |
| 1:A:307:PHE:O | 1:A:308:ASN:HB2 | 2.16 | 0.44 |
| 1:B:101:ALA:HB3 | 1:B:377:GLN:O | 2.18 | 0.44 |
| 1:C:130:GLU:HB2 | 1:C:260:LEU:HD13 | 2.00 | 0.44 |
| 1:D:22:VAL:O | 1:D:23:SER:C | 2.55 | 0.44 |
| 1:D:28:VAL:HG22 | 1:D:381:ILE:HD11 | 2.00 | 0.44 |
| 1:D:117:ILE:HD11 | 1:E:260:LEU:CD2 | 2.41 | 0.44 |
| 1:E:42:LEU:HD23 | 1:E:42:LEU:HA | 1.48 | 0.44 |
| 1:E:76:HIS:HB2 | 1:E:450:ASN:HA | 1.98 | 0.44 |
| 1:E:99:VAL:HG11 | 1:E:323:ILE:CG2 | 2.31 | 0.44 |
| 1:F:57:ASN:HD21 | 1:F:59:LYS:N | 2.11 | 0.44 |
| 1:F:117:ILE:HG12 | 1:F:149:MET:O | 2.18 | 0.44 |
| 1:F:237:MET:HB3 | 1:F:246:LEU:HD22 | 1.98 | 0.44 |
| 1:F:395:ASN:ND2 | 1:F:397:THR:OG1 | 2.50 | 0.44 |
| 1:G:395:ASN:C | 1:G:395:ASN:ND2 | 2.71 | 0.44 |
| 1:H:135:TYR:HE2 | 1:H:287:ALA:HB2 | 1.81 | 0.44 |
| 1:H:308:ASN:ND2 | 1:I:251:ARG:HH22 | 2.12 | 0.44 |
| 1:I:193:THR:CG2 | 1:I:230:LYS:HD2 | 2.45 | 0.44 |
| 1:J:57:ASN:ND2 | 1:J:59:LYS:H | 2.16 | 0.44 |
| 1:J:58:ASN:OD1 | 1:J:58:ASN:N | 2.50 | 0.44 |
| 1:K:213:LEU:HD12 | 1:O:344:LEU:CD1 | 2.42 | 0.44 |
| 1:K:237:MET:CE | 1:K:246:LEU:HD13 | 2.48 | 0.44 |
| 1:K:364:LEU:HD23 | 1:K:364:LEU:HA | 1.72 | 0.44 |
| 1:K:369:GLU:OE1 | 1:L:190:LEU:CD2 | 2.66 | 0.44 |
| 1:L:33:ILE:HD12 | 1:L:33:ILE:HG23 | 1.77 | 0.44 |
| 1:M:22:VAL:O | 1:M:23:SER:C | 2.55 | 0.44 |
| 1:M:363:TYR:CE2 | 1:N:185:CYS:HB2 | 2.52 | 0.44 |
| 1:N:31:THR:HG23 | 1:N:379:CYS:HA | 2.00 | 0.44 |
| 1:N:74:ARG:CB | 1:N:330:PHE:HE2 | 2.31 | 0.44 |
| 1:O:331:VAL:CG1 | 1:O:331:VAL:CA | 2.82 | 0.44 |
| 1:O:398:ILE:CD1 | 1:O:398:ILE:HA | 2.48 | 0.44 |
| 1:O:463:PRO:CA | 1:O:466:ARG:HH21 | 2.31 | 0.44 |
| 1:A:155:GLN:CG | 1:A:307:PHE:HE1 | 2.30 | 0.44 |
| 1:A:188:LEU:CD1 | 1:A:213:LEU:HD11 | 2.48 | 0.44 |
| 1:A:462:PHE:O | 1:A:466:ARG:HG3 | 2.18 | 0.44 |
| 1:C:117:ILE:HG21 | 1:C:117:ILE:HD13 | 1.66 | 0.44 |
| 1:C:381:ILE:O | 1:C:383:LEU:HD12 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:21:VAL:C | 1:D:22:VAL:HG13 | 2.39 | 0.44 |
| 1:D:103:VAL:HG21 | 1:D:468:PHE:CZ | 2.53 | 0.44 |
| 1:D:120:HIS:HB2 | 1:D:221:PRO:HA | 1.99 | 0.44 |
| 1:D:155:GLN:HG2 | 1:D:307:PHE:HE1 | 1.83 | 0.44 |
| 1:D:178:VAL:CG2 | 1:D:178:VAL:N | 2.80 | 0.44 |
| 1:E:36:HIS:CG | 1:E:37:ALA:N | 2.85 | 0.44 |
| 1:E:96:GLN:CB | 1:E:382:THR:HG22 | 2.29 | 0.44 |
| 1:F:141:VAL:HG13 | 1:J:357:ASN:H | 1.83 | 0.44 |
| 1:F:166:GLY:O | 1:F:192:ASN:HA | 2.18 | 0.44 |
| 1:G:394:MET:HE2 | 1:G:394:MET:HB3 | 1.89 | 0.44 |
| 1:I:85:PHE:HA | 1:I:86:PRO:HD2 | 1.70 | 0.44 |
| 1:I:110:GLY:C | 1:I:111:GLN:HG2 | 2.37 | 0.44 |
| 1:I:444:TYR:HB3 | 1:I:446:PHE:CZ | 2.53 | 0.44 |
| 1:J:316:ALA:C | 1:J:318:GLY:H | 2.21 | 0.44 |
| 1:J:364:LEU:HD23 | 1:J:364:LEU:HA | 1.61 | 0.44 |
| 1:K:44:ALA:HB3 | 1:K:368:GLU:HB2 | 2.00 | 0.44 |
| 1:L:348:ILE:HD11 | 1:M:181:GLN:HE22 | 1.83 | 0.44 |
| 1:L:463:PRO:HA | 1:L:466:ARG:HE | 1.82 | 0.44 |
| 1:M:208:MET:HB2 | 1:M:209:ASP:H | 1.45 | 0.44 |
| 1:M:383:LEU:HD22 | 1:M:388:MET:CE | 2.44 | 0.44 |
| 1:N:117:ILE:O | 1:N:117:ILE:HG23 | 2.17 | 0.44 |
| 1:N:325:TRP:HB3 | 1:N:398:ILE:CD1 | 2.47 | 0.44 |
| 1:N:348:ILE:HD12 | 1:N:348:ILE:HA | 1.81 | 0.44 |
| 1:O:42:LEU:HD13 | 1:O:447:TRP:CZ2 | 2.52 | 0.44 |
| 1:O:129:THR:HG1 | 1:O:260:LEU:C | 2.19 | 0.44 |
| 1:O:390:TYR:O | 1:O:392:HIS:N | 2.51 | 0.44 |
| 1:O:459:LEU:C | 1:O:461:GLN:N | 2.71 | 0.44 |
| 1:A:150:ASP:HB3 | 1:B:257:VAL:HG21 | 1.99 | 0.44 |
| 1:A:283:THR:HG1 | 1:E:142:ASP:CG | 2.22 | 0.44 |
| 1:A:399:LEU:HA | 1:A:402:TRP:CE3 | 2.50 | 0.44 |
| 1:B:154:THR:H | 1:B:336:THR:CG2 | 2.31 | 0.44 |
| 1:B:178:VAL:C | 1:B:180:VAL:H | 2.20 | 0.44 |
| 1:B:365:ARG:HD3 | 1:B:365:ARG:HA | 1.77 | 0.44 |
| 1:B:399:LEU:O | 1:B:402:TRP:HB2 | 2.17 | 0.44 |
| 1:C:54:LYS:HB3 | 1:C:57:ASN:HD22 | 1.82 | 0.44 |
| 1:C:345:CYS:HA | 1:C:361:LYS:O | 2.17 | 0.44 |
| 1:D:143:ASN:O | 1:D:144:ARG:C | 2.54 | 0.44 |
| 1:D:148:SER:OG | 1:E:129:THR:CB | 2.64 | 0.44 |
| 1:D:384:THR:HG23 | 1:D:387:VAL:HG23 | 2.00 | 0.44 |
| 1:D:398:ILE:HG22 | 1:D:402:TRP:CZ3 | 2.53 | 0.44 |
| 1:E:322:GLY:C | 1:E:323:ILE:HD13 | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:397:THR:O | 1:F:401:ASP:N | 2.47 | 0.44 |
| 1:G:24:THR:O | 1:G:28:VAL:N | 2.45 | 0.44 |
| 1:G:271:VAL:HG12 | 1:G:276:TYR:CE2 | 2.52 | 0.44 |
| 1:H:97:ARG:HA | 1:H:97:ARG:HH11 | 1.82 | 0.44 |
| 1:H:329:LEU:HD23 | 1:H:329:LEU:HA | 1.59 | 0.44 |
| 1:I:344:LEU:HD21 | 1:I:365:ARG:CG | 2.48 | 0.44 |
| 1:I:396:SER:OG | 1:I:397:THR:N | 2.51 | 0.44 |
| 1:J:30:ARG:HH11 | 1:J:377:GLN:NE2 | 2.16 | 0.44 |
| 1:J:68:LEU:HD13 | 1:J:151:TYR:CD1 | 2.52 | 0.44 |
| 1:J:96:GLN:C | 1:J:96:GLN:HA | 2.14 | 0.44 |
| 1:J:153:GLN:H | 1:J:297:GLY:HA3 | 1.82 | 0.44 |
| 1:J:180:VAL:HG12 | 1:J:181:GLN:H | 1.82 | 0.44 |
| 1:K:54:LYS:HE3 | 1:K:55:PRO:CD | 2.33 | 0.44 |
| 1:K:109:ARG:NE | 1:K:335:ASP:OD2 | 2.49 | 0.44 |
| 1:K:185:CYS:HA | 1:K:186:PRO:HD3 | 1.81 | 0.44 |
| 1:K:190:LEU:CD2 | 1:O:369:GLU:OE1 | 2.65 | 0.44 |
| 1:L:351:SER:HB2 | 1:L:352:GLU:OE1 | 2.17 | 0.44 |
| 1:M:22:VAL:N | 1:M:390:TYR:OH | 2.47 | 0.44 |
| 1:M:120:HIS:CE1 | 1:M:122:LEU:H | 2.34 | 0.44 |
| 1:M:365:ARG:HH11 | 1:M:365:ARG:CG | 2.29 | 0.44 |
| 1:N:92:ASN:HA | 1:N:93:PRO:HD2 | 1.45 | 0.44 |
| 1:N:135:TYR:HE2 | 1:N:287:ALA:HB2 | 1.83 | 0.44 |
| 1:N:196:GLN:NE2 | 1:N:444:TYR:HD2 | 2.16 | 0.44 |
| 1:N:219:GLU:O | 1:N:220:VAL:CG1 | 2.66 | 0.44 |
| 1:O:63:PRO:O | 1:O:65:VAL:HG23 | 2.18 | 0.44 |
| 1:A:72:VAL:HG22 | 1:A:332:THR:HG23 | 1.99 | 0.44 |
| 1:B:54:LYS:CB | 1:B:57:ASN:HD22 | 2.31 | 0.44 |
| 1:B:106:GLU:HG3 | 1:B:309:LYS:C | 2.38 | 0.44 |
| 1:B:214:GLN:CD | 1:B:219:GLU:HB2 | 2.37 | 0.44 |
| 1:B:256:PHE:CD2 | 1:B:296:SER:HB3 | 2.52 | 0.44 |
| 1:C:170:GLY:HA2 | 1:C:213:LEU:CD2 | 2.42 | 0.44 |
| 1:C:391:ILE:HG21 | 1:C:402:TRP:HZ3 | 1.82 | 0.44 |
| 1:D:125:LYS:NZ | 1:D:127:ASP:HA | 2.33 | 0.44 |
| 1:D:152:LYS:CB | 1:D:255:MET:HB2 | 2.27 | 0.44 |
| 1:D:164:PRO:HG2 | 1:D:195:ILE:HB | 2.00 | 0.44 |
| 1:D:234:TYR:O | 1:D:236:LYS:N | 2.51 | 0.44 |
| 1:D:301:THR:CG2 | 1:D:301:THR:HB | 2.19 | 0.44 |
| 1:E:166:GLY:N | 1:E:193:THR:O | 2.50 | 0.44 |
| 1:E:262:ASN:ND2 | 1:E:288:SER:HB3 | 2.31 | 0.44 |
| 1:E:447:TRP:HD1 | 1:E:448:GLU:N | 2.15 | 0.44 |
| 1:F:34:TYR:CE2 | 1:F:377:GLN:CB | 2.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:163:PRO:N | 1:F:330:PHE:CD1 | 2.86 | 0.44 |
| 1:F:241:PRO:HG2 | 1:F:242:TYR:H | 1.83 | 0.44 |
| 1:G:61:LEU:O | 1:G:61:LEU:HD12 | 2.18 | 0.44 |
| 1:G:384:THR:O | 1:G:388:MET:HB2 | 2.18 | 0.44 |
| 1:H:79:ASP:HA | 1:H:327:ASN:ND2 | 2.33 | 0.44 |
| 1:H:167:GLU:HG2 | 1:H:231:TYR:O | 2.18 | 0.44 |
| 1:H:204:GLY:HA3 | 1:H:295:PRO:HG3 | 1.99 | 0.44 |
| 1:H:228:ILE:HD12 | 1:H:228:ILE:N | 2.32 | 0.44 |
| 1:I:34:TYR:CD2 | 1:I:377:GLN:HB2 | 2.52 | 0.44 |
| 1:I:165:ILE:O | 1:I:165:ILE:HG22 | 2.16 | 0.44 |
| 1:I:344:LEU:HD21 | 1:I:365:ARG:HG2 | 2.00 | 0.44 |
| 1:K:85:PHE:CE2 | 1:K:378:LEU:HD22 | 2.53 | 0.44 |
| 1:K:257:VAL:HG13 | 1:O:115:VAL:CG2 | 2.48 | 0.44 |
| 1:L:158:LEU:CD2 | 1:L:249:TYR:HB2 | 2.47 | 0.44 |
| 1:M:270:ASN:O | 1:M:272:PRO:HD3 | 2.18 | 0.44 |
| 1:M:272:PRO:O | 1:M:275:LEU:HG | 2.17 | 0.44 |
| 1:M:281:GLY:O | 1:M:282:SER:C | 2.56 | 0.44 |
| 1:M:312:TRP:CH2 | 1:M:468:PHE:HA | 2.52 | 0.44 |
| 1:M:459:LEU:C | 1:M:461:GLN:H | 2.20 | 0.44 |
| 1:N:149:MET:HE3 | 1:N:295:PRO:HD2 | 1.99 | 0.44 |
| 1:N:442:LYS:HB3 | 1:N:443:LYS:HD3 | 1.99 | 0.44 |
| 1:O:219:GLU:O | 1:O:220:VAL:HG13 | 2.17 | 0.44 |
| 1:A:43:LEU:HD21 | 1:B:190:LEU:HB2 | 1.99 | 0.43 |
| 1:A:220:VAL:O | 1:A:221:PRO:C | 2.55 | 0.43 |
| 1:C:246:LEU:H | 1:C:246:LEU:CD2 | 2.28 | 0.43 |
| 1:E:72:VAL:HG23 | 1:E:72:VAL:H | 1.62 | 0.43 |
| 1:E:155:GLN:OE1 | 1:E:305:GLN:HA | 2.18 | 0.43 |
| 1:F:117:ILE:HD12 | 1:G:293:PRO:HB3 | 2.00 | 0.43 |
| 1:F:163:PRO:HA | 1:F:330:PHE:CD1 | 2.53 | 0.43 |
| 1:F:299:MET:HA | 1:G:255:MET:O | 2.18 | 0.43 |
| 1:G:42:LEU:HB3 | 1:G:447:TRP:CZ2 | 2.53 | 0.43 |
| 1:G:73:PHE:N | 1:G:73:PHE:CD1 | 2.85 | 0.43 |
| 1:G:459:LEU:C | 1:G:461:GLN:N | 2.71 | 0.43 |
| 1:H:24:THR:O | 1:H:26:GLU:N | 2.51 | 0.43 |
| 1:I:75:ILE:HG21 | 1:I:451:LEU:CD1 | 2.43 | 0.43 |
| 1:J:42:LEU:HB3 | 1:J:447:TRP:CZ2 | 2.53 | 0.43 |
| 1:J:69:GLN:HA | 1:J:199:ASP:O | 2.17 | 0.43 |
| 1:J:102:CYS:SG | 1:J:105:VAL:HG23 | 2.58 | 0.43 |
| 1:J:210:PHE:CD1 | 1:J:224:ILE:HB | 2.52 | 0.43 |
| 1:K:24:THR:CG2 | 1:K:320:ASN:HA | 2.48 | 0.43 |
| 1:K:149:MET:HE1 | 1:K:205:PHE:HZ | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:21:VAL:CG1 | 1:L:22:VAL:N | 2.81 | 0.43 |
| 1:L:34:TYR:CD2 | 1:L:377:GLN:HB2 | 2.49 | 0.43 |
| 1:L:117:ILE:HD11 | 1:M:260:LEU:HD23 | 1.99 | 0.43 |
| 1:L:247:PHE:CD1 | 1:L:248:PHE:N | 2.85 | 0.43 |
| 1:L:281:GLY:H | 1:L:284:ALA:CB | 2.31 | 0.43 |
| 1:N:33:ILE:HB | 1:N:378:LEU:HB3 | 2.00 | 0.43 |
| 1:N:35:TYR:O | 1:N:376:PHE:N | 2.40 | 0.43 |
| 1:N:217:LYS:O | 1:N:218:SER:CB | 2.66 | 0.43 |
| 1:N:219:GLU:C | 1:N:220:VAL:CG1 | 2.85 | 0.43 |
| 1:N:365:ARG:HD3 | 1:N:365:ARG:HA | 1.65 | 0.43 |
| 1:O:114:GLY:HA3 | 1:O:340:THR:OG1 | 2.18 | 0.43 |
| 1:O:189:GLU:O | 1:O:191:ILE:HG13 | 2.17 | 0.43 |
| 1:O:384:THR:OG1 | 1:O:387:VAL:HG23 | 2.18 | 0.43 |
| 1:A:472:LEU:HD23 | 1:F:138:ASN:HD22 | 1.83 | 0.43 |
| 1:B:24:THR:CG2 | 1:B:320:ASN:HA | 2.48 | 0.43 |
| 1:B:46:GLY:N | 1:B:65:VAL:HG21 | 2.33 | 0.43 |
| 1:C:210:PHE:CD1 | 1:C:224:ILE:HB | 2.53 | 0.43 |
| 1:C:273:ASP:OD2 | 1:C:273:ASP:N | 2.50 | 0.43 |
| 1:D:149:MET:HB2 | 1:D:150:ASP:H | 1.64 | 0.43 |
| 1:D:271:VAL:HA | 1:D:272:PRO:HD3 | 1.85 | 0.43 |
| 1:D:459:LEU:C | 1:D:461:GLN:H | 2.20 | 0.43 |
| 1:E:66:SER:OG | 1:E:67:GLY:N | 2.48 | 0.43 |
| 1:F:44:ALA:HB3 | 1:F:368:GLU:HB2 | 2.00 | 0.43 |
| 1:F:154:THR:H | 1:F:336:THR:HG23 | 1.80 | 0.43 |
| 1:G:46:GLY:HA3 | 1:G:65:VAL:HB | 2.00 | 0.43 |
| 1:G:156:LEU:HD12 | 1:G:156:LEU:O | 2.17 | 0.43 |
| 1:G:247:PHE:HD1 | 1:G:248:PHE:N | 2.16 | 0.43 |
| 1:H:306:ILE:HD12 | 1:H:306:ILE:HG23 | 1.67 | 0.43 |
| 1:I:329:LEU:HD23 | 1:I:329:LEU:HA | 1.63 | 0.43 |
| 1:I:464:LEU:CD2 | 1:I:464:LEU:O | 2.65 | 0.43 |
| 1:J:188:LEU:HD11 | 1:J:213:LEU:CD1 | 2.45 | 0.43 |
| 1:J:351:SER:O | 1:J:352:GLU:O | 2.36 | 0.43 |
| 1:J:465:GLY:O | 1:J:467:LYS:N | 2.51 | 0.43 |
| 1:K:33:ILE:HA | 1:K:33:ILE:HD13 | 1.53 | 0.43 |
| 1:L:117:ILE:HD12 | 1:M:293:PRO:HB3 | 2.00 | 0.43 |
| 1:L:163:PRO:HB3 | 1:L:330:PHE:CE1 | 2.53 | 0.43 |
| 1:L:214:GLN:OE1 | 1:L:219:GLU:HB2 | 2.17 | 0.43 |
| 1:M:344:LEU:HD13 | 1:N:213:LEU:HD12 | 2.00 | 0.43 |
| 1:M:440:PRO:C | 1:M:443:LYS:NZ | 2.72 | 0.43 |
| 1:N:27:TYR:CE2 | 1:N:390:TYR:CE2 | 3.06 | 0.43 |
| 1:N:150:ASP:O | 1:N:150:ASP:CG | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:205:PHE:HE2 | 1:O:293:PRO:O | 2.01 | 0.43 |
| 1:A:153:GLN:H | 1:A:297:GLY:HA3 | 1.83 | 0.43 |
| 1:A:223:ASP:OD1 | 1:A:223:ASP:C | 2.54 | 0.43 |
| 1:B:259:HIS:HE1 | 1:C:130:GLU:HG2 | 1.83 | 0.43 |
| 1:B:306:ILE:HG23 | 1:B:306:ILE:HD12 | 1.72 | 0.43 |
| 1:B:461:GLN:HA | 1:B:461:GLN:NE2 | 2.31 | 0.43 |
| 1:C:114:GLY:HA3 | 1:C:340:THR:OG1 | 2.18 | 0.43 |
| 1:C:291:TYR:CD1 | 1:C:291:TYR:N | 2.83 | 0.43 |
| 1:D:62:VAL:HG13 | 1:D:63:PRO:HD2 | 1.99 | 0.43 |
| 1:D:391:ILE:HG21 | 1:D:391:ILE:HD13 | 1.75 | 0.43 |
| 1:E:120:HIS:ND1 | 1:E:122:LEU:N | 2.63 | 0.43 |
| 1:F:73:PHE:N | 1:F:73:PHE:CD1 | 2.86 | 0.43 |
| 1:G:105:VAL:HG22 | 1:G:374:PHE:HD2 | 1.82 | 0.43 |
| 1:G:373:GLN:C | 1:G:374:PHE:CD1 | 2.92 | 0.43 |
| 1:H:62:VAL:HA | 1:H:63:PRO:HD3 | 1.80 | 0.43 |
| 1:H:65:VAL:O | 1:H:366:HIS:HB3 | 2.18 | 0.43 |
| 1:H:97:ARG:HA | 1:H:97:ARG:NH1 | 2.33 | 0.43 |
| 1:H:147:ILE:HA | 1:I:129:THR:O | 2.18 | 0.43 |
| 1:I:470:LEU:CD2 | 1:I:470:LEU:O | 2.67 | 0.43 |
| 1:J:247:PHE:HD1 | 1:J:248:PHE:H | 1.64 | 0.43 |
| 1:L:107:VAL:HG23 | 1:L:311:TYR:HE1 | 1.84 | 0.43 |
| 1:M:68:LEU:HD13 | 1:M:151:TYR:CD1 | 2.54 | 0.43 |
| 1:O:297:GLY:O | 1:O:298:SER:O | 2.36 | 0.43 |
| 1:A:74:ARG:HH12 | 1:A:441:LEU:HB2 | 1.83 | 0.43 |
| 1:A:120:HIS:ND1 | 1:A:122:LEU:N | 2.56 | 0.43 |
| 1:A:152:LYS:NZ | 1:A:253:GLU:OE1 | 2.49 | 0.43 |
| 1:B:80:PRO:HB3 | 1:B:100:TRP:NE1 | 2.34 | 0.43 |
| 1:B:103:VAL:HA | 1:B:313:LEU:HB2 | 2.01 | 0.43 |
| 1:B:440:PRO:O | 1:B:443:LYS:NZ | 2.52 | 0.43 |
| 1:C:149:MET:HE2 | 1:C:205:PHE:CZ | 2.54 | 0.43 |
| 1:C:150:ASP:CG | 1:D:257:VAL:HG21 | 2.39 | 0.43 |
| 1:D:117:ILE:O | 1:D:117:ILE:CG2 | 2.67 | 0.43 |
| 1:D:267:VAL:HG11 | 1:D:270:ASN:CG | 2.39 | 0.43 |
| 1:D:361:LYS:CG | 1:D:361:LYS:CE | 2.87 | 0.43 |
| 1:D:365:ARG:HH11 | 1:D:365:ARG:HG3 | 1.83 | 0.43 |
| 1:E:74:ARG:CG | 1:E:330:PHE:HE2 | 2.32 | 0.43 |
| 1:E:162:LYS:HG2 | 1:E:244:ASP:HB3 | 2.00 | 0.43 |
| 1:F:98:LEU:HD22 | 1:F:379:CYS:O | 2.18 | 0.43 |
| 1:G:46:GLY:N | 1:G:65:VAL:HB | 2.33 | 0.43 |
| 1:H:299:MET:HA | 1:I:256:PHE:HB3 | 1.99 | 0.43 |
| 1:I:179:ALA:C | 1:I:180:VAL:CG2 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:23:SER:OG | 1:K:25:ASP:HB2 | 2.18 | 0.43 |
| 1:K:113:LEU:HD21 | 1:K:305:GLN:NE2 | 2.33 | 0.43 |
| 1:K:232:PRO:HB2 | 1:K:234:TYR:CZ | 2.53 | 0.43 |
| 1:K:463:PRO:CA | 1:K:466:ARG:HH21 | 2.31 | 0.43 |
| 1:L:42:LEU:HD13 | 1:L:447:TRP:CE2 | 2.53 | 0.43 |
| 1:L:80:PRO:C | 1:L:82:LYS:N | 2.72 | 0.43 |
| 1:L:117:ILE:H | 1:L:117:ILE:HG22 | 1.43 | 0.43 |
| 1:M:279:GLY:C | 1:M:284:ALA:HB2 | 2.38 | 0.43 |
| 1:M:363:TYR:CD2 | 1:N:185:CYS:HB2 | 2.53 | 0.43 |
| 1:M:363:TYR:CG | 1:N:185:CYS:HB2 | 2.54 | 0.43 |
| 1:N:141:VAL:HG12 | 1:N:142:ASP:N | 2.33 | 0.43 |
| 1:N:154:THR:N | 1:N:336:THR:HG21 | 2.15 | 0.43 |
| 1:O:55:PRO:HG2 | 1:O:56:ASN:ND2 | 2.33 | 0.43 |
| 1:O:104:GLY:O | 1:O:374:PHE:CA | 2.63 | 0.43 |
| 1:O:220:VAL:HB | 1:O:224:ILE:HD12 | 2.01 | 0.43 |
| 1:A:42:LEU:CD1 | 1:A:73:PHE:HE2 | 2.32 | 0.43 |
| 1:A:300:VAL:H | 1:A:300:VAL:HG22 | 1.44 | 0.43 |
| 1:B:120:HIS:HB3 | 1:B:123:LEU:HB2 | 2.00 | 0.43 |
| 1:C:46:GLY:HA3 | 1:C:65:VAL:CG2 | 2.49 | 0.43 |
| 1:C:166:GLY:N | 1:C:195:ILE:HD11 | 2.33 | 0.43 |
| 1:C:373:GLN:C | 1:C:464:LEU:HD12 | 2.39 | 0.43 |
| 1:D:72:VAL:HG21 | 1:D:195:ILE:O | 2.18 | 0.43 |
| 1:D:149:MET:HA | 1:E:260:LEU:HD21 | 2.00 | 0.43 |
| 1:E:129:THR:HG21 | 1:E:291:TYR:HD2 | 1.82 | 0.43 |
| 1:E:343:SER:HB3 | 1:E:364:LEU:CD2 | 2.49 | 0.43 |
| 1:F:163:PRO:HB3 | 1:F:330:PHE:CE1 | 2.54 | 0.43 |
| 1:F:193:THR:HG23 | 1:F:230:LYS:HD2 | 2.00 | 0.43 |
| 1:F:470:LEU:O | 1:F:470:LEU:HD23 | 2.19 | 0.43 |
| 1:G:27:TYR:CE2 | 1:G:390:TYR:HE2 | 2.35 | 0.43 |
| 1:G:66:SER:OG | 1:G:68:LEU:N | 2.51 | 0.43 |
| 1:G:77:LEU:O | 1:G:327:ASN:HB3 | 2.19 | 0.43 |
| 1:H:149:MET:HE3 | 1:H:295:PRO:HD2 | 2.01 | 0.43 |
| 1:H:344:LEU:HD13 | 1:I:213:LEU:HD11 | 1.96 | 0.43 |
| 1:H:372:LEU:N | 1:H:372:LEU:HD23 | 2.32 | 0.43 |
| 1:H:398:ILE:HG22 | 1:H:402:TRP:CZ3 | 2.53 | 0.43 |
| 1:I:221:PRO:HD2 | 1:I:224:ILE:HD11 | 2.01 | 0.43 |
| 1:I:240:GLU:HG3 | 1:I:243:GLY:HA2 | 2.00 | 0.43 |
| 1:J:120:HIS:HA | 1:J:222:LEU:HD13 | 1.99 | 0.43 |
| 1:J:354:THR:O | 1:J:356:LYS:HG3 | 2.18 | 0.43 |
| 1:K:302:SER:CB | 1:L:253:GLU:H | 2.32 | 0.43 |
| 1:L:246:LEU:O | 1:L:246:LEU:HG | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:130:GLU:CB | 1:M:260:LEU:HD13 | 2.42 | 0.43 |
| 1:M:251:ARG:O | 1:M:252:ARG:HB2 | 2.17 | 0.43 |
| 1:N:68:LEU:HD23 | 1:N:201:VAL:HG21 | 2.00 | 0.43 |
| 1:N:456:SER:HB3 | 1:N:462:PHE:HE1 | 1.83 | 0.43 |
| 1:O:71:ARG:HB3 | 1:O:73:PHE:CE1 | 2.54 | 0.43 |
| 1:A:113:LEU:HA | 1:A:337:THR:O | 2.18 | 0.43 |
| 1:A:163:PRO:HA | 1:A:330:PHE:CD1 | 2.53 | 0.43 |
| 1:B:34:TYR:HA | 1:B:376:PHE:O | 2.19 | 0.43 |
| 1:B:106:GLU:HG3 | 1:B:309:LYS:O | 2.18 | 0.43 |
| 1:C:300:VAL:O | 1:C:300:VAL:CG2 | 2.54 | 0.43 |
| 1:C:342:MET:HB2 | 1:D:208:MET:HE1 | 2.01 | 0.43 |
| 1:D:260:LEU:O | 1:D:261:PHE:HD2 | 2.01 | 0.43 |
| 1:E:117:ILE:CD1 | 1:E:117:ILE:CG2 | 2.96 | 0.43 |
| 1:E:171:LYS:HG3 | 1:E:187:PRO:HD2 | 2.01 | 0.43 |
| 1:F:139:ALA:O | 1:F:140:GLY:C | 2.57 | 0.43 |
| 1:F:178:VAL:C | 1:F:180:VAL:H | 2.19 | 0.43 |
| 1:F:462:PHE:O | 1:F:466:ARG:HG3 | 2.19 | 0.43 |
| 1:G:125:LYS:HD3 | 1:G:127:ASP:N | 2.33 | 0.43 |
| 1:G:153:GLN:HA | 1:G:336:THR:OG1 | 2.18 | 0.43 |
| 1:G:280:SER:C | 1:G:284:ALA:HB2 | 2.39 | 0.43 |
| 1:H:151:TYR:HD2 | 1:H:203:THR:O | 2.02 | 0.43 |
| 1:H:397:THR:HB | 1:H:401:ASP:OD2 | 2.18 | 0.43 |
| 1:I:49:TYR:CE1 | 1:I:364:LEU:CD1 | 3.02 | 0.43 |
| 1:I:99:VAL:HG12 | 1:I:100:TRP:O | 2.18 | 0.43 |
| 1:I:158:LEU:HB2 | 1:I:332:THR:HB | 1.99 | 0.43 |
| 1:I:378:LEU:HD12 | 1:I:378:LEU:C | 2.34 | 0.43 |
| 1:J:240:GLU:HG3 | 1:J:243:GLY:N | 2.34 | 0.43 |
| 1:L:76:HIS:HB2 | 1:L:450:ASN:HA | 2.00 | 0.43 |
| 1:L:96:GLN:HA | 1:L:381:ILE:O | 2.17 | 0.43 |
| 1:L:181:GLN:O | 1:L:182:PRO:C | 2.55 | 0.43 |
| 1:L:365:ARG:HA | 1:L:365:ARG:HD3 | 1.74 | 0.43 |
| 1:M:188:LEU:HD13 | 1:M:188:LEU:HA | 1.62 | 0.43 |
| 1:M:447:TRP:CD1 | 1:M:447:TRP:C | 2.92 | 0.43 |
| 1:N:32:ASN:CB | 1:N:32:ASN:ND2 | 2.71 | 0.43 |
| 1:N:80:PRO:HG2 | 1:N:98:LEU:HB2 | 2.01 | 0.43 |
| 1:N:159:ILE:HG22 | 1:N:247:PHE:HE1 | 1.83 | 0.43 |
| 1:O:49:TYR:O | 1:O:223:ASP:HA | 2.18 | 0.43 |
| 1:O:54:LYS:CG | 1:O:56:ASN:OD1 | 2.61 | 0.43 |
| 1:O:386:ASP:OD2 | 1:O:386:ASP:N | 2.51 | 0.43 |
| 1:A:42:LEU:HA | 1:A:42:LEU:HD23 | 1.54 | 0.43 |
| 1:A:51:PRO:C | 1:A:52:ILE:HD12 | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:398:ILE:HG23 | 1:B:398:ILE:HD12 | 1.50 | 0.43 |
| 1:D:149:MET:CE | 1:D:205:PHE:CZ | 3.01 | 0.43 |
| 1:D:345:CYS:HA | 1:D:361:LYS:O | 2.18 | 0.43 |
| 1:E:201:VAL:O | 1:E:229:CYS:SG | 2.69 | 0.43 |
| 1:F:260:LEU:HD23 | 1:J:117:ILE:CD1 | 2.37 | 0.43 |
| 1:F:272:PRO:HD2 | 1:F:275:LEU:CD1 | 2.49 | 0.43 |
| 1:G:34:TYR:CD2 | 1:G:377:GLN:HB2 | 2.53 | 0.43 |
| 1:G:214:GLN:HE22 | 1:G:219:GLU:HB2 | 1.83 | 0.43 |
| 1:G:316:ALA:O | 1:G:318:GLY:N | 2.51 | 0.43 |
| 1:H:34:TYR:CE2 | 1:H:377:GLN:CG | 3.01 | 0.43 |
| 1:H:117:ILE:HD11 | 1:I:260:LEU:HD23 | 2.00 | 0.43 |
| 1:J:72:VAL:HG22 | 1:J:332:THR:HG23 | 1.99 | 0.43 |
| 1:J:74:ARG:CD | 1:J:74:ARG:HB2 | 2.47 | 0.43 |
| 1:J:188:LEU:HD13 | 1:J:188:LEU:HA | 1.55 | 0.43 |
| 1:J:329:LEU:HA | 1:J:329:LEU:HD23 | 1.27 | 0.43 |
| 1:J:359:ASN:CG | 1:J:359:ASN:O | 2.57 | 0.43 |
| 1:K:54:LYS:HG2 | 1:K:57:ASN:HB3 | 2.00 | 0.43 |
| 1:K:54:LYS:HB3 | 1:K:57:ASN:HD22 | 1.84 | 0.43 |
| 1:K:173:SER:HA | 1:K:174:PRO:HD3 | 1.55 | 0.43 |
| 1:K:183:GLY:O | 1:K:185:CYS:N | 2.51 | 0.43 |
| 1:K:262:ASN:ND2 | 1:K:288:SER:HB3 | 2.34 | 0.43 |
| 1:K:459:LEU:O | 1:K:460:ASP:C | 2.56 | 0.43 |
| 1:K:459:LEU:C | 1:K:461:GLN:N | 2.70 | 0.43 |
| 1:L:22:VAL:O | 1:L:23:SER:C | 2.56 | 0.43 |
| 1:L:75:ILE:HG12 | 1:L:374:PHE:CZ | 2.54 | 0.43 |
| 1:L:163:PRO:N | 1:L:330:PHE:HD1 | 2.16 | 0.43 |
| 1:L:184:ASP:O | 1:L:185:CYS:O | 2.36 | 0.43 |
| 1:L:348:ILE:HG13 | 1:L:348:ILE:O | 2.17 | 0.43 |
| 1:M:240:GLU:HG3 | 1:M:243:GLY:H | 1.83 | 0.43 |
| 1:N:24:THR:HG23 | 1:N:320:ASN:HA | 1.98 | 0.43 |
| 1:N:30:ARG:HD3 | 1:N:377:GLN:HE22 | 1.83 | 0.43 |
| 1:O:36:HIS:HB2 | 1:O:459:LEU:HD22 | 2.01 | 0.43 |
| 1:O:106:GLU:HG3 | 1:O:309:LYS:O | 2.18 | 0.43 |
| 1:O:125:LYS:C | 1:O:125:LYS:CD | 2.87 | 0.43 |
| 1:A:52:ILE:HG12 | 1:B:269:GLU:CD | 2.39 | 0.43 |
| 1:A:148:SER:HB3 | 1:B:291:TYR:CD2 | 2.53 | 0.43 |
| 1:A:283:THR:OG1 | 1:E:142:ASP:OD1 | 2.35 | 0.43 |
| 1:A:302:SER:N | 1:B:253:GLU:O | 2.50 | 0.43 |
| 1:A:383:LEU:HB3 | 1:A:388:MET:HG3 | 2.00 | 0.43 |
| 1:B:33:ILE:CD1 | 1:B:33:ILE:HA | 2.49 | 0.43 |
| 1:B:92:ASN:HD21 | 1:B:94:ASP:HB2 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:188:LEU:CD1 | 1:B:213:LEU:HD11 | 2.48 | 0.43 |
| 1:B:219:GLU:O | 1:B:220:VAL:CG1 | 2.66 | 0.43 |
| 1:C:35:TYR:O | 1:C:375:ILE:HA | 2.19 | 0.43 |
| 1:D:37:ALA:CB | 1:D:451:LEU:HD13 | 2.47 | 0.43 |
| 1:D:60:ILE:H | 1:D:60:ILE:HG12 | 1.51 | 0.43 |
| 1:D:224:ILE:H | 1:D:224:ILE:HG12 | 1.51 | 0.43 |
| 1:E:47:HIS:CE1 | 1:E:49:TYR:HD1 | 2.37 | 0.43 |
| 1:E:124:ASN:HD22 | 1:E:216:ASN:ND2 | 2.17 | 0.43 |
| 1:F:142:ASP:OD1 | 1:G:279:GLY:HA2 | 2.19 | 0.43 |
| 1:G:92:ASN:ND2 | 1:G:95:THR:H | 2.17 | 0.43 |
| 1:G:126:LEU:HB3 | 1:G:262:ASN:HB3 | 2.00 | 0.43 |
| 1:G:348:ILE:HG22 | 1:G:359:ASN:HA | 2.00 | 0.43 |
| 1:G:463:PRO:CG | 1:G:464:LEU:H | 2.02 | 0.43 |
| 1:I:46:GLY:HA3 | 1:I:65:VAL:HG23 | 2.00 | 0.43 |
| 1:I:149:MET:HA | 1:J:260:LEU:HD21 | 2.00 | 0.43 |
| 1:I:359:ASN:O | 1:I:359:ASN:CG | 2.56 | 0.43 |
| 1:J:54:LYS:CG | 1:J:56:ASN:OD1 | 2.63 | 0.43 |
| 1:J:149:MET:HE3 | 1:J:294:THR:HG22 | 2.01 | 0.43 |
| 1:J:156:LEU:C | 1:J:156:LEU:CD1 | 2.82 | 0.43 |
| 1:K:68:LEU:CD2 | 1:K:201:VAL:HG21 | 2.42 | 0.43 |
| 1:K:326:GLY:O | 1:K:327:ASN:CB | 2.65 | 0.43 |
| 1:L:152:LYS:CE | 1:L:152:LYS:CG | 2.80 | 0.43 |
| 1:L:185:CYS:HA | 1:L:186:PRO:HD3 | 1.51 | 0.43 |
| 1:M:24:THR:HG23 | 1:M:320:ASN:HA | 2.00 | 0.43 |
| 1:M:68:LEU:HD23 | 1:M:68:LEU:HA | 2.00 | 0.43 |
| 1:M:293:PRO:O | 1:M:293:PRO:CG | 2.66 | 0.43 |
| 1:O:92:ASN:C | 1:O:94:ASP:H | 2.22 | 0.43 |
| 1:O:180:VAL:HG13 | 1:O:184:ASP:CB | 2.37 | 0.43 |
| 1:O:220:VAL:HB | 1:O:224:ILE:CD1 | 2.48 | 0.43 |
| 1:O:262:ASN:HD22 | 1:O:263:ARG:N | 2.17 | 0.43 |
| 1:B:92:ASN:HA | 1:B:93:PRO:HD2 | 1.85 | 0.43 |
| 1:B:99:VAL:HG12 | 1:B:100:TRP:N | 2.34 | 0.43 |
| 1:B:395:ASN:ND2 | 1:B:397:THR:OG1 | 2.51 | 0.43 |
| 1:C:155:GLN:OE1 | 1:C:306:ILE:N | 2.48 | 0.43 |
| 1:C:181:GLN:O | 1:C:182:PRO:C | 2.57 | 0.43 |
| 1:D:75:ILE:HB | 1:D:329:LEU:CB | 2.48 | 0.43 |
| 1:D:175:CYS:HB3 | 1:D:177:GLN:OE1 | 2.19 | 0.43 |
| 1:E:39:THR:CG2 | 1:E:449:VAL:CG1 | 2.97 | 0.43 |
| 1:E:156:LEU:HD13 | 1:E:158:LEU:HG | 2.01 | 0.43 |
| 1:E:247:PHE:HD1 | 1:E:248:PHE:N | 2.15 | 0.43 |
| 1:E:272:PRO:HD2 | 1:E:275:LEU:HD12 | 1.98 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:148:SER:OG | 1:G:129:THR:HB | 2.18 | 0.43 |
| 1:G:356:LYS:O | 1:G:359:ASN:HB3 | 2.18 | 0.43 |
| 1:H:92:ASN:HA | 1:H:93:PRO:HD2 | 1.76 | 0.43 |
| 1:H:300:VAL:CG1 | 1:H:337:THR:HG22 | 2.48 | 0.43 |
| 1:H:446:PHE:O | 1:H:448:GLU:N | 2.52 | 0.43 |
| 1:I:41:ARG:HH22 | 1:J:192:ASN:HD21 | 1.67 | 0.43 |
| 1:I:116:GLY:N | 1:I:339:SER:OG | 2.52 | 0.43 |
| 1:I:300:VAL:HG11 | 1:I:337:THR:HA | 2.01 | 0.43 |
| 1:J:21:VAL:C | 1:J:22:VAL:HG13 | 2.39 | 0.43 |
| 1:J:24:THR:HG21 | 1:J:323:ILE:HG13 | 1.99 | 0.43 |
| 1:J:345:CYS:SG | 1:J:345:CYS:O | 2.76 | 0.43 |
| 1:L:30:ARG:HH11 | 1:L:377:GLN:HE22 | 1.66 | 0.43 |
| 1:L:73:PHE:HA | 1:L:447:TRP:HB3 | 2.01 | 0.43 |
| 1:M:320:ASN:OD1 | 1:M:320:ASN:C | 2.57 | 0.43 |
| 1:M:372:LEU:HB3 | 1:M:374:PHE:CE1 | 2.53 | 0.43 |
| 1:N:34:TYR:CE2 | 1:N:377:GLN:CB | 2.96 | 0.43 |
| 1:N:120:HIS:ND1 | 1:N:121:PRO:CD | 2.82 | 0.43 |
| 1:N:125:LYS:HG3 | 1:N:261:PHE:CD1 | 2.54 | 0.43 |
| 1:N:383:LEU:HD22 | 1:N:388:MET:CE | 2.49 | 0.43 |
| 1:N:459:LEU:C | 1:N:461:GLN:N | 2.71 | 0.43 |
| 1:A:115:VAL:N | 1:B:255:MET:CE | 2.78 | 0.43 |
| 1:A:123:LEU:HD23 | 1:A:147:ILE:HG21 | 2.00 | 0.43 |
| 1:A:149:MET:HE2 | 1:A:205:PHE:CZ | 2.54 | 0.43 |
| 1:A:173:SER:HA | 1:A:174:PRO:HD2 | 1.48 | 0.43 |
| 1:A:255:MET:SD | 1:E:114:GLY:HA2 | 2.59 | 0.43 |
| 1:A:257:VAL:H | 1:A:257:VAL:HG22 | 1.40 | 0.43 |
| 1:B:271:VAL:HA | 1:B:272:PRO:HD3 | 1.64 | 0.43 |
| 1:B:465:GLY:O | 1:B:466:ARG:C | 2.56 | 0.43 |
| 1:C:68:LEU:HD13 | 1:C:151:TYR:CD1 | 2.54 | 0.43 |
| 1:D:79:ASP:HA | 1:D:80:PRO:HD3 | 1.77 | 0.43 |
| 1:D:158:LEU:HB2 | 1:D:332:THR:OG1 | 2.19 | 0.43 |
| 1:D:461:GLN:NE2 | 1:E:21:VAL:HB | 2.33 | 0.43 |
| 1:E:54:LYS:O | 1:E:57:ASN:O | 2.36 | 0.43 |
| 1:E:120:HIS:CE1 | 1:E:122:LEU:H | 2.37 | 0.43 |
| 1:E:451:LEU:O | 1:E:454:LYS:N | 2.50 | 0.43 |
| 1:F:153:GLN:NE2 | 1:F:300:VAL:HA | 2.32 | 0.43 |
| 1:F:155:GLN:HB3 | 1:F:252:ARG:HB3 | 2.01 | 0.43 |
| 1:F:166:GLY:N | 1:F:195:ILE:HG13 | 2.33 | 0.43 |
| 1:F:256:PHE:CE2 | 1:F:296:SER:OG | 2.65 | 0.43 |
| 1:F:323:ILE:HD12 | 1:F:323:ILE:HG23 | 1.84 | 0.43 |
| 1:F:374:PHE:HB3 | 1:F:376:PHE:CE1 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:75:ILE:CG2 | 1:G:451:LEU:HD12 | 2.49 | 0.43 |
| 1:G:178:VAL:C | 1:G:180:VAL:H | 2.19 | 0.43 |
| 1:G:459:LEU:C | 1:G:461:GLN:H | 2.23 | 0.43 |
| 1:H:33:ILE:HD13 | 1:H:33:ILE:HA | 1.72 | 0.43 |
| 1:I:44:ALA:HB3 | 1:I:368:GLU:HB2 | 2.01 | 0.43 |
| 1:I:218:SER:C | 1:I:219:GLU:HG2 | 2.39 | 0.43 |
| 1:I:241:PRO:CG | 1:I:242:TYR:H | 2.28 | 0.43 |
| 1:I:390:TYR:C | 1:I:392:HIS:N | 2.70 | 0.43 |
| 1:J:124:ASN:C | 1:J:124:ASN:OD1 | 2.56 | 0.43 |
| 1:J:156:LEU:HD12 | 1:J:157:CYS:N | 2.33 | 0.43 |
| 1:K:280:SER:CA | 1:K:284:ALA:HB2 | 2.49 | 0.43 |
| 1:L:66:SER:OG | 1:L:68:LEU:N | 2.52 | 0.43 |
| 1:L:358:THR:HA | 1:M:266:THR:CG2 | 2.49 | 0.43 |
| 1:M:80:PRO:C | 1:M:82:LYS:H | 2.21 | 0.43 |
| 1:M:87:ASP:C | 1:M:88:THR:HG23 | 2.38 | 0.43 |
| 1:O:223:ASP:OD1 | 1:O:224:ILE:N | 2.52 | 0.43 |
| 1:A:33:ILE:HB | 1:A:378:LEU:HB3 | 2.01 | 0.42 |
| 1:A:139:ALA:CB | 1:A:143:ASN:HD21 | 2.31 | 0.42 |
| 1:A:286:LEU:CD1 | 1:E:122:LEU:CD2 | 2.87 | 0.42 |
| 1:A:290:ASN:N | 1:A:290:ASN:ND2 | 2.66 | 0.42 |
| 1:C:54:LYS:HZ3 | 1:C:54:LYS:CA | 2.25 | 0.42 |
| 1:D:150:ASP:OD1 | 1:E:257:VAL:HG21 | 2.18 | 0.42 |
| 1:D:348:ILE:HD12 | 1:D:348:ILE:HA | 1.71 | 0.42 |
| 1:E:36:HIS:ND1 | 1:E:36:HIS:C | 2.71 | 0.42 |
| 1:E:80:PRO:HB2 | 1:E:98:LEU:HB3 | 2.01 | 0.42 |
| 1:E:317:GLN:H | 1:E:317:GLN:HG3 | 1.50 | 0.42 |
| 1:E:384:THR:H | 1:E:387:VAL:HB | 1.84 | 0.42 |
| 1:F:105:VAL:HG22 | 1:F:374:PHE:CD2 | 2.54 | 0.42 |
| 1:F:144:ARG:HD3 | 1:J:355:TYR:CE1 | 2.53 | 0.42 |
| 1:F:259:HIS:HE1 | 1:G:130:GLU:OE1 | 2.02 | 0.42 |
| 1:G:363:TYR:HE2 | 1:H:269:GLU:HG3 | 1.84 | 0.42 |
| 1:H:81:ASN:ND2 | 1:H:402:TRP:CD1 | 2.87 | 0.42 |
| 1:H:90:PHE:HD1 | 1:H:91:TYR:HB3 | 1.84 | 0.42 |
| 1:H:126:LEU:HD23 | 1:H:262:ASN:OD1 | 2.19 | 0.42 |
| 1:H:241:PRO:HG2 | 1:H:242:TYR:H | 1.84 | 0.42 |
| 1:H:395:ASN:O | 1:H:398:ILE:HG12 | 2.18 | 0.42 |
| 1:I:85:PHE:C | 1:I:87:ASP:H | 2.22 | 0.42 |
| 1:J:43:LEU:HA | 1:J:368:GLU:O | 2.19 | 0.42 |
| 1:K:48:PRO:HB3 | 1:K:341:ASN:ND2 | 2.32 | 0.42 |
| 1:K:109:ARG:HE | 1:K:338:ARG:HD2 | 1.83 | 0.42 |
| 1:K:259:HIS:CA | 1:K:260:LEU:HD12 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:383:LEU:HD23 | 1:L:388:MET:CE | 2.49 | 0.42 |
| 1:M:156:LEU:HD12 | 1:M:157:CYS:N | 2.34 | 0.42 |
| 1:M:303:ASP:N | 1:M:303:ASP:OD1 | 2.52 | 0.42 |
| 1:N:208:MET:SD | 1:N:210:PHE:CE2 | 3.12 | 0.42 |
| 1:N:292:PHE:O | 1:N:292:PHE:CG | 2.71 | 0.42 |
| 1:A:120:HIS:CG | 1:A:222:LEU:CD1 | 3.02 | 0.42 |
| 1:A:151:TYR:OH | 1:A:221:PRO:HB2 | 2.18 | 0.42 |
| 1:B:54:LYS:HZ2 | 1:B:54:LYS:HB2 | 1.84 | 0.42 |
| 1:B:164:PRO:HG2 | 1:B:195:ILE:HB | 2.00 | 0.42 |
| 1:B:459:LEU:C | 1:B:461:GLN:N | 2.72 | 0.42 |
| 1:C:74:ARG:O | 1:C:449:VAL:HG23 | 2.19 | 0.42 |
| 1:C:147:ILE:HD13 | 1:C:261:PHE:CE1 | 2.55 | 0.42 |
| 1:C:181:GLN:OE1 | 1:C:182:PRO:O | 2.36 | 0.42 |
| 1:C:219:GLU:O | 1:C:220:VAL:HG13 | 2.18 | 0.42 |
| 1:C:333:VAL:CG1 | 1:C:334:VAL:N | 2.82 | 0.42 |
| 1:C:355:TYR:C | 1:C:355:TYR:CD2 | 2.93 | 0.42 |
| 1:D:71:ARG:HH11 | 1:D:71:ARG:HG2 | 1.84 | 0.42 |
| 1:D:159:ILE:O | 1:D:247:PHE:CD1 | 2.71 | 0.42 |
| 1:E:33:ILE:HA | 1:E:33:ILE:HD13 | 2.01 | 0.42 |
| 1:E:54:LYS:HB2 | 1:E:57:ASN:HD22 | 1.84 | 0.42 |
| 1:E:113:LEU:N | 1:E:113:LEU:HD12 | 2.34 | 0.42 |
| 1:E:216:ASN:O | 1:E:217:LYS:HB3 | 2.20 | 0.42 |
| 1:E:320:ASN:ND2 | 1:E:325:TRP:NE1 | 2.66 | 0.42 |
| 1:F:166:GLY:HA2 | 1:F:232:PRO:HA | 2.01 | 0.42 |
| 1:F:278:LYS:HB2 | 1:I:354:THR:HG22 | 2.01 | 0.42 |
| 1:G:381:ILE:O | 1:G:383:LEU:HD12 | 2.18 | 0.42 |
| 1:H:92:ASN:HD21 | 1:H:94:ASP:HB2 | 1.83 | 0.42 |
| 1:H:185:CYS:SG | 1:H:186:PRO:HD2 | 2.59 | 0.42 |
| 1:I:57:ASN:HD21 | 1:I:59:LYS:CB | 2.32 | 0.42 |
| 1:I:397:THR:O | 1:I:398:ILE:C | 2.58 | 0.42 |
| 1:J:263:ARG:HG2 | 1:J:292:PHE:HD2 | 1.84 | 0.42 |
| 1:J:300:VAL:HG22 | 1:J:300:VAL:H | 1.41 | 0.42 |
| 1:K:21:VAL:CG1 | 1:K:390:TYR:OH | 2.60 | 0.42 |
| 1:K:29:ALA:CB | 1:K:380:LYS:O | 2.66 | 0.42 |
| 1:K:33:ILE:HD12 | 1:K:33:ILE:HG23 | 1.76 | 0.42 |
| 1:K:66:SER:C | 1:K:68:LEU:H | 2.21 | 0.42 |
| 1:K:142:ASP:CG | 1:L:283:THR:HG1 | 2.18 | 0.42 |
| 1:K:155:GLN:HG3 | 1:K:307:PHE:HE1 | 1.84 | 0.42 |
| 1:K:260:LEU:HD23 | 1:O:117:ILE:HD11 | 2.00 | 0.42 |
| 1:K:391:ILE:HG21 | 1:K:391:ILE:HD13 | 1.85 | 0.42 |
| 1:L:151:TYR:CD2 | 1:L:203:THR:HB | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:224:ILE:O | 1:L:226:THR:N | 2.52 | 0.42 |
| 1:L:451:LEU:HA | 1:L:451:LEU:HD23 | 1.79 | 0.42 |
| 1:M:191:ILE:HG21 | 1:M:191:ILE:HD13 | 1.69 | 0.42 |
| 1:M:386:ASP:OD2 | 1:M:386:ASP:N | 2.52 | 0.42 |
| 1:N:228:ILE:CD1 | 1:N:228:ILE:N | 2.82 | 0.42 |
| 1:N:375:ILE:HD11 | 1:N:465:GLY:HA2 | 2.00 | 0.42 |
| 1:N:399:LEU:HA | 1:N:402:TRP:HE3 | 1.83 | 0.42 |
| 1:O:71:ARG:HH12 | 1:O:198:GLY:H | 1.68 | 0.42 |
| 1:O:266:THR:OG1 | 1:O:266:THR:O | 2.38 | 0.42 |
| 1:A:153:GLN:NE2 | 1:A:300:VAL:HG12 | 2.34 | 0.42 |
| 1:A:300:VAL:HG22 | 1:B:255:MET:O | 2.18 | 0.42 |
| 1:A:390:TYR:C | 1:A:392:HIS:H | 2.21 | 0.42 |
| 1:A:450:ASN:ND2 | 1:A:452:LYS:HD2 | 2.35 | 0.42 |
| 1:B:42:LEU:HD13 | 1:B:73:PHE:HE2 | 1.83 | 0.42 |
| 1:B:209:ASP:O | 1:B:213:LEU:HD23 | 2.20 | 0.42 |
| 1:B:241:PRO:C | 1:B:243:GLY:N | 2.72 | 0.42 |
| 1:C:153:GLN:NE2 | 1:C:300:VAL:HG12 | 2.34 | 0.42 |
| 1:C:399:LEU:O | 1:C:402:TRP:HB2 | 2.19 | 0.42 |
| 1:D:196:GLN:NE2 | 1:D:444:TYR:CD2 | 2.81 | 0.42 |
| 1:F:106:GLU:HB3 | 1:F:373:GLN:HB2 | 2.01 | 0.42 |
| 1:G:49:TYR:HE1 | 1:G:364:LEU:HD13 | 1.84 | 0.42 |
| 1:G:54:LYS:HG2 | 1:G:56:ASN:OD1 | 2.19 | 0.42 |
| 1:G:168:HIS:CE1 | 1:G:191:ILE:HB | 2.54 | 0.42 |
| 1:H:21:VAL:CG1 | 1:H:390:TYR:OH | 2.63 | 0.42 |
| 1:H:104:GLY:CA | 1:H:375:ILE:HB | 2.49 | 0.42 |
| 1:H:263:ARG:HD3 | 1:H:292:PHE:CD2 | 2.54 | 0.42 |
| 1:I:80:PRO:HG2 | 1:I:98:LEU:O | 2.19 | 0.42 |
| 1:J:52:ILE:HD12 | 1:J:52:ILE:N | 2.34 | 0.42 |
| 1:J:61:LEU:HD12 | 1:J:61:LEU:O | 2.18 | 0.42 |
| 1:K:45:VAL:CG2 | 1:L:169:TRP:CZ3 | 3.02 | 0.42 |
| 1:K:272:PRO:HB2 | 1:K:275:LEU:HG | 2.01 | 0.42 |
| 1:L:50:PHE:HB2 | 1:L:51:PRO:HD2 | 2.02 | 0.42 |
| 1:L:226:THR:HG21 | 1:M:275:LEU:HD23 | 2.00 | 0.42 |
| 1:M:299:MET:CE | 1:N:298:SER:CB | 2.98 | 0.42 |
| 1:N:80:PRO:C | 1:N:82:LYS:N | 2.71 | 0.42 |
| 1:N:124:ASN:OD1 | 1:N:264:ALA:N | 2.34 | 0.42 |
| 1:N:142:ASP:OD1 | 1:O:279:GLY:HA2 | 2.18 | 0.42 |
| 1:N:357:ASN:H | 1:O:141:VAL:HG13 | 1.85 | 0.42 |
| 1:O:156:LEU:HD22 | 1:O:234:TYR:OH | 2.19 | 0.42 |
| 1:O:169:TRP:HD1 | 1:O:207:ALA:O | 2.02 | 0.42 |
| 1:O:277:ILE:HG21 | 1:O:277:ILE:HD13 | 1.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:348:ILE:HG22 | 1:O:359:ASN:OD1 | 2.19 | 0.42 |
| 1:A:52:ILE:CD1 | 1:A:52:ILE:H | 2.27 | 0.42 |
| 1:A:119:GLY:N | 1:A:221:PRO:HB3 | 2.34 | 0.42 |
| 1:A:274:ASP:OD1 | 1:A:274:ASP:N | 2.51 | 0.42 |
| 1:A:323:ILE:HG21 | 1:A:325:TRP:CE2 | 2.54 | 0.42 |
| 1:A:395:ASN:HB3 | 1:A:398:ILE:HG12 | 2.02 | 0.42 |
| 1:B:54:LYS:CB | 1:B:54:LYS:HZ2 | 2.32 | 0.42 |
| 1:B:166:GLY:HA2 | 1:B:232:PRO:HA | 2.02 | 0.42 |
| 1:B:233:ASP:OD2 | 1:B:236:LYS:HB2 | 2.19 | 0.42 |
| 1:C:169:TRP:N | 1:C:208:MET:HA | 2.32 | 0.42 |
| 1:D:311:TYR:CD2 | 1:D:311:TYR:N | 2.82 | 0.42 |
| 1:F:76:HIS:HB2 | 1:F:450:ASN:HA | 2.01 | 0.42 |
| 1:F:356:LYS:O | 1:F:359:ASN:N | 2.50 | 0.42 |
| 1:F:373:GLN:C | 1:F:374:PHE:CD1 | 2.93 | 0.42 |
| 1:G:98:LEU:HD13 | 1:G:378:LEU:HD11 | 2.00 | 0.42 |
| 1:G:208:MET:SD | 1:G:210:PHE:HE2 | 2.42 | 0.42 |
| 1:G:220:VAL:HB | 1:G:224:ILE:HG13 | 2.00 | 0.42 |
| 1:G:248:PHE:CE2 | 1:G:311:TYR:CB | 3.02 | 0.42 |
| 1:G:361:LYS:CA | 1:H:266:THR:HG1 | 2.19 | 0.42 |
| 1:H:271:VAL:O | 1:H:272:PRO:C | 2.57 | 0.42 |
| 1:H:345:CYS:HA | 1:H:361:LYS:O | 2.19 | 0.42 |
| 1:I:40:SER:O | 1:I:41:ARG:HB2 | 2.19 | 0.42 |
| 1:I:200:MET:HB2 | 1:I:228:ILE:O | 2.20 | 0.42 |
| 1:I:306:ILE:HD12 | 1:I:306:ILE:HG23 | 1.60 | 0.42 |
| 1:J:31:THR:HG23 | 1:J:378:LEU:O | 2.19 | 0.42 |
| 1:J:42:LEU:HD22 | 1:J:447:TRP:CZ2 | 2.54 | 0.42 |
| 1:J:126:LEU:HA | 1:J:126:LEU:HD12 | 1.72 | 0.42 |
| 1:J:155:GLN:HE21 | 1:J:155:GLN:HB2 | 1.53 | 0.42 |
| 1:K:71:ARG:HB3 | 1:K:73:PHE:CE1 | 2.55 | 0.42 |
| 1:K:123:LEU:O | 1:K:125:LYS:N | 2.52 | 0.42 |
| 1:K:124:ASN:OD1 | 1:K:264:ALA:N | 2.51 | 0.42 |
| 1:L:240:GLU:CD | 1:L:241:PRO:HD2 | 2.40 | 0.42 |
| 1:L:278:LYS:HB3 | 1:O:354:THR:HG22 | 2.01 | 0.42 |
| 1:N:106:GLU:HG3 | 1:N:309:LYS:O | 2.18 | 0.42 |
| 1:N:313:LEU:CD2 | 1:N:313:LEU:HD11 | 2.48 | 0.42 |
| 1:O:365:ARG:HD3 | 1:O:365:ARG:HA | 1.65 | 0.42 |
| 1:A:71:ARG:HD3 | 1:A:197:ASP:OD1 | 2.20 | 0.42 |
| 1:A:216:ASN:ND2 | 1:A:219:GLU:OE2 | 2.52 | 0.42 |
| 1:A:237:MET:CE | 1:A:246:LEU:HD13 | 2.50 | 0.42 |
| 1:A:305:GLN:HE22 | 1:A:337:THR:HG21 | 1.84 | 0.42 |
| 1:A:342:MET:SD | 1:B:208:MET:CE | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:54:LYS:HB3 | 1:B:57:ASN:HB3 | 2.02 | 0.42 |
| 1:B:90:PHE:CD1 | 1:B:91:TYR:HB3 | 2.54 | 0.42 |
| 1:B:180:VAL:HG12 | 1:B:181:GLN:N | 2.34 | 0.42 |
| 1:B:358:THR:HA | 1:C:266:THR:HG22 | 2.01 | 0.42 |
| 1:C:78:PRO:HD2 | 1:C:455:PHE:CZ | 2.54 | 0.42 |
| 1:C:162:LYS:HA | 1:C:162:LYS:HD3 | 1.83 | 0.42 |
| 1:D:42:LEU:HA | 1:D:42:LEU:HD23 | 1.73 | 0.42 |
| 1:E:85:PHE:C | 1:E:87:ASP:H | 2.23 | 0.42 |
| 1:E:105:VAL:HG22 | 1:E:374:PHE:CE2 | 2.55 | 0.42 |
| 1:F:126:LEU:HB3 | 1:F:127:ASP:H | 1.34 | 0.42 |
| 1:F:193:THR:HG23 | 1:F:230:LYS:CD | 2.49 | 0.42 |
| 1:F:222:LEU:HA | 1:F:225:CYS:SG | 2.59 | 0.42 |
| 1:G:194:VAL:HG21 | 1:G:444:TYR:CZ | 2.55 | 0.42 |
| 1:G:345:CYS:SG | 1:H:216:ASN:N | 2.88 | 0.42 |
| 1:G:464:LEU:HD23 | 1:G:464:LEU:HA | 1.80 | 0.42 |
| 1:H:106:GLU:HG3 | 1:H:310:PRO:CA | 2.49 | 0.42 |
| 1:J:48:PRO:HB3 | 1:J:341:ASN:ND2 | 2.35 | 0.42 |
| 1:K:122:LEU:CD1 | 1:L:286:LEU:HD11 | 2.48 | 0.42 |
| 1:K:219:GLU:HB3 | 1:K:263:ARG:NH1 | 2.34 | 0.42 |
| 1:K:231:TYR:CD1 | 1:K:232:PRO:HD2 | 2.54 | 0.42 |
| 1:K:242:TYR:CE2 | 1:K:394:MET:HB2 | 2.55 | 0.42 |
| 1:L:120:HIS:ND1 | 1:L:122:LEU:N | 2.49 | 0.42 |
| 1:L:188:LEU:HA | 1:L:188:LEU:HD13 | 1.81 | 0.42 |
| 1:L:395:ASN:ND2 | 1:L:397:THR:OG1 | 2.52 | 0.42 |
| 1:M:115:VAL:HG22 | 1:N:255:MET:HE1 | 2.00 | 0.42 |
| 1:N:77:LEU:HA | 1:N:78:PRO:HD2 | 1.79 | 0.42 |
| 1:N:154:THR:H | 1:N:336:THR:HG23 | 1.81 | 0.42 |
| 1:O:36:HIS:ND1 | 1:O:36:HIS:C | 2.72 | 0.42 |
| 1:O:297:GLY:C | 1:O:298:SER:O | 2.56 | 0.42 |
| 1:O:320:ASN:ND2 | 1:O:325:TRP:NE1 | 2.66 | 0.42 |
| 1:O:356:LYS:HB2 | 1:O:359:ASN:HB3 | 2.01 | 0.42 |
| 1:A:80:PRO:HB2 | 1:A:98:LEU:HB2 | 2.02 | 0.42 |
| 1:A:167:GLU:HG2 | 1:A:231:TYR:O | 2.20 | 0.42 |
| 1:A:178:VAL:CG1 | 1:A:178:VAL:HB | 2.20 | 0.42 |
| 1:A:348:ILE:O | 1:A:348:ILE:HG13 | 2.19 | 0.42 |
| 1:B:125:LYS:HE2 | 1:B:127:ASP:O | 2.20 | 0.42 |
| 1:B:384:THR:H | 1:B:387:VAL:HB | 1.85 | 0.42 |
| 1:C:75:ILE:HB | 1:C:329:LEU:HB3 | 2.01 | 0.42 |
| 1:C:143:ASN:OD1 | 1:C:143:ASN:N | 2.52 | 0.42 |
| 1:C:358:THR:HA | 1:D:266:THR:CG2 | 2.48 | 0.42 |
| 1:D:302:SER:O | 1:D:304:ALA:N | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:90:PHE:HE1 | 1:E:98:LEU:HD11 | 1.84 | 0.42 |
| 1:E:216:ASN:OD1 | 1:E:218:SER:N | 2.53 | 0.42 |
| 1:E:223:ASP:OD1 | 1:E:224:ILE:HG12 | 2.19 | 0.42 |
| 1:F:81:ASN:OD1 | 1:F:98:LEU:N | 2.52 | 0.42 |
| 1:F:231:TYR:CD1 | 1:J:112:PRO:HB3 | 2.55 | 0.42 |
| 1:G:92:ASN:ND2 | 1:G:94:ASP:HB2 | 2.29 | 0.42 |
| 1:G:149:MET:CE | 1:G:205:PHE:HE1 | 2.31 | 0.42 |
| 1:H:96:GLN:HA | 1:H:381:ILE:O | 2.19 | 0.42 |
| 1:H:96:GLN:CA | 1:H:382:THR:HA | 2.50 | 0.42 |
| 1:I:98:LEU:HA | 1:I:379:CYS:O | 2.19 | 0.42 |
| 1:I:120:HIS:CE1 | 1:I:218:SER:HB3 | 2.55 | 0.42 |
| 1:I:472:LEU:HD22 | 1:M:138:ASN:HD22 | 1.71 | 0.42 |
| 1:K:21:VAL:CG1 | 1:K:22:VAL:N | 2.83 | 0.42 |
| 1:K:61:LEU:C | 1:K:62:VAL:HG23 | 2.39 | 0.42 |
| 1:K:150:ASP:OD1 | 1:L:257:VAL:HG21 | 2.19 | 0.42 |
| 1:L:105:VAL:HG12 | 1:L:106:GLU:N | 2.35 | 0.42 |
| 1:L:149:MET:HE2 | 1:L:205:PHE:HE1 | 1.83 | 0.42 |
| 1:L:307:PHE:CD1 | 1:L:307:PHE:N | 2.86 | 0.42 |
| 1:L:323:ILE:HG23 | 1:L:323:ILE:HD12 | 1.44 | 0.42 |
| 1:L:398:ILE:HD12 | 1:L:398:ILE:HG23 | 1.12 | 0.42 |
| 1:L:464:LEU:C | 1:L:464:LEU:HD22 | 2.39 | 0.42 |
| 1:M:54:LYS:CE | 1:M:55:PRO:HD2 | 2.48 | 0.42 |
| 1:M:137:ALA:CB | 1:M:137:ALA:HA | 2.21 | 0.42 |
| 1:M:233:ASP:O | 1:M:234:TYR:C | 2.58 | 0.42 |
| 1:M:257:VAL:H | 1:M:257:VAL:HG22 | 1.29 | 0.42 |
| 1:M:262:ASN:HD21 | 1:M:288:SER:CB | 2.32 | 0.42 |
| 1:M:395:ASN:O | 1:M:398:ILE:CG1 | 2.67 | 0.42 |
| 1:N:69:GLN:HA | 1:N:199:ASP:O | 2.19 | 0.42 |
| 1:N:155:GLN:HB3 | 1:N:252:ARG:HB3 | 2.02 | 0.42 |
| 1:O:66:SER:C | 1:O:68:LEU:H | 2.22 | 0.42 |
| 1:O:105:VAL:HG12 | 1:O:106:GLU:N | 2.33 | 0.42 |
| 1:O:120:HIS:HB2 | 1:O:221:PRO:HA | 2.00 | 0.42 |
| 1:O:149:MET:HE2 | 1:O:205:PHE:CZ | 2.54 | 0.42 |
| 1:O:325:TRP:HB3 | 1:O:398:ILE:HD11 | 2.02 | 0.42 |
| 1:A:133:SER:O | 1:A:134:ALA:HB2 | 2.20 | 0.42 |
| 1:A:139:ALA:O | 1:A:141:VAL:N | 2.53 | 0.42 |
| 1:A:149:MET:HA | 1:B:260:LEU:CD2 | 2.48 | 0.42 |
| 1:B:24:THR:O | 1:B:25:ASP:C | 2.57 | 0.42 |
| 1:B:81:ASN:ND2 | 1:B:402:TRP:HD1 | 2.15 | 0.42 |
| 1:B:141:VAL:HG12 | 1:B:142:ASP:N | 2.26 | 0.42 |
| 1:B:336:THR:O | 1:B:338:ARG:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:52:ILE:HG12 | 1:D:269:GLU:OE2 | 2.20 | 0.42 |
| 1:C:292:PHE:CD1 | 1:C:292:PHE:C | 2.93 | 0.42 |
| 1:C:342:MET:SD | 1:D:208:MET:CE | 3.07 | 0.42 |
| 1:C:356:LYS:NZ | 1:C:356:LYS:HD2 | 2.29 | 0.42 |
| 1:C:390:TYR:HB3 | 1:C:391:ILE:H | 1.69 | 0.42 |
| 1:D:240:GLU:HG3 | 1:D:243:GLY:N | 2.35 | 0.42 |
| 1:E:168:HIS:HB2 | 1:E:208:MET:HA | 2.01 | 0.42 |
| 1:F:24:THR:O | 1:F:26:GLU:N | 2.53 | 0.42 |
| 1:F:77:LEU:HA | 1:F:78:PRO:HD2 | 1.85 | 0.42 |
| 1:F:367:GLY:C | 1:F:368:GLU:HG2 | 2.40 | 0.42 |
| 1:G:196:GLN:CA | 1:G:199:ASP:OD2 | 2.67 | 0.42 |
| 1:G:317:GLN:NE2 | 1:G:317:GLN:C | 2.73 | 0.42 |
| 1:G:375:ILE:CG1 | 1:G:464:LEU:HD13 | 2.46 | 0.42 |
| 1:H:77:LEU:HD21 | 1:H:376:PHE:CZ | 2.53 | 0.42 |
| 1:H:121:PRO:HG3 | 1:I:289:SER:HB2 | 2.02 | 0.42 |
| 1:H:348:ILE:HD12 | 1:I:182:PRO:O | 2.19 | 0.42 |
| 1:H:365:ARG:HH11 | 1:H:365:ARG:HG3 | 1.84 | 0.42 |
| 1:I:219:GLU:CA | 1:I:263:ARG:HH12 | 2.31 | 0.42 |
| 1:I:240:GLU:HG3 | 1:I:243:GLY:CA | 2.50 | 0.42 |
| 1:J:155:GLN:OE1 | 1:J:305:GLN:HA | 2.20 | 0.42 |
| 1:J:185:CYS:SG | 1:J:186:PRO:HD2 | 2.59 | 0.42 |
| 1:K:36:HIS:ND1 | 1:K:37:ALA:N | 2.68 | 0.42 |
| 1:K:110:GLY:O | 1:K:111:GLN:NE2 | 2.53 | 0.42 |
| 1:K:121:PRO:HG2 | 1:L:289:SER:HB2 | 2.01 | 0.42 |
| 1:K:440:PRO:O | 1:K:443:LYS:NZ | 2.53 | 0.42 |
| 1:L:120:HIS:HE2 | 1:L:218:SER:HB3 | 1.84 | 0.42 |
| 1:M:57:ASN:CG | 1:M:58:ASN:N | 2.73 | 0.42 |
| 1:N:68:LEU:CB | 1:N:201:VAL:CG2 | 2.96 | 0.42 |
| 1:N:150:ASP:O | 1:N:296:SER:HA | 2.18 | 0.42 |
| 1:N:262:ASN:ND2 | 1:N:288:SER:CB | 2.67 | 0.42 |
| 1:O:35:TYR:O | 1:O:375:ILE:HA | 2.20 | 0.42 |
| 1:O:43:LEU:HD12 | 1:O:369:GLU:HA | 2.02 | 0.42 |
| 1:O:366:HIS:CD2 | 1:O:367:GLY:N | 2.87 | 0.42 |
| 1:A:149:MET:CE | 1:A:205:PHE:CZ | 3.03 | 0.42 |
| 1:A:381:ILE:CG2 | 1:A:381:ILE:C | 2.88 | 0.42 |
| 1:B:42:LEU:HD22 | 1:B:447:TRP:HZ2 | 1.83 | 0.42 |
| 1:B:440:PRO:HA | 1:B:443:LYS:HZ1 | 1.84 | 0.42 |
| 1:C:163:PRO:HA | 1:C:164:PRO:HD2 | 1.80 | 0.42 |
| 1:C:185:CYS:HA | 1:C:186:PRO:HD3 | 1.71 | 0.42 |
| 1:C:255:MET:HG3 | 1:C:295:PRO:HB2 | 2.01 | 0.42 |
| 1:C:317:GLN:C | 1:C:317:GLN:HE21 | 2.23 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:373:GLN:HB3 | 1:C:464:LEU:HG | 2.02 | 0.42 |
| 1:D:164:PRO:HG3 | 1:D:332:THR:HG21 | 2.02 | 0.42 |
| 1:D:358:THR:HG22 | 1:E:266:THR:HG22 | 2.01 | 0.42 |
| 1:E:39:THR:CG2 | 1:E:449:VAL:HG11 | 2.50 | 0.42 |
| 1:E:165:ILE:CD1 | 1:E:165:ILE:CB | 2.85 | 0.42 |
| 1:F:46:GLY:O | 1:F:365:ARG:HA | 2.20 | 0.42 |
| 1:F:99:VAL:HG11 | 1:F:323:ILE:CG2 | 2.41 | 0.42 |
| 1:G:42:LEU:CD1 | 1:G:73:PHE:HE2 | 2.33 | 0.42 |
| 1:G:66:SER:HA | 1:G:366:HIS:ND1 | 2.34 | 0.42 |
| 1:G:85:PHE:CE1 | 1:G:98:LEU:CD1 | 3.02 | 0.42 |
| 1:H:35:TYR:O | 1:H:376:PHE:N | 2.39 | 0.42 |
| 1:H:74:ARG:NH2 | 1:H:441:LEU:HD12 | 2.34 | 0.42 |
| 1:H:440:PRO:C | 1:H:443:LYS:NZ | 2.73 | 0.42 |
| 1:I:147:ILE:HA | 1:J:129:THR:O | 2.20 | 0.42 |
| 1:I:329:LEU:HD13 | 1:I:374:PHE:HE2 | 1.82 | 0.42 |
| 1:I:338:ARG:HH11 | 1:I:338:ARG:HG3 | 1.85 | 0.42 |
| 1:J:276:TYR:CD1 | 1:J:277:ILE:N | 2.87 | 0.42 |
| 1:L:213:LEU:HA | 1:L:213:LEU:HD13 | 1.78 | 0.42 |
| 1:M:53:LYS:HD3 | 1:M:58:ASN:HA | 2.02 | 0.42 |
| 1:M:54:LYS:HG3 | 1:M:55:PRO:CD | 2.50 | 0.42 |
| 1:M:107:VAL:O | 1:M:307:PHE:HB3 | 2.20 | 0.42 |
| 1:M:149:MET:CE | 1:M:205:PHE:CE1 | 3.02 | 0.42 |
| 1:N:61:LEU:CD1 | 1:N:61:LEU:O | 2.63 | 0.42 |
| 1:N:365:ARG:NH1 | 1:N:365:ARG:HG2 | 2.35 | 0.42 |
| 1:O:188:LEU:HD13 | 1:O:188:LEU:HA | 1.86 | 0.42 |
| 1:O:398:ILE:CD1 | 1:O:398:ILE:CG2 | 2.97 | 0.42 |
| 1:A:96:GLN:HA | 1:A:382:THR:HA | 2.00 | 0.42 |
| 1:A:185:CYS:HB2 | 1:E:363:TYR:CE2 | 2.55 | 0.42 |
| 1:B:464:LEU:O | 1:B:464:LEU:HD23 | 2.20 | 0.42 |
| 1:C:45:VAL:HG21 | 1:D:169:TRP:CH2 | 2.54 | 0.42 |
| 1:C:274:ASP:OD1 | 1:C:274:ASP:N | 2.52 | 0.42 |
| 1:C:276:TYR:C | 1:C:277:ILE:CG1 | 2.88 | 0.42 |
| 1:C:472:LEU:CD2 | 1:H:138:ASN:HD22 | 2.32 | 0.42 |
| 1:F:122:LEU:HD11 | 1:G:286:LEU:CD1 | 2.48 | 0.42 |
| 1:F:125:LYS:HE3 | 1:F:261:PHE:CD2 | 2.54 | 0.42 |
| 1:F:375:ILE:HG12 | 1:F:464:LEU:CD1 | 2.44 | 0.42 |
| 1:G:57:ASN:HD21 | 1:G:59:LYS:CB | 2.32 | 0.42 |
| 1:G:113:LEU:HD13 | 1:H:253:GLU:CD | 2.39 | 0.42 |
| 1:G:210:PHE:HE1 | 1:G:224:ILE:HD12 | 1.85 | 0.42 |
| 1:I:180:VAL:HG13 | 1:I:184:ASP:CB | 2.50 | 0.42 |
| 1:I:281:GLY:N | 1:I:284:ALA:CB | 2.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:105:VAL:HG22 | 1:J:374:PHE:CD2 | 2.55 | 0.42 |
| 1:J:220:VAL:O | 1:J:221:PRO:O | 2.37 | 0.42 |
| 1:K:186:PRO:HD2 | 1:O:344:LEU:HD12 | 2.01 | 0.42 |
| 1:K:235:ILE:HD11 | 1:O:109:ARG:O | 2.20 | 0.42 |
| 1:L:43:LEU:HD12 | 1:L:43:LEU:HA | 1.62 | 0.42 |
| 1:L:183:GLY:O | 1:L:184:ASP:C | 2.57 | 0.42 |
| 1:L:471:GLN:CD | 1:L:471:GLN:C | 2.78 | 0.42 |
| 1:M:143:ASN:O | 1:M:144:ARG:C | 2.59 | 0.42 |
| 1:N:80:PRO:C | 1:N:82:LYS:H | 2.22 | 0.42 |
| 1:N:123:LEU:O | 1:N:125:LYS:N | 2.53 | 0.42 |
| 1:O:21:VAL:HG13 | 1:O:390:TYR:OH | 2.20 | 0.42 |
| 1:A:85:PHE:CZ | 1:A:378:LEU:HD22 | 2.55 | 0.42 |
| 1:A:222:LEU:HD12 | 1:A:222:LEU:HA | 1.77 | 0.42 |
| 1:A:271:VAL:CG2 | 1:E:222:LEU:HD21 | 2.50 | 0.42 |
| 1:B:117:ILE:HD11 | 1:C:260:LEU:CD2 | 2.41 | 0.42 |
| 1:B:117:ILE:H | 1:B:117:ILE:HG22 | 1.57 | 0.42 |
| 1:C:99:VAL:HG12 | 1:C:100:TRP:O | 2.20 | 0.42 |
| 1:C:325:TRP:CE2 | 1:C:394:MET:HE1 | 2.55 | 0.42 |
| 1:D:290:ASN:N | 1:D:290:ASN:HD22 | 2.18 | 0.42 |
| 1:D:344:LEU:CD1 | 1:E:213:LEU:HD13 | 2.49 | 0.42 |
| 1:E:117:ILE:CD1 | 1:E:117:ILE:HG21 | 2.50 | 0.42 |
| 1:G:30:ARG:HG2 | 1:G:377:GLN:NE2 | 2.35 | 0.42 |
| 1:G:250:LEU:HD12 | 1:G:250:LEU:C | 2.40 | 0.42 |
| 1:H:31:THR:HG23 | 1:H:31:THR:H | 1.59 | 0.42 |
| 1:H:54:LYS:HB2 | 1:H:57:ASN:HD22 | 1.85 | 0.42 |
| 1:H:73:PHE:CD1 | 1:H:73:PHE:N | 2.86 | 0.42 |
| 1:H:98:LEU:HD13 | 1:H:378:LEU:HD11 | 2.02 | 0.42 |
| 1:H:280:SER:CA | 1:H:284:ALA:HB2 | 2.50 | 0.42 |
| 1:I:112:PRO:HB2 | 1:J:202:ASP:OD2 | 2.20 | 0.42 |
| 1:I:365:ARG:NH2 | 1:J:269:GLU:OE1 | 2.47 | 0.42 |
| 1:I:392:HIS:HB2 | 1:I:399:LEU:HD11 | 2.02 | 0.42 |
| 1:I:398:ILE:HG22 | 1:I:402:TRP:CH2 | 2.55 | 0.42 |
| 1:J:34:TYR:CE2 | 1:J:377:GLN:HG3 | 2.55 | 0.42 |
| 1:K:21:VAL:C | 1:K:22:VAL:CG1 | 2.88 | 0.42 |
| 1:K:208:MET:SD | 1:O:342:MET:HB2 | 2.60 | 0.42 |
| 1:K:323:ILE:CG2 | 1:K:325:TRP:CZ3 | 3.03 | 0.42 |
| 1:L:163:PRO:N | 1:L:330:PHE:CD1 | 2.87 | 0.42 |
| 1:L:208:MET:CG | 1:L:210:PHE:CE2 | 3.02 | 0.42 |
| 1:M:320:ASN:ND2 | 1:M:325:TRP:NE1 | 2.68 | 0.42 |
| 1:N:39:THR:H | 1:N:39:THR:HG23 | 1.37 | 0.42 |
| 1:N:148:SER:HG | 1:O:129:THR:HB | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:219:GLU:HB3 | 1:N:263:ARG:NH2 | 2.35 | 0.42 |
| 1:O:59:LYS:HE2 | 1:O:59:LYS:HB3 | 1.89 | 0.42 |
| 1:O:68:LEU:HD23 | 1:O:201:VAL:HG21 | 2.01 | 0.42 |
| 1:O:234:TYR:O | 1:O:235:ILE:C | 2.58 | 0.42 |
| 1:A:120:HIS:HA | 1:A:121:PRO:HD3 | 1.92 | 0.41 |
| 1:B:54:LYS:NZ | 1:B:54:LYS:CA | 2.81 | 0.41 |
| 1:B:71:ARG:HA | 1:B:71:ARG:HD3 | 1.60 | 0.41 |
| 1:B:81:ASN:HD21 | 1:B:402:TRP:HE1 | 1.67 | 0.41 |
| 1:B:348:ILE:HD11 | 1:C:181:GLN:HE22 | 1.85 | 0.41 |
| 1:C:87:ASP:O | 1:C:88:THR:CG2 | 2.68 | 0.41 |
| 1:C:326:GLY:O | 1:C:327:ASN:CB | 2.68 | 0.41 |
| 1:C:459:LEU:C | 1:C:461:GLN:N | 2.68 | 0.41 |
| 1:D:240:GLU:HG3 | 1:D:243:GLY:H | 1.84 | 0.41 |
| 1:E:27:TYR:CE2 | 1:E:390:TYR:HE2 | 2.37 | 0.41 |
| 1:E:280:SER:CA | 1:E:284:ALA:HB2 | 2.50 | 0.41 |
| 1:E:305:GLN:C | 1:E:306:ILE:HD13 | 2.41 | 0.41 |
| 1:F:35:TYR:CD1 | 1:F:100:TRP:HH2 | 2.38 | 0.41 |
| 1:F:47:HIS:HA | 1:F:48:PRO:HD2 | 1.54 | 0.41 |
| 1:G:107:VAL:O | 1:G:307:PHE:HB3 | 2.19 | 0.41 |
| 1:H:117:ILE:HD11 | 1:I:260:LEU:CB | 2.45 | 0.41 |
| 1:H:122:LEU:HD13 | 1:H:144:ARG:HH22 | 1.82 | 0.41 |
| 1:H:399:LEU:H | 1:H:399:LEU:HG | 1.68 | 0.41 |
| 1:I:107:VAL:HG13 | 1:I:372:LEU:HD21 | 2.02 | 0.41 |
| 1:I:126:LEU:N | 1:I:262:ASN:O | 2.52 | 0.41 |
| 1:I:273:ASP:N | 1:I:273:ASP:OD2 | 2.52 | 0.41 |
| 1:J:73:PHE:HD1 | 1:J:73:PHE:H | 1.64 | 0.41 |
| 1:J:124:ASN:OD1 | 1:J:264:ALA:N | 2.52 | 0.41 |
| 1:J:355:TYR:CD2 | 1:J:355:TYR:C | 2.93 | 0.41 |
| 1:J:443:LYS:HD3 | 1:J:443:LYS:H | 1.85 | 0.41 |
| 1:L:277:ILE:HD13 | 1:L:277:ILE:HG21 | 1.86 | 0.41 |
| 1:M:121:PRO:O | 1:M:122:LEU:HD23 | 2.19 | 0.41 |
| 1:M:169:TRP:HD1 | 1:M:207:ALA:O | 2.02 | 0.41 |
| 1:N:47:HIS:HA | 1:N:48:PRO:HD2 | 1.42 | 0.41 |
| 1:N:217:LYS:CD | 1:O:274:ASP:O | 2.44 | 0.41 |
| 1:O:43:LEU:HD12 | 1:O:43:LEU:HA | 1.95 | 0.41 |
| 1:O:46:GLY:N | 1:O:65:VAL:HG21 | 2.35 | 0.41 |
| 1:A:100:TRP:CZ2 | 1:A:455:PHE:CE2 | 3.08 | 0.41 |
| 1:A:139:ALA:C | 1:A:141:VAL:H | 2.24 | 0.41 |
| 1:A:157:CYS:HB2 | 1:A:307:PHE:HE2 | 1.84 | 0.41 |
| 1:A:184:ASP:O | 1:A:185:CYS:C | 2.56 | 0.41 |
| 1:A:256:PHE:CE1 | 1:A:257:VAL:O | 2.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:306:ILE:HD12 | 1:A:306:ILE:HG23 | 1.30 | 0.41 |
| 1:B:21:VAL:C | 1:B:22:VAL:HG13 | 2.39 | 0.41 |
| 1:B:139:ALA:HB1 | 1:B:143:ASN:OD1 | 2.20 | 0.41 |
| 1:C:35:TYR:CE2 | 1:C:457:ALA:CB | 2.94 | 0.41 |
| 1:C:50:PHE:CB | 1:C:51:PRO:HD2 | 2.50 | 0.41 |
| 1:C:115:VAL:H | 1:D:255:MET:CE | 2.33 | 0.41 |
| 1:C:372:LEU:HD23 | 1:C:372:LEU:HA | 1.72 | 0.41 |
| 1:D:383:LEU:HD23 | 1:D:388:MET:CE | 2.49 | 0.41 |
| 1:D:385:ALA:O | 1:D:389:THR:HG23 | 2.19 | 0.41 |
| 1:G:113:LEU:HA | 1:G:337:THR:O | 2.21 | 0.41 |
| 1:G:325:TRP:HB3 | 1:G:398:ILE:HD11 | 2.02 | 0.41 |
| 1:G:386:ASP:OD2 | 1:G:386:ASP:N | 2.52 | 0.41 |
| 1:G:438:GLU:HG2 | 1:G:442:LYS:NZ | 2.36 | 0.41 |
| 1:I:42:LEU:HD23 | 1:I:42:LEU:HA | 1.74 | 0.41 |
| 1:I:348:ILE:HD12 | 1:I:348:ILE:HA | 1.90 | 0.41 |
| 1:J:42:LEU:HB3 | 1:J:447:TRP:CH2 | 2.55 | 0.41 |
| 1:J:317:GLN:HE21 | 1:J:317:GLN:HB2 | 1.70 | 0.41 |
| 1:K:158:LEU:HD23 | 1:K:249:TYR:HB2 | 2.02 | 0.41 |
| 1:L:165:ILE:O | 1:L:165:ILE:HG22 | 2.19 | 0.41 |
| 1:L:276:TYR:HB2 | 1:L:277:ILE:H | 1.54 | 0.41 |
| 1:M:24:THR:CG2 | 1:M:320:ASN:HA | 2.50 | 0.41 |
| 1:M:75:ILE:HG12 | 1:M:374:PHE:CZ | 2.55 | 0.41 |
| 1:M:126:LEU:HD13 | 1:M:264:ALA:CB | 2.49 | 0.41 |
| 1:M:173:SER:HA | 1:M:174:PRO:HD3 | 1.57 | 0.41 |
| 1:M:302:SER:C | 1:M:304:ALA:N | 2.67 | 0.41 |
| 1:M:363:TYR:CD1 | 1:N:185:CYS:HB2 | 2.56 | 0.41 |
| 1:N:92:ASN:C | 1:N:94:ASP:N | 2.73 | 0.41 |
| 1:O:71:ARG:HA | 1:O:71:ARG:NH1 | 2.29 | 0.41 |
| 1:O:73:PHE:O | 1:O:330:PHE:HD2 | 2.03 | 0.41 |
| 1:O:156:LEU:HD12 | 1:O:156:LEU:O | 2.20 | 0.41 |
| 1:A:67:GLY:C | 1:A:68:LEU:HG | 2.41 | 0.41 |
| 1:A:92:ASN:N | 1:A:96:GLN:OE1 | 2.44 | 0.41 |
| 1:A:153:GLN:N | 1:A:297:GLY:HA3 | 2.34 | 0.41 |
| 1:A:279:GLY:HA2 | 1:E:142:ASP:OD1 | 2.20 | 0.41 |
| 1:B:166:GLY:CA | 1:B:195:ILE:HD11 | 2.50 | 0.41 |
| 1:D:237:MET:HB3 | 1:D:246:LEU:HD21 | 2.03 | 0.41 |
| 1:D:259:HIS:C | 1:D:260:LEU:HD12 | 2.41 | 0.41 |
| 1:D:451:LEU:HA | 1:D:454:LYS:CG | 2.51 | 0.41 |
| 1:F:70:TYR:HE1 | 1:F:201:VAL:HA | 1.85 | 0.41 |
| 1:F:151:TYR:OH | 1:F:221:PRO:CB | 2.68 | 0.41 |
| 1:F:357:ASN:H | 1:G:141:VAL:HG13 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:468:PHE:O | 1:F:468:PHE:CD1 | 2.74 | 0.41 |
| 1:G:237:MET:CB | 1:G:246:LEU:HD22 | 2.46 | 0.41 |
| 1:H:106:GLU:HG3 | 1:H:310:PRO:HA | 2.01 | 0.41 |
| 1:H:202:ASP:OD1 | 1:H:206:GLY:O | 2.38 | 0.41 |
| 1:I:158:LEU:CD2 | 1:I:249:TYR:HB2 | 2.51 | 0.41 |
| 1:I:262:ASN:HD22 | 1:I:262:ASN:C | 2.20 | 0.41 |
| 1:J:124:ASN:OD1 | 1:J:124:ASN:O | 2.39 | 0.41 |
| 1:K:164:PRO:HG3 | 1:K:332:THR:HG21 | 2.00 | 0.41 |
| 1:K:246:LEU:O | 1:K:246:LEU:CD2 | 2.56 | 0.41 |
| 1:L:101:ALA:O | 1:L:376:PHE:HA | 2.20 | 0.41 |
| 1:L:173:SER:HA | 1:L:174:PRO:HD2 | 1.53 | 0.41 |
| 1:L:381:ILE:HD13 | 1:L:381:ILE:HG21 | 1.61 | 0.41 |
| 1:M:57:ASN:HD21 | 1:M:59:LYS:HB3 | 1.85 | 0.41 |
| 1:M:70:TYR:OH | 1:M:230:LYS:O | 2.16 | 0.41 |
| 1:M:167:GLU:HB2 | 1:M:190:LEU:HD11 | 2.01 | 0.41 |
| 1:M:306:ILE:HG23 | 1:M:306:ILE:HD12 | 1.74 | 0.41 |
| 1:N:120:HIS:ND1 | 1:N:121:PRO:HD2 | 2.35 | 0.41 |
| 1:N:159:ILE:HG22 | 1:N:247:PHE:CE1 | 2.55 | 0.41 |
| 1:O:120:HIS:CE1 | 1:O:122:LEU:H | 2.35 | 0.41 |
| 1:O:126:LEU:N | 1:O:262:ASN:O | 2.51 | 0.41 |
| 1:A:92:ASN:HA | 1:A:93:PRO:HD2 | 1.79 | 0.41 |
| 1:C:42:LEU:HD22 | 1:C:447:TRP:HZ2 | 1.85 | 0.41 |
| 1:C:97:ARG:HG3 | 1:C:383:LEU:HD11 | 2.02 | 0.41 |
| 1:C:154:THR:H | 1:C:336:THR:CG2 | 2.33 | 0.41 |
| 1:D:50:PHE:HB2 | 1:D:51:PRO:HD2 | 2.02 | 0.41 |
| 1:D:70:TYR:CZ | 1:D:230:LYS:O | 2.73 | 0.41 |
| 1:D:85:PHE:CZ | 1:D:378:LEU:HD22 | 2.56 | 0.41 |
| 1:D:109:ARG:N | 1:D:308:ASN:OD1 | 2.47 | 0.41 |
| 1:D:281:GLY:O | 1:D:284:ALA:HB3 | 2.20 | 0.41 |
| 1:E:81:ASN:O | 1:E:82:LYS:HG3 | 2.21 | 0.41 |
| 1:E:228:ILE:N | 1:E:228:ILE:HD12 | 2.36 | 0.41 |
| 1:E:465:GLY:O | 1:E:467:LYS:N | 2.54 | 0.41 |
| 1:F:116:GLY:HA3 | 1:F:339:SER:HB2 | 2.02 | 0.41 |
| 1:F:319:HIS:CE1 | 1:J:466:ARG:HD3 | 2.55 | 0.41 |
| 1:G:111:GLN:HB2 | 1:G:338:ARG:HD3 | 2.02 | 0.41 |
| 1:G:117:ILE:HG13 | 1:G:149:MET:O | 2.19 | 0.41 |
| 1:G:373:GLN:O | 1:G:374:PHE:CG | 2.73 | 0.41 |
| 1:H:39:THR:H | 1:H:39:THR:HG23 | 1.61 | 0.41 |
| 1:H:80:PRO:HG2 | 1:H:98:LEU:O | 2.20 | 0.41 |
| 1:I:52:ILE:HB | 1:I:62:VAL:HB | 2.03 | 0.41 |
| 1:I:109:ARG:N | 1:I:308:ASN:OD1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:188:LEU:HD13 | 1:I:188:LEU:HA | 1.76 | 0.41 |
| 1:I:194:VAL:H | 1:I:194:VAL:HG23 | 1.67 | 0.41 |
| 1:J:105:VAL:HG11 | 1:J:159:ILE:HD11 | 2.02 | 0.41 |
| 1:J:279:GLY:HA3 | 1:J:283:THR:O | 2.21 | 0.41 |
| 1:L:52:ILE:O | 1:L:52:ILE:HG22 | 2.21 | 0.41 |
| 1:L:96:GLN:CA | 1:L:382:THR:HA | 2.49 | 0.41 |
| 1:L:323:ILE:O | 1:L:325:TRP:N | 2.51 | 0.41 |
| 1:M:50:PHE:CB | 1:M:51:PRO:HD2 | 2.48 | 0.41 |
| 1:M:463:PRO:HB3 | 1:M:466:ARG:NH2 | 2.30 | 0.41 |
| 1:M:465:GLY:O | 1:M:466:ARG:C | 2.58 | 0.41 |
| 1:N:70:TYR:CE1 | 1:N:201:VAL:HA | 2.55 | 0.41 |
| 1:O:120:HIS:ND1 | 1:O:121:PRO:N | 2.69 | 0.41 |
| 1:O:457:ALA:O | 1:O:459:LEU:CD2 | 2.68 | 0.41 |
| 1:O:459:LEU:N | 1:O:459:LEU:CD2 | 2.64 | 0.41 |
| 1:A:130:GLU:HG2 | 1:E:259:HIS:CE1 | 2.56 | 0.41 |
| 1:B:77:LEU:HA | 1:B:78:PRO:HD2 | 1.81 | 0.41 |
| 1:B:117:ILE:O | 1:B:117:ILE:CG2 | 2.68 | 0.41 |
| 1:B:259:HIS:CE1 | 1:C:130:GLU:CG | 3.01 | 0.41 |
| 1:B:320:ASN:ND2 | 1:B:323:ILE:HB | 2.35 | 0.41 |
| 1:B:329:LEU:HD23 | 1:B:329:LEU:HA | 1.85 | 0.41 |
| 1:C:31:THR:HG23 | 1:C:379:CYS:HA | 2.02 | 0.41 |
| 1:C:49:TYR:HB2 | 1:C:50:PHE:CD2 | 2.54 | 0.41 |
| 1:C:271:VAL:HA | 1:C:272:PRO:HD3 | 1.81 | 0.41 |
| 1:C:364:LEU:O | 1:C:365:ARG:HD3 | 2.20 | 0.41 |
| 1:D:22:VAL:N | 1:D:390:TYR:OH | 2.47 | 0.41 |
| 1:D:118:SER:HB2 | 1:D:151:TYR:CE1 | 2.55 | 0.41 |
| 1:D:256:PHE:O | 1:D:295:PRO:HA | 2.21 | 0.41 |
| 1:E:54:LYS:HG3 | 1:E:55:PRO:CD | 2.50 | 0.41 |
| 1:E:375:ILE:HG21 | 1:E:468:PHE:CD2 | 2.56 | 0.41 |
| 1:F:280:SER:O | 1:F:280:SER:OG | 2.38 | 0.41 |
| 1:F:300:VAL:HG23 | 1:F:300:VAL:O | 2.19 | 0.41 |
| 1:G:34:TYR:HA | 1:G:376:PHE:O | 2.20 | 0.41 |
| 1:G:69:GLN:HB3 | 1:G:198:GLY:HA2 | 2.02 | 0.41 |
| 1:G:74:ARG:HA | 1:G:330:PHE:CD2 | 2.55 | 0.41 |
| 1:G:201:VAL:CG2 | 1:G:201:VAL:C | 2.89 | 0.41 |
| 1:G:323:ILE:C | 1:G:325:TRP:H | 2.24 | 0.41 |
| 1:G:451:LEU:HA | 1:G:454:LYS:HG2 | 2.01 | 0.41 |
| 1:H:110:GLY:O | 1:H:111:GLN:NE2 | 2.50 | 0.41 |
| 1:J:80:PRO:HB2 | 1:J:98:LEU:HB3 | 2.02 | 0.41 |
| 1:J:222:LEU:HA | 1:J:222:LEU:HD12 | 1.85 | 0.41 |
| 1:K:257:VAL:HG21 | 1:O:150:ASP:CB | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:147:ILE:HG23 | 1:N:129:THR:O | 2.20 | 0.41 |
| 1:N:24:THR:O | 1:N:25:ASP:C | 2.58 | 0.41 |
| 1:N:119:GLY:O | 1:N:221:PRO:HB3 | 2.21 | 0.41 |
| 1:N:397:THR:HB | 1:N:401:ASP:OD2 | 2.20 | 0.41 |
| 1:O:39:THR:CG2 | 1:O:449:VAL:HG11 | 2.50 | 0.41 |
| 1:O:271:VAL:HG13 | 1:O:275:LEU:HD12 | 2.01 | 0.41 |
| 1:A:120:HIS:ND1 | 1:A:121:PRO:N | 2.69 | 0.41 |
| 1:A:255:MET:CG | 1:A:256:PHE:H | 2.15 | 0.41 |
| 1:A:372:LEU:HD23 | 1:A:372:LEU:HA | 1.75 | 0.41 |
| 1:B:151:TYR:OH | 1:B:221:PRO:CB | 2.69 | 0.41 |
| 1:C:224:ILE:HG21 | 1:C:224:ILE:HD13 | 1.76 | 0.41 |
| 1:D:125:LYS:HZ3 | 1:D:127:ASP:HA | 1.85 | 0.41 |
| 1:D:162:LYS:O | 1:D:330:PHE:HD1 | 2.04 | 0.41 |
| 1:D:259:HIS:HB3 | 1:D:260:LEU:H | 1.67 | 0.41 |
| 1:E:158:LEU:HD23 | 1:E:249:TYR:HB2 | 2.01 | 0.41 |
| 1:F:68:LEU:HD22 | 1:F:203:THR:HG22 | 2.02 | 0.41 |
| 1:F:96:GLN:NE2 | 1:F:382:THR:HG22 | 2.36 | 0.41 |
| 1:F:267:VAL:H | 1:F:267:VAL:HG23 | 1.47 | 0.41 |
| 1:G:121:PRO:HG3 | 1:H:289:SER:CB | 2.51 | 0.41 |
| 1:G:201:VAL:HG23 | 1:G:202:ASP:O | 2.21 | 0.41 |
| 1:G:219:GLU:CB | 1:G:263:ARG:NH2 | 2.83 | 0.41 |
| 1:G:248:PHE:CE2 | 1:G:311:TYR:CG | 3.08 | 0.41 |
| 1:G:391:ILE:HD12 | 1:G:402:TRP:CZ3 | 2.55 | 0.41 |
| 1:I:106:GLU:HB3 | 1:I:373:GLN:HG3 | 2.02 | 0.41 |
| 1:I:175:CYS:C | 1:I:177:GLN:H | 2.23 | 0.41 |
| 1:I:185:CYS:HA | 1:I:186:PRO:HD3 | 1.88 | 0.41 |
| 1:I:193:THR:CG2 | 1:I:193:THR:HB | 2.19 | 0.41 |
| 1:I:369:GLU:OE1 | 1:J:190:LEU:CD2 | 2.67 | 0.41 |
| 1:J:34:TYR:OH | 1:J:377:GLN:OE1 | 2.08 | 0.41 |
| 1:J:191:ILE:HG21 | 1:J:191:ILE:HD13 | 1.85 | 0.41 |
| 1:K:46:GLY:N | 1:K:65:VAL:HB | 2.35 | 0.41 |
| 1:K:96:GLN:HE21 | 1:K:382:THR:HG23 | 1.85 | 0.41 |
| 1:K:258:ARG:HG3 | 1:K:259:HIS:ND1 | 2.36 | 0.41 |
| 1:L:137:ALA:O | 1:L:138:ASN:C | 2.59 | 0.41 |
| 1:L:391:ILE:HD13 | 1:L:402:TRP:HH2 | 1.86 | 0.41 |
| 1:M:42:LEU:HD13 | 1:M:447:TRP:CZ2 | 2.55 | 0.41 |
| 1:M:57:ASN:HD21 | 1:M:59:LYS:N | 2.18 | 0.41 |
| 1:M:72:VAL:HG21 | 1:M:195:ILE:O | 2.21 | 0.41 |
| 1:N:111:GLN:HG2 | 1:N:369:GLU:HB3 | 2.01 | 0.41 |
| 1:N:390:TYR:HB3 | 1:N:391:ILE:H | 1.73 | 0.41 |
| 1:O:74:ARG:HH21 | 1:O:441:LEU:HD12 | 1.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:163:PRO:HA | 1:O:330:PHE:CD1 | 2.55 | 0.41 |
| 1:A:68:LEU:HD23 | 1:A:201:VAL:CG2 | 2.39 | 0.41 |
| 1:A:168:HIS:HB2 | 1:A:208:MET:CA | 2.50 | 0.41 |
| 1:A:443:LYS:HZ3 | 1:A:443:LYS:HG2 | 1.86 | 0.41 |
| 1:B:47:HIS:HD2 | 1:C:269:GLU:OE2 | 2.03 | 0.41 |
| 1:B:367:GLY:O | 1:B:368:GLU:HG2 | 2.21 | 0.41 |
| 1:B:459:LEU:HB3 | 1:B:465:GLY:HA3 | 2.02 | 0.41 |
| 1:C:217:LYS:HD3 | 1:D:274:ASP:O | 2.21 | 0.41 |
| 1:D:219:GLU:HB3 | 1:D:263:ARG:NH2 | 2.36 | 0.41 |
| 1:D:219:GLU:O | 1:D:220:VAL:HG13 | 2.20 | 0.41 |
| 1:D:235:ILE:O | 1:D:235:ILE:HG22 | 2.21 | 0.41 |
| 1:D:463:PRO:HA | 1:D:466:ARG:HE | 1.85 | 0.41 |
| 1:E:235:ILE:CD1 | 1:E:235:ILE:CA | 2.99 | 0.41 |
| 1:E:312:TRP:HH2 | 1:E:468:PHE:HB2 | 1.78 | 0.41 |
| 1:F:220:VAL:O | 1:F:221:PRO:O | 2.38 | 0.41 |
| 1:F:248:PHE:CE2 | 1:F:311:TYR:HB3 | 2.54 | 0.41 |
| 1:F:253:GLU:O | 1:J:302:SER:N | 2.50 | 0.41 |
| 1:G:36:HIS:ND1 | 1:G:37:ALA:N | 2.69 | 0.41 |
| 1:G:251:ARG:HH11 | 1:G:251:ARG:HD2 | 1.63 | 0.41 |
| 1:H:384:THR:N | 1:H:387:VAL:HB | 2.35 | 0.41 |
| 1:I:23:SER:O | 1:I:26:GLU:N | 2.42 | 0.41 |
| 1:I:174:PRO:HB3 | 1:I:175:CYS:H | 1.56 | 0.41 |
| 1:J:105:VAL:CG2 | 1:J:105:VAL:CA | 2.82 | 0.41 |
| 1:K:329:LEU:HA | 1:K:329:LEU:HD23 | 1.80 | 0.41 |
| 1:L:126:LEU:HD12 | 1:L:126:LEU:HA | 1.94 | 0.41 |
| 1:L:201:VAL:HG11 | 1:L:334:VAL:CG1 | 2.50 | 0.41 |
| 1:M:289:SER:O | 1:M:291:TYR:CD1 | 2.74 | 0.41 |
| 1:M:458:ASP:C | 1:M:460:ASP:H | 2.23 | 0.41 |
| 1:O:158:LEU:O | 1:O:331:VAL:HA | 2.20 | 0.41 |
| 1:O:262:ASN:HD22 | 1:O:262:ASN:C | 2.24 | 0.41 |
| 1:O:329:LEU:HD13 | 1:O:374:PHE:CE2 | 2.56 | 0.41 |
| 1:O:390:TYR:C | 1:O:392:HIS:N | 2.74 | 0.41 |
| 1:O:459:LEU:C | 1:O:461:GLN:H | 2.22 | 0.41 |
| 1:O:463:PRO:HG2 | 1:O:464:LEU:H | 1.85 | 0.41 |
| 1:A:41:ARG:HG2 | 1:A:42:LEU:O | 2.20 | 0.41 |
| 1:A:61:LEU:O | 1:A:62:VAL:CG2 | 2.69 | 0.41 |
| 1:A:80:PRO:C | 1:A:82:LYS:N | 2.74 | 0.41 |
| 1:A:129:THR:HB | 1:E:148:SER:OG | 2.20 | 0.41 |
| 1:A:186:PRO:HD2 | 1:E:344:LEU:HD12 | 2.03 | 0.41 |
| 1:B:34:TYR:CE2 | 1:B:377:GLN:HB2 | 2.55 | 0.41 |
| 1:B:43:LEU:CD1 | 1:B:369:GLU:HG3 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:323:ILE:HG21 | 1:B:325:TRP:CZ2 | 2.56 | 0.41 |
| 1:B:344:LEU:HD13 | 1:C:213:LEU:CD1 | 2.51 | 0.41 |
| 1:B:345:CYS:HG | 1:C:216:ASN:HB2 | 1.79 | 0.41 |
| 1:C:216:ASN:CG | 1:C:219:GLU:OE2 | 2.59 | 0.41 |
| 1:D:355:TYR:CD2 | 1:D:355:TYR:C | 2.94 | 0.41 |
| 1:D:372:LEU:HB3 | 1:D:374:PHE:HE1 | 1.85 | 0.41 |
| 1:D:461:GLN:HE22 | 1:E:21:VAL:H | 1.69 | 0.41 |
| 1:E:178:VAL:C | 1:E:180:VAL:H | 2.24 | 0.41 |
| 1:E:438:GLU:HG2 | 1:E:439:ASP:N | 2.36 | 0.41 |
| 1:F:120:HIS:CE1 | 1:F:122:LEU:H | 2.37 | 0.41 |
| 1:F:166:GLY:HA3 | 1:F:195:ILE:HD11 | 2.02 | 0.41 |
| 1:F:223:ASP:OD1 | 1:F:224:ILE:N | 2.53 | 0.41 |
| 1:G:72:VAL:HA | 1:G:332:THR:HG23 | 2.03 | 0.41 |
| 1:G:105:VAL:CG2 | 1:G:105:VAL:CA | 2.84 | 0.41 |
| 1:H:96:GLN:HB3 | 1:H:382:THR:CG2 | 2.43 | 0.41 |
| 1:I:92:ASN:HA | 1:I:93:PRO:HD2 | 1.72 | 0.41 |
| 1:I:297:GLY:C | 1:I:298:SER:O | 2.59 | 0.41 |
| 1:J:39:THR:H | 1:J:39:THR:HG23 | 1.61 | 0.41 |
| 1:J:54:LYS:HA | 1:J:54:LYS:HZ2 | 1.84 | 0.41 |
| 1:J:471:GLN:O | 1:J:472:LEU:OXT | 2.38 | 0.41 |
| 1:K:121:PRO:HG3 | 1:L:289:SER:HB2 | 2.03 | 0.41 |
| 1:K:144:ARG:CZ | 1:O:355:TYR:HB2 | 2.50 | 0.41 |
| 1:L:80:PRO:CG | 1:L:98:LEU:O | 2.68 | 0.41 |
| 1:L:324:CYS:O | 1:L:325:TRP:C | 2.59 | 0.41 |
| 1:L:457:ALA:O | 1:L:459:LEU:HD23 | 2.21 | 0.41 |
| 1:M:117:ILE:CG1 | 1:M:149:MET:O | 2.69 | 0.41 |
| 1:M:180:VAL:CG1 | 1:M:181:GLN:N | 2.82 | 0.41 |
| 1:M:365:ARG:HA | 1:M:365:ARG:HD3 | 1.86 | 0.41 |
| 1:N:119:GLY:HA3 | 1:O:291:TYR:CE1 | 2.56 | 0.41 |
| 1:N:302:SER:C | 1:N:304:ALA:N | 2.71 | 0.41 |
| 1:N:312:TRP:CE3 | 1:N:312:TRP:HA | 2.54 | 0.41 |
| 1:O:221:PRO:HD2 | 1:O:224:ILE:HD11 | 2.03 | 0.41 |
| 1:A:101:ALA:HB3 | 1:A:377:GLN:HB3 | 2.03 | 0.41 |
| 1:A:241:PRO:HG2 | 1:A:242:TYR:N | 2.32 | 0.41 |
| 1:B:71:ARG:HA | 1:B:71:ARG:NH1 | 2.18 | 0.41 |
| 1:B:74:ARG:CB | 1:B:330:PHE:HE2 | 2.34 | 0.41 |
| 1:B:184:ASP:O | 1:B:185:CYS:C | 2.58 | 0.41 |
| 1:B:248:PHE:CE2 | 1:B:311:TYR:CG | 3.09 | 0.41 |
| 1:B:360:PHE:CE2 | 1:C:216:ASN:HA | 2.56 | 0.41 |
| 1:C:39:THR:HG22 | 1:C:449:VAL:CG1 | 2.51 | 0.41 |
| 1:C:316:ALA:HB3 | 1:C:321:ASN:OD1 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:325:TRP:CE2 | 1:C:394:MET:CE | 3.04 | 0.41 |
| 1:C:348:ILE:CG2 | 1:C:359:ASN:OD1 | 2.59 | 0.41 |
| 1:C:351:SER:O | 1:C:352:GLU:O | 2.39 | 0.41 |
| 1:D:80:PRO:O | 1:D:82:LYS:N | 2.54 | 0.41 |
| 1:D:231:TYR:HA | 1:D:232:PRO:HD3 | 1.93 | 0.41 |
| 1:D:307:PHE:O | 1:D:308:ASN:CB | 2.67 | 0.41 |
| 1:D:395:ASN:HB3 | 1:D:398:ILE:CG1 | 2.45 | 0.41 |
| 1:E:68:LEU:HD23 | 1:E:201:VAL:HG21 | 2.03 | 0.41 |
| 1:E:79:ASP:O | 1:E:80:PRO:C | 2.57 | 0.41 |
| 1:E:133:SER:O | 1:E:134:ALA:HB2 | 2.21 | 0.41 |
| 1:E:151:TYR:CD2 | 1:E:203:THR:CB | 2.94 | 0.41 |
| 1:E:163:PRO:HB3 | 1:E:330:PHE:CE1 | 2.56 | 0.41 |
| 1:E:390:TYR:C | 1:E:392:HIS:N | 2.73 | 0.41 |
| 1:E:451:LEU:HD23 | 1:E:451:LEU:HA | 1.76 | 0.41 |
| 1:F:49:TYR:HE1 | 1:F:364:LEU:CD1 | 2.34 | 0.41 |
| 1:F:258:ARG:HG3 | 1:F:259:HIS:ND1 | 2.35 | 0.41 |
| 1:G:103:VAL:HG23 | 1:G:104:GLY:N | 2.36 | 0.41 |
| 1:G:115:VAL:H | 1:H:255:MET:CE | 2.34 | 0.41 |
| 1:G:152:LYS:O | 1:G:152:LYS:CG | 2.65 | 0.41 |
| 1:G:161:CYS:SG | 1:G:244:ASP:O | 2.67 | 0.41 |
| 1:G:219:GLU:H | 1:G:219:GLU:HG2 | 1.63 | 0.41 |
| 1:G:299:MET:HA | 1:H:256:PHE:HB3 | 2.02 | 0.41 |
| 1:H:103:VAL:HG22 | 1:H:375:ILE:HG22 | 2.02 | 0.41 |
| 1:H:119:GLY:O | 1:H:222:LEU:N | 2.41 | 0.41 |
| 1:H:224:ILE:HD13 | 1:H:224:ILE:HG21 | 1.74 | 0.41 |
| 1:H:439:ASP:O | 1:H:442:LYS:HB2 | 2.21 | 0.41 |
| 1:H:461:GLN:NE2 | 1:I:21:VAL:HG23 | 2.36 | 0.41 |
| 1:I:33:ILE:O | 1:I:377:GLN:HA | 2.21 | 0.41 |
| 1:I:75:ILE:HB | 1:I:329:LEU:CB | 2.50 | 0.41 |
| 1:I:333:VAL:CG1 | 1:I:334:VAL:N | 2.82 | 0.41 |
| 1:I:373:GLN:CB | 1:I:464:LEU:HD12 | 2.50 | 0.41 |
| 1:I:381:ILE:HD13 | 1:I:381:ILE:HG21 | 1.47 | 0.41 |
| 1:J:74:ARG:HD2 | 1:J:330:PHE:CZ | 2.56 | 0.41 |
| 1:J:98:LEU:CD2 | 1:J:379:CYS:O | 2.66 | 0.41 |
| 1:J:105:VAL:HG11 | 1:J:159:ILE:CD1 | 2.51 | 0.41 |
| 1:K:30:ARG:HH11 | 1:K:377:GLN:HE22 | 1.67 | 0.41 |
| 1:K:135:TYR:CE2 | 1:K:287:ALA:HB2 | 2.53 | 0.41 |
| 1:K:301:THR:OG1 | 1:K:302:SER:N | 2.52 | 0.41 |
| 1:L:49:TYR:CE2 | 1:L:118:SER:HB3 | 2.56 | 0.41 |
| 1:L:109:ARG:NH1 | 1:L:370:TYR:CZ | 2.88 | 0.41 |
| 1:L:121:PRO:CD | 1:L:222:LEU:CD1 | 2.99 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:316:ALA:CB | 1:L:321:ASN:OD1 | 2.67 | 0.41 |
| 1:L:320:ASN:OD1 | 1:L:323:ILE:HG12 | 2.21 | 0.41 |
| 1:M:40:SER:O | 1:M:41:ARG:HB2 | 2.20 | 0.41 |
| 1:M:76:HIS:HB2 | 1:M:450:ASN:HA | 2.03 | 0.41 |
| 1:M:150:ASP:HB3 | 1:N:257:VAL:HG21 | 2.02 | 0.41 |
| 1:M:321:ASN:CG | 1:M:321:ASN:O | 2.59 | 0.41 |
| 1:M:323:ILE:HG21 | 1:M:325:TRP:CE2 | 2.56 | 0.41 |
| 1:M:328:GLN:HE21 | 1:M:328:GLN:HB2 | 1.34 | 0.41 |
| 1:M:399:LEU:HA | 1:M:402:TRP:CE3 | 2.51 | 0.41 |
| 1:N:52:ILE:HD13 | 1:N:52:ILE:H | 1.86 | 0.41 |
| 1:N:68:LEU:HA | 1:N:201:VAL:HG21 | 2.02 | 0.41 |
| 1:N:170:GLY:HA2 | 1:N:213:LEU:HD21 | 2.03 | 0.41 |
| 1:N:234:TYR:CD1 | 1:N:251:ARG:NH2 | 2.89 | 0.41 |
| 1:N:277:ILE:HD13 | 1:N:277:ILE:HG21 | 1.44 | 0.41 |
| 1:N:471:GLN:CD | 1:N:472:LEU:N | 2.74 | 0.41 |
| 1:O:217:LYS:O | 1:O:217:LYS:CG | 2.65 | 0.41 |
| 1:A:185:CYS:SG | 1:E:344:LEU:CD1 | 3.08 | 0.41 |
| 1:A:185:CYS:HA | 1:A:186:PRO:HD3 | 1.95 | 0.41 |
| 1:B:241:PRO:C | 1:B:243:GLY:H | 2.24 | 0.41 |
| 1:B:364:LEU:O | 1:B:365:ARG:CD | 2.69 | 0.41 |
| 1:C:70:TYR:CG | 1:C:195:ILE:CG2 | 3.04 | 0.41 |
| 1:D:166:GLY:H | 1:D:195:ILE:HG13 | 1.84 | 0.41 |
| 1:D:231:TYR:CD1 | 1:D:232:PRO:HD2 | 2.56 | 0.41 |
| 1:F:372:LEU:HD23 | 1:F:372:LEU:HA | 1.78 | 0.41 |
| 1:F:398:ILE:HG23 | 1:F:398:ILE:HD12 | 1.88 | 0.41 |
| 1:G:24:THR:HG22 | 1:G:27:TYR:OH | 2.20 | 0.41 |
| 1:G:126:LEU:HD12 | 1:G:126:LEU:HA | 1.65 | 0.41 |
| 1:G:219:GLU:O | 1:G:263:ARG:NH2 | 2.37 | 0.41 |
| 1:G:398:ILE:HG22 | 1:G:402:TRP:CZ3 | 2.56 | 0.41 |
| 1:H:90:PHE:CD1 | 1:H:91:TYR:HB3 | 2.56 | 0.41 |
| 1:H:152:LYS:HE2 | 1:H:154:THR:OG1 | 2.21 | 0.41 |
| 1:H:162:LYS:HG2 | 1:H:244:ASP:HB3 | 2.02 | 0.41 |
| 1:J:76:HIS:O | 1:J:451:LEU:HB2 | 2.21 | 0.41 |
| 1:K:30:ARG:CD | 1:K:30:ARG:CB | 2.86 | 0.41 |
| 1:K:66:SER:N | 1:K:69:GLN:NE2 | 2.63 | 0.41 |
| 1:K:115:VAL:HG21 | 1:L:257:VAL:HG13 | 2.02 | 0.41 |
| 1:K:234:TYR:O | 1:K:236:LYS:N | 2.54 | 0.41 |
| 1:L:263:ARG:HD3 | 1:L:292:PHE:CD2 | 2.56 | 0.41 |
| 1:M:71:ARG:HG3 | 1:M:370:TYR:OH | 2.21 | 0.41 |
| 1:M:149:MET:CE | 1:M:205:PHE:HE1 | 2.34 | 0.41 |
| 1:M:294:THR:OG1 | 1:M:294:THR:O | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:85:PHE:CE2 | 1:O:378:LEU:HD22 | 2.56 | 0.41 |
| 1:O:246:LEU:HD23 | 1:O:246:LEU:O | 2.21 | 0.41 |
| 1:A:117:ILE:CG2 | 1:B:293:PRO:HD3 | 2.50 | 0.40 |
| 1:A:123:LEU:HD23 | 1:A:147:ILE:HB | 2.03 | 0.40 |
| 1:A:155:GLN:HE21 | 1:A:155:GLN:HB2 | 1.60 | 0.40 |
| 1:A:255:MET:SD | 1:E:115:VAL:HG22 | 2.61 | 0.40 |
| 1:A:260:LEU:HD21 | 1:E:149:MET:HA | 2.03 | 0.40 |
| 1:A:351:SER:HB2 | 1:A:352:GLU:H | 1.75 | 0.40 |
| 1:B:122:LEU:HD11 | 1:C:286:LEU:CD1 | 2.42 | 0.40 |
| 1:B:316:ALA:CB | 1:B:321:ASN:OD1 | 2.70 | 0.40 |
| 1:B:451:LEU:O | 1:B:454:LYS:CB | 2.59 | 0.40 |
| 1:C:41:ARG:HG2 | 1:C:41:ARG:O | 2.13 | 0.40 |
| 1:C:46:GLY:N | 1:C:65:VAL:HB | 2.35 | 0.40 |
| 1:C:137:ALA:O | 1:C:138:ASN:C | 2.58 | 0.40 |
| 1:C:325:TRP:NE1 | 1:C:394:MET:HE3 | 2.37 | 0.40 |
| 1:C:463:PRO:CA | 1:C:466:ARG:HH21 | 2.34 | 0.40 |
| 1:D:122:LEU:HD21 | 1:E:286:LEU:HD12 | 2.03 | 0.40 |
| 1:D:151:TYR:OH | 1:D:221:PRO:HG2 | 2.22 | 0.40 |
| 1:E:154:THR:O | 1:E:334:VAL:HG12 | 2.21 | 0.40 |
| 1:E:216:ASN:ND2 | 1:E:219:GLU:OE2 | 2.54 | 0.40 |
| 1:E:247:PHE:CD1 | 1:E:247:PHE:N | 2.87 | 0.40 |
| 1:E:255:MET:HG2 | 1:E:256:PHE:N | 2.36 | 0.40 |
| 1:E:262:ASN:HD22 | 1:E:263:ARG:N | 2.19 | 0.40 |
| 1:F:260:LEU:N | 1:F:260:LEU:CD1 | 2.65 | 0.40 |
| 1:F:276:TYR:HA | 1:J:217:LYS:HG2 | 2.02 | 0.40 |
| 1:G:392:HIS:HB2 | 1:G:399:LEU:HD11 | 2.03 | 0.40 |
| 1:H:185:CYS:HA | 1:H:186:PRO:HD3 | 1.79 | 0.40 |
| 1:H:193:THR:OG1 | 1:H:194:VAL:N | 2.53 | 0.40 |
| 1:H:242:TYR:CD2 | 1:H:394:MET:HG3 | 2.57 | 0.40 |
| 1:H:336:THR:HG23 | 1:H:336:THR:H | 1.47 | 0.40 |
| 1:H:355:TYR:CE1 | 1:I:144:ARG:HD3 | 2.56 | 0.40 |
| 1:H:373:GLN:HB3 | 1:H:464:LEU:CD1 | 2.39 | 0.40 |
| 1:I:196:GLN:HA | 1:I:446:PHE:CE2 | 2.55 | 0.40 |
| 1:I:306:ILE:HD13 | 1:I:306:ILE:N | 2.17 | 0.40 |
| 1:J:316:ALA:C | 1:J:318:GLY:N | 2.73 | 0.40 |
| 1:L:162:LYS:HA | 1:L:162:LYS:HD3 | 1.88 | 0.40 |
| 1:L:440:PRO:C | 1:L:443:LYS:NZ | 2.75 | 0.40 |
| 1:M:85:PHE:HA | 1:M:86:PRO:HD2 | 1.92 | 0.40 |
| 1:M:172:GLY:O | 1:M:173:SER:O | 2.39 | 0.40 |
| 1:M:387:VAL:HG13 | 1:M:391:ILE:CD1 | 2.51 | 0.40 |
| 1:M:387:VAL:O | 1:M:391:ILE:HG13 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:443:LYS:HD3 | 1:M:443:LYS:H | 1.84 | 0.40 |
| 1:N:119:GLY:O | 1:N:221:PRO:CA | 2.69 | 0.40 |
| 1:O:76:HIS:HB2 | 1:O:450:ASN:HA | 2.03 | 0.40 |
| 1:A:141:VAL:O | 1:A:142:ASP:CB | 2.66 | 0.40 |
| 1:A:224:ILE:H | 1:A:224:ILE:HG12 | 1.76 | 0.40 |
| 1:B:43:LEU:HD12 | 1:B:369:GLU:HA | 2.04 | 0.40 |
| 1:B:163:PRO:CA | 1:B:330:PHE:CD1 | 3.05 | 0.40 |
| 1:B:339:SER:O | 1:B:340:THR:C | 2.59 | 0.40 |
| 1:C:33:ILE:O | 1:C:377:GLN:HA | 2.21 | 0.40 |
| 1:C:120:HIS:HA | 1:C:222:LEU:HD13 | 2.03 | 0.40 |
| 1:C:231:TYR:HA | 1:C:232:PRO:HD3 | 1.80 | 0.40 |
| 1:C:328:GLN:HE21 | 1:C:328:GLN:HB2 | 1.51 | 0.40 |
| 1:C:398:ILE:HG22 | 1:C:402:TRP:CZ3 | 2.56 | 0.40 |
| 1:C:451:LEU:HA | 1:C:454:LYS:HG2 | 2.01 | 0.40 |
| 1:C:458:ASP:OD2 | 1:C:458:ASP:N | 2.55 | 0.40 |
| 1:C:461:GLN:HE22 | 1:D:21:VAL:CG2 | 2.34 | 0.40 |
| 1:D:33:ILE:HD12 | 1:D:33:ILE:HG23 | 1.84 | 0.40 |
| 1:D:293:PRO:O | 1:D:293:PRO:HG2 | 2.21 | 0.40 |
| 1:E:27:TYR:CZ | 1:E:390:TYR:HE2 | 2.39 | 0.40 |
| 1:G:28:VAL:HG22 | 1:G:381:ILE:HD11 | 2.03 | 0.40 |
| 1:G:71:ARG:NH1 | 1:G:198:GLY:N | 2.50 | 0.40 |
| 1:G:115:VAL:N | 1:H:255:MET:SD | 2.93 | 0.40 |
| 1:G:317:GLN:C | 1:G:317:GLN:HE21 | 2.25 | 0.40 |
| 1:H:81:ASN:ND2 | 1:H:402:TRP:HD1 | 2.19 | 0.40 |
| 1:H:103:VAL:HG22 | 1:H:375:ILE:O | 2.21 | 0.40 |
| 1:I:50:PHE:HB2 | 1:I:51:PRO:HD2 | 2.02 | 0.40 |
| 1:I:99:VAL:CG2 | 1:I:402:TRP:HZ2 | 2.34 | 0.40 |
| 1:I:470:LEU:O | 1:I:470:LEU:HD23 | 2.21 | 0.40 |
| 1:J:233:ASP:OD2 | 1:J:236:LYS:HB2 | 2.21 | 0.40 |
| 1:K:42:LEU:HD23 | 1:K:42:LEU:HA | 1.83 | 0.40 |
| 1:K:92:ASN:C | 1:K:94:ASP:N | 2.75 | 0.40 |
| 1:K:397:THR:O | 1:K:401:ASP:OD2 | 2.40 | 0.40 |
| 1:L:302:SER:O | 1:L:304:ALA:N | 2.53 | 0.40 |
| 1:M:61:LEU:O | 1:M:62:VAL:HG23 | 2.22 | 0.40 |
| 1:M:343:SER:C | 1:M:344:LEU:HD23 | 2.38 | 0.40 |
| 1:N:96:GLN:HA | 1:N:382:THR:HA | 2.02 | 0.40 |
| 1:N:345:CYS:SG | 1:O:216:ASN:N | 2.91 | 0.40 |
| 1:O:62:VAL:HA | 1:O:63:PRO:HD3 | 1.96 | 0.40 |
| 1:O:165:ILE:O | 1:O:165:ILE:HG22 | 2.17 | 0.40 |
| 1:O:451:LEU:HA | 1:O:454:LYS:CG | 2.51 | 0.40 |
| 1:A:71:ARG:HA | 1:A:71:ARG:HD3 | 1.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:98:LEU:HB3 | 1:A:378:LEU:HD11 | 2.04 | 0.40 |
| 1:A:217:LYS:HG2 | 1:B:276:TYR:HA | 2.03 | 0.40 |
| 1:A:443:LYS:CD | 1:A:443:LYS:H | 2.32 | 0.40 |
| 1:B:258:ARG:HB2 | 1:B:296:SER:HB2 | 2.03 | 0.40 |
| 1:B:391:ILE:HD13 | 1:B:402:TRP:HH2 | 1.87 | 0.40 |
| 1:D:36:HIS:ND1 | 1:D:36:HIS:C | 2.74 | 0.40 |
| 1:D:62:VAL:CG1 | 1:D:63:PRO:CD | 2.99 | 0.40 |
| 1:D:155:GLN:HB3 | 1:D:252:ARG:HB3 | 2.03 | 0.40 |
| 1:D:176:THR:CA | 1:D:176:THR:CG2 | 2.84 | 0.40 |
| 1:D:246:LEU:HD23 | 1:D:246:LEU:N | 2.10 | 0.40 |
| 1:E:83:PHE:HD2 | 1:E:85:PHE:CZ | 2.40 | 0.40 |
| 1:E:306:ILE:HD13 | 1:E:306:ILE:N | 2.27 | 0.40 |
| 1:E:320:ASN:ND2 | 1:E:325:TRP:CD1 | 2.90 | 0.40 |
| 1:E:389:THR:CG2 | 1:E:389:THR:CA | 2.82 | 0.40 |
| 1:F:94:ASP:C | 1:F:95:THR:CG2 | 2.87 | 0.40 |
| 1:F:252:ARG:CD | 1:F:306:ILE:HD11 | 2.42 | 0.40 |
| 1:H:143:ASN:O | 1:H:144:ARG:O | 2.39 | 0.40 |
| 1:H:196:GLN:O | 1:H:197:ASP:C | 2.59 | 0.40 |
| 1:H:262:ASN:HD22 | 1:H:263:ARG:N | 2.19 | 0.40 |
| 1:H:335:ASP:OD2 | 1:H:338:ARG:HD2 | 2.21 | 0.40 |
| 1:I:74:ARG:CZ | 1:I:441:LEU:HD12 | 2.50 | 0.40 |
| 1:I:103:VAL:CG2 | 1:I:375:ILE:HG22 | 2.51 | 0.40 |
| 1:I:174:PRO:HD3 | 1:I:187:PRO:HG2 | 2.00 | 0.40 |
| 1:I:343:SER:HB3 | 1:I:364:LEU:CD2 | 2.51 | 0.40 |
| 1:I:398:ILE:CG2 | 1:I:402:TRP:CZ3 | 3.02 | 0.40 |
| 1:I:461:GLN:HE21 | 1:I:461:GLN:HA | 1.85 | 0.40 |
| 1:J:50:PHE:CB | 1:J:51:PRO:CD | 2.96 | 0.40 |
| 1:J:345:CYS:HA | 1:J:361:LYS:O | 2.21 | 0.40 |
| 1:K:21:VAL:HA | 1:K:390:TYR:HE1 | 1.86 | 0.40 |
| 1:K:147:ILE:CG2 | 1:K:148:SER:N | 2.84 | 0.40 |
| 1:K:178:VAL:CG1 | 1:K:178:VAL:HB | 2.20 | 0.40 |
| 1:K:207:ALA:O | 1:K:208:MET:CB | 2.65 | 0.40 |
| 1:K:217:LYS:HG2 | 1:L:276:TYR:HA | 2.04 | 0.40 |
| 1:K:290:ASN:HA | 1:O:364:LEU:CD1 | 2.50 | 0.40 |
| 1:K:346:ALA:CB | 1:K:346:ALA:N | 2.71 | 0.40 |
| 1:L:59:LYS:NZ | 1:L:59:LYS:CD | 2.73 | 0.40 |
| 1:L:85:PHE:CZ | 1:L:378:LEU:HD22 | 2.57 | 0.40 |
| 1:L:375:ILE:HG21 | 1:L:468:PHE:CE2 | 2.55 | 0.40 |
| 1:M:120:HIS:ND1 | 1:M:121:PRO:CD | 2.85 | 0.40 |
| 1:M:120:HIS:ND1 | 1:M:121:PRO:N | 2.69 | 0.40 |
| 1:N:90:PHE:CD1 | 1:N:90:PHE:C | 2.95 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:276:TYR:O | 1:N:277:ILE:HG12 | 2.22 | 0.40 |
| 1:N:384:THR:HG23 | 1:N:387:VAL:HG21 | 2.03 | 0.40 |
| 1:N:398:ILE:HG22 | 1:N:402:TRP:CH2 | 2.56 | 0.40 |
| 1:O:143:ASN:N | 1:O:143:ASN:OD1 | 2.53 | 0.40 |
| 1:O:440:PRO:O | 1:O:443:LYS:NZ | 2.49 | 0.40 |
| 1:A:293:PRO:CD | 1:A:293:PRO:O | 2.69 | 0.40 |
| 1:A:348:ILE:HG22 | 1:A:359:ASN:OD1 | 2.21 | 0.40 |
| 1:A:443:LYS:NZ | 1:A:443:LYS:CG | 2.85 | 0.40 |
| 1:B:231:TYR:HA | 1:B:232:PRO:HD3 | 1.88 | 0.40 |
| 1:B:302:SER:C | 1:B:304:ALA:H | 2.24 | 0.40 |
| 1:B:333:VAL:HG12 | 1:B:334:VAL:N | 2.37 | 0.40 |
| 1:C:85:PHE:HA | 1:C:86:PRO:HD2 | 1.88 | 0.40 |
| 1:C:149:MET:CE | 1:C:294:THR:HG22 | 2.52 | 0.40 |
| 1:C:194:VAL:HG21 | 1:C:444:TYR:CZ | 2.57 | 0.40 |
| 1:C:217:LYS:O | 1:C:218:SER:CB | 2.68 | 0.40 |
| 1:C:246:LEU:HD12 | 1:C:249:TYR:CD2 | 2.57 | 0.40 |
| 1:C:250:LEU:O | 1:C:250:LEU:CD1 | 2.68 | 0.40 |
| 1:C:280:SER:O | 1:C:281:GLY:C | 2.60 | 0.40 |
| 1:C:440:PRO:CA | 1:C:443:LYS:NZ | 2.82 | 0.40 |
| 1:C:454:LYS:HA | 1:C:454:LYS:HD2 | 1.93 | 0.40 |
| 1:D:121:PRO:C | 1:D:122:LEU:HD23 | 2.41 | 0.40 |
| 1:D:152:LYS:CE | 1:D:253:GLU:OE1 | 2.70 | 0.40 |
| 1:D:196:GLN:HB3 | 1:D:445:THR:O | 2.20 | 0.40 |
| 1:D:241:PRO:HG2 | 1:D:242:TYR:N | 2.34 | 0.40 |
| 1:D:259:HIS:CE1 | 1:E:130:GLU:HG2 | 2.56 | 0.40 |
| 1:E:154:THR:O | 1:E:336:THR:HG23 | 2.21 | 0.40 |
| 1:F:65:VAL:CA | 1:F:69:GLN:HE22 | 2.21 | 0.40 |
| 1:F:129:THR:HG22 | 1:J:146:CYS:O | 2.22 | 0.40 |
| 1:F:135:TYR:HE2 | 1:F:287:ALA:HB2 | 1.85 | 0.40 |
| 1:F:142:ASP:OD1 | 1:G:283:THR:OG1 | 2.34 | 0.40 |
| 1:G:46:GLY:CA | 1:G:63:PRO:O | 2.67 | 0.40 |
| 1:G:111:GLN:HA | 1:G:112:PRO:HD2 | 1.86 | 0.40 |
| 1:G:117:ILE:CG1 | 1:G:149:MET:O | 2.70 | 0.40 |
| 1:G:233:ASP:OD2 | 1:G:236:LYS:HB2 | 2.22 | 0.40 |
| 1:G:465:GLY:O | 1:G:468:PHE:N | 2.55 | 0.40 |
| 1:H:70:TYR:CE1 | 1:H:230:LYS:O | 2.74 | 0.40 |
| 1:H:302:SER:C | 1:H:304:ALA:H | 2.25 | 0.40 |
| 1:H:372:LEU:HD23 | 1:H:372:LEU:HA | 1.64 | 0.40 |
| 1:I:62:VAL:HG13 | 1:I:63:PRO:CD | 2.51 | 0.40 |
| 1:I:208:MET:N | 1:I:229:CYS:O | 2.55 | 0.40 |
| 1:I:312:TRP:HA | 1:I:312:TRP:HE3 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:35:TYR:CZ | 1:M:457:ALA:HB2 | 2.56 | 0.40 |
| 1:M:96:GLN:NE2 | 1:M:382:THR:CG2 | 2.84 | 0.40 |
| 1:M:115:VAL:N | 1:N:255:MET:CE | 2.73 | 0.40 |
| 1:M:246:LEU:HD23 | 1:M:246:LEU:N | 2.36 | 0.40 |
| 1:N:46:GLY:O | 1:N:365:ARG:HD3 | 2.22 | 0.40 |
| 1:N:123:LEU:HD23 | 1:N:147:ILE:HB | 2.03 | 0.40 |
| 1:N:217:LYS:O | 1:N:218:SER:HB3 | 2.21 | 0.40 |
| 1:O:85:PHE:CE1 | 1:O:98:LEU:HD13 | 2.57 | 0.40 |
| 1:O:99:VAL:HG21 | 1:O:325:TRP:CZ3 | 2.56 | 0.40 |
| 1:O:107:VAL:HB | 1:O:307:PHE:HD2 | 1.86 | 0.40 |
| 1:O:222:LEU:HA | 1:O:225:CYS:SG | 2.61 | 0.40 |
| 1:A:60:ILE:O | 1:A:60:ILE:CG1 | 2.69 | 0.40 |
| 1:A:121:PRO:HG2 | 1:B:289:SER:HB2 | 2.03 | 0.40 |
| 1:B:177:GLN:O | 1:B:178:VAL:C | 2.60 | 0.40 |
| 1:B:188:LEU:HD13 | 1:B:188:LEU:HA | 1.69 | 0.40 |
| 1:C:152:LYS:NZ | 1:C:253:GLU:OE1 | 2.54 | 0.40 |
| 1:C:159:ILE:HG21 | 1:C:159:ILE:HD13 | 1.80 | 0.40 |
| 1:C:300:VAL:HG22 | 1:C:300:VAL:H | 1.42 | 0.40 |
| 1:C:315:ARG:O | 1:C:316:ALA:HB2 | 2.21 | 0.40 |
| 1:C:354:THR:HG22 | 1:E:278:LYS:CB | 2.50 | 0.40 |
| 1:D:277:ILE:HD13 | 1:D:277:ILE:HG21 | 1.77 | 0.40 |
| 1:E:80:PRO:HD3 | 1:E:327:ASN:OD1 | 2.21 | 0.40 |
| 1:E:149:MET:HE3 | 1:E:294:THR:CG2 | 2.11 | 0.40 |
| 1:E:196:GLN:HB3 | 1:E:445:THR:O | 2.21 | 0.40 |
| 1:F:66:SER:OG | 1:F:68:LEU:N | 2.54 | 0.40 |
| 1:F:141:VAL:CG1 | 1:F:142:ASP:N | 2.81 | 0.40 |
| 1:F:185:CYS:HB2 | 1:J:363:TYR:CD2 | 2.56 | 0.40 |
| 1:F:389:THR:O | 1:F:392:HIS:HB3 | 2.22 | 0.40 |
| 1:G:80:PRO:HB2 | 1:G:98:LEU:CB | 2.52 | 0.40 |
| 1:G:92:ASN:HA | 1:G:93:PRO:HD2 | 1.68 | 0.40 |
| 1:G:160:GLY:HA3 | 1:G:245:SER:O | 2.21 | 0.40 |
| 1:G:312:TRP:HA | 1:G:312:TRP:HE3 | 1.85 | 0.40 |
| 1:H:272:PRO:HD2 | 1:H:275:LEU:HD11 | 2.02 | 0.40 |
| 1:H:400:GLU:C | 1:H:402:TRP:N | 2.74 | 0.40 |
| 1:I:152:LYS:HB3 | 1:I:255:MET:CB | 2.49 | 0.40 |
| 1:I:246:LEU:HD23 | 1:I:246:LEU:O | 2.21 | 0.40 |
| 1:J:80:PRO:O | 1:J:85:PHE:HE1 | 2.05 | 0.40 |
| 1:J:147:ILE:HG22 | 1:J:148:SER:H | 1.85 | 0.40 |
| 1:J:372:LEU:HD23 | 1:J:372:LEU:HA | 1.76 | 0.40 |
| 1:K:91:TYR:HD1 | 1:K:96:GLN:HG3 | 1.86 | 0.40 |
| 1:K:255:MET:HE3 | 1:O:115:VAL:H | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:106:GLU:HG3 | 1:L:310:PRO:HA | 2.03 | 0.40 |
| 1:L:109:ARG:NH1 | 1:L:370:TYR:CE1 | 2.89 | 0.40 |
| 1:L:263:ARG:NE | 1:L:292:PHE:CD2 | 2.89 | 0.40 |
| 1:M:98:LEU:HD13 | 1:M:378:LEU:CD2 | 2.35 | 0.40 |
| 1:M:214:GLN:HE22 | 1:M:219:GLU:HB2 | 1.86 | 0.40 |
| 1:M:259:HIS:CE1 | 1:N:130:GLU:HG2 | 2.57 | 0.40 |
| 1:M:384:THR:H | 1:M:387:VAL:HB | 1.87 | 0.40 |
| 1:N:178:VAL:C | 1:N:180:VAL:N | 2.74 | 0.40 |
| 1:N:216:ASN:CG | 1:N:219:GLU:HG2 | 2.42 | 0.40 |
| 1:N:271:VAL:HA | 1:N:272:PRO:HD3 | 1.88 | 0.40 |
| 1:N:451:LEU:HD22 | 1:N:454:LYS:HB2 | 2.04 | 0.40 |
| 1:O:307:PHE:CD1 | 1:O:307:PHE:N | 2.89 | 0.40 |

All (47) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:177:GLN:OE1 | 1:M:87:ASP:N[3_645] | 1.49 | 0.71 |
| 1:E:177:GLN:OE1 | 1:M:86:PRO:C[3_645] | 1.62 | 0.58 |
| 1:I:177:GLN:CG | 1:J:95:THR:C[3_645] | 1.66 | 0.54 |
| 1:D:175:CYS:O | 1:N:88:THR:CG2[3_545] | 1.72 | 0.48 |
| 1:D:177:GLN:N | 1:N:88:THR:CA[3_545] | 1.73 | 0.47 |
| 1:I:177:GLN:CG | 1:J:95:THR:O[3_645] | 1.80 | 0.40 |
| 1:I:177:GLN:CG | 1:J:96:GLN:N[3_645] | 1.81 | 0.39 |
| 1:E:177:GLN:OE1 | 1:M:86:PRO:CA[3_645] | 1.82 | 0.38 |
| 1:E:177:GLN:OE1 | 1:M:86:PRO:N[3_645] | 1.82 | 0.38 |
| 1:I:177:GLN:CA | 1:J:96:GLN:N[3_645] | 1.82 | 0.38 |
| 1:D:177:GLN:CA | 1:N:88:THR:O[3_545] | 1.84 | 0.36 |
| 1:I:177:GLN:N | 1:J:92:ASN:O[3_645] | 1.86 | 0.34 |
| 1:I:177:GLN:O | 1:J:92:ASN:O[3_645] | 1.87 | 0.33 |
| 1:I:178:VAL:CA | 1:J:92:ASN:ND2[3_645] | 1.92 | 0.28 |
| 1:E:177:GLN:CD | 1:M:87:ASP:N[3_645] | 1.93 | 0.27 |
| 1:I:177:GLN:O | 1:J:94:ASP:N[3_645] | 1.97 | 0.23 |
| 1:I:178:VAL:O | 1:J:94:ASP:N[3_645] | 1.99 | 0.21 |
| 1:F:384:THR:N | 1:H:176:THR:O[3_555] | 2.02 | 0.18 |
| 1:I:176:THR:O | 1:J:96:GLN:C[3_645] | 2.02 | 0.18 |
| 1:I:177:GLN:CG | 1:J:96:GLN:CA[3_645] | 2.03 | 0.17 |
| 1:I:176:THR:O | 1:J:96:GLN:CG[3_645] | 2.05 | 0.15 |
| 1:I:176:THR:OG1 | 1:J:98:LEU:CG[3_645] | 2.05 | 0.15 |
| 1:I:177:GLN:N | 1:J:96:GLN:O[3_645] | 2.05 | 0.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:177:GLN:C | 1:J:92:ASN:O[3_645] | 2.05 | 0.15 |
| 1:I:175:CYS:CA | 1:J:97:ARG:NE[3_645] | 2.07 | 0.13 |
| 1:I:176:THR:O | 1:J:96:GLN:CB[3_645] | 2.07 | 0.13 |
| 1:I:177:GLN:CB | 1:J:96:GLN:O[3_645] | 2.07 | 0.13 |
| 1:D:176:THR:CG2 | 1:N:87:ASP:O[3_545] | 2.08 | 0.12 |
| 1:F:384:THR:O | 1:H:176:THR:O[3_555] | 2.09 | 0.11 |
| 1:D:177:GLN:N | 1:N:88:THR:CB[3_545] | 2.10 | 0.10 |
| 1:I:176:THR:C | 1:J:96:GLN:C[3_645] | 2.10 | 0.10 |
| 1:D:176:THR:OG1 | 1:N:87:ASP:N[3_545] | 2.11 | 0.09 |
| 1:D:177:GLN:CA | 1:N:88:THR:C[3_545] | 2.11 | 0.09 |
| 1:F:385:ALA:O | 1:H:177:GLN:NE2[3_555] | 2.11 | 0.09 |
| 1:I:178:VAL:N | 1:J:95:THR:N[3_645] | 2.11 | 0.09 |
| 1:D:177:GLN:N | 1:N:88:THR:CG2[3_545] | 2.12 | 0.08 |
| 1:F:383:LEU:C | 1:H:177:GLN:N[3_555] | 2.12 | 0.08 |
| 1:D:176:THR:CA | 1:N:87:ASP:O[3_545] | 2.13 | 0.07 |
| 1:I:176:THR:C | 1:J:96:GLN:O[3_645] | 2.14 | 0.06 |
| 1:I:177:GLN:CB | 1:J:95:THR:C[3_645] | 2.15 | 0.05 |
| 1:I:177:GLN:OE1 | 1:J:383:LEU:CD1[3_645] | 2.16 | 0.04 |
| 1:I:177:GLN:CB | 1:J:96:GLN:N[3_645] | 2.16 | 0.04 |
| 1:I:174:PRO:O | 1:J:97:ARG:NH2[3_645] | 2.17 | 0.03 |
| 1:I:179:ALA:N | 1:J:92:ASN:CA[3_645] | 2.17 | 0.03 |
| 1:D:176:THR:OG1 | 1:N:85:PHE:C[3_545] | 2.19 | 0.01 |
| 1:D:177:GLN:O | 1:N:88:THR:CB[3_545] | 2.19 | 0.01 |
| 1:F:384:THR:N | 1:H:176:THR:C[3_555] | 2.19 | 0.01 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 415/424 (98%) | 316 (76%) | 69 (17%) | 30 (7%) | 1 14 |
| 1 | B | 415/424 (98%) | 327 (79%) | 64 (15%) | 24 (6%) | 1 19 |
| 1 | C | 415/424 (98%) | 322 (78%) | 63 (15%) | 30 (7%) | 1 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | D | 415/424 (98%) | 309 (74%) | 76 (18%) | 30 (7%) | 1 | 14 |
| 1 | E | 415/424 (98%) | 321 (77%) | 66 (16%) | 28 (7%) | 1 | 16 |
| 1 | F | 415/424 (98%) | 325 (78%) | 63 (15%) | 27 (6%) | 1 | 17 |
| 1 | G | 415/424 (98%) | 310 (75%) | 71 (17%) | 34 (8%) | 1 | 11 |
| 1 | H | 415/424 (98%) | 322 (78%) | 59 (14%) | 34 (8%) | 1 | 11 |
| 1 | I | 415/424 (98%) | 321 (77%) | 64 (15%) | 30 (7%) | 1 | 14 |
| 1 | J | 415/424 (98%) | 316 (76%) | 65 (16%) | 34 (8%) | 1 | 11 |
| 1 | K | 415/424 (98%) | 322 (78%) | 66 (16%) | 27 (6%) | 1 | 17 |
| 1 | L | 415/424 (98%) | 321 (77%) | 67 (16%) | 27 (6%) | 1 | 17 |
| 1 | M | 415/424 (98%) | 319 (77%) | 72 (17%) | 24 (6%) | 1 | 19 |
| 1 | N | 415/424 (98%) | 319 (77%) | 67 (16%) | 29 (7%) | 1 | 15 |
| 1 | O | 415/424 (98%) | 325 (78%) | 59 (14%) | 31 (8%) | 1 | 13 |
| All | All | 6225/6360 (98%) | 4795 (77%) | 991 (16%) | 439 (7%) | 1 | 15 |

All (439) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 140 | GLY |
| 1 | A | 174 | PRO |
| 1 | A | 180 | VAL |
| 1 | A | 299 | MET |
| 1 | A | 303 | ASP |
| 1 | A | 458 | ASP |
| 1 | B | 140 | GLY |
| 1 | B | 173 | SER |
| 1 | B | 174 | PRO |
| 1 | B | 185 | CYS |
| 1 | B | 218 | SER |
| 1 | B | 352 | GLU |
| 1 | C | 140 | GLY |
| 1 | C | 151 | TYR |
| 1 | C | 173 | SER |
| 1 | C | 174 | PRO |
| 1 | C | 178 | VAL |
| 1 | C | 180 | VAL |
| 1 | C | 303 | ASP |
| 1 | C | 352 | GLU |
| 1 | C | 391 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 144 | ARG |
| 1 | D | 174 | PRO |
| 1 | D | 180 | VAL |
| 1 | D | 218 | SER |
| 1 | D | 337 | THR |
| 1 | D | 351 | SER |
| 1 | E | 140 | GLY |
| 1 | E | 173 | SER |
| 1 | E | 174 | PRO |
| 1 | E | 180 | VAL |
| 1 | E | 184 | ASP |
| 1 | E | 185 | CYS |
| 1 | E | 303 | ASP |
| 1 | F | 93 | PRO |
| 1 | F | 140 | GLY |
| 1 | F | 173 | SER |
| 1 | F | 174 | PRO |
| 1 | F | 176 | THR |
| 1 | F | 180 | VAL |
| 1 | G | 81 | ASN |
| 1 | G | 140 | GLY |
| 1 | G | 144 | ARG |
| 1 | G | 173 | SER |
| 1 | G | 174 | PRO |
| 1 | G | 178 | VAL |
| 1 | G | 180 | VAL |
| 1 | G | 352 | GLU |
| 1 | G | 391 | ILE |
| 1 | H | 138 | ASN |
| 1 | H | 140 | GLY |
| 1 | H | 144 | ARG |
| 1 | H | 174 | PRO |
| 1 | H | 178 | VAL |
| 1 | H | 179 | ALA |
| 1 | H | 180 | VAL |
| 1 | I | 140 | GLY |
| 1 | I | 173 | SER |
| 1 | I | 174 | PRO |
| 1 | I | 176 | THR |
| 1 | I | 179 | ALA |
| 1 | I | 180 | VAL |
| 1 | I | 184 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 235 | ILE |
| 1 | I | 303 | ASP |
| 1 | J | 81 | ASN |
| 1 | J | 138 | ASN |
| 1 | J | 174 | PRO |
| 1 | J | 179 | ALA |
| 1 | J | 180 | VAL |
| 1 | J | 184 | ASP |
| 1 | J | 185 | CYS |
| 1 | J | 241 | PRO |
| 1 | J | 242 | TYR |
| 1 | J | 351 | SER |
| 1 | K | 124 | ASN |
| 1 | K | 140 | GLY |
| 1 | K | 144 | ARG |
| 1 | K | 173 | SER |
| 1 | K | 174 | PRO |
| 1 | K | 180 | VAL |
| 1 | K | 218 | SER |
| 1 | L | 124 | ASN |
| 1 | L | 140 | GLY |
| 1 | L | 173 | SER |
| 1 | L | 174 | PRO |
| 1 | L | 179 | ALA |
| 1 | L | 180 | VAL |
| 1 | L | 225 | CYS |
| 1 | M | 138 | ASN |
| 1 | M | 140 | GLY |
| 1 | M | 173 | SER |
| 1 | M | 174 | PRO |
| 1 | M | 180 | VAL |
| 1 | M | 184 | ASP |
| 1 | M | 221 | PRO |
| 1 | M | 303 | ASP |
| 1 | M | 466 | ARG |
| 1 | N | 140 | GLY |
| 1 | N | 173 | SER |
| 1 | N | 174 | PRO |
| 1 | N | 180 | VAL |
| 1 | N | 201 | VAL |
| 1 | N | 218 | SER |
| 1 | N | 303 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 391 | ILE |
| 1 | N | 466 | ARG |
| 1 | O | 140 | GLY |
| 1 | O | 151 | TYR |
| 1 | O | 173 | SER |
| 1 | O | 174 | PRO |
| 1 | O | 178 | VAL |
| 1 | O | 180 | VAL |
| 1 | O | 218 | SER |
| 1 | O | 324 | CYS |
| 1 | O | 352 | GLU |
| 1 | A | 144 | ARG |
| 1 | A | 178 | VAL |
| 1 | A | 184 | ASP |
| 1 | A | 218 | SER |
| 1 | A | 245 | SER |
| 1 | B | 178 | VAL |
| 1 | B | 180 | VAL |
| 1 | B | 184 | ASP |
| 1 | B | 221 | PRO |
| 1 | B | 235 | ILE |
| 1 | B | 241 | PRO |
| 1 | B | 303 | ASP |
| 1 | C | 131 | ASN |
| 1 | C | 138 | ASN |
| 1 | C | 184 | ASP |
| 1 | C | 245 | SER |
| 1 | C | 278 | LYS |
| 1 | C | 316 | ALA |
| 1 | C | 357 | ASN |
| 1 | D | 140 | GLY |
| 1 | D | 151 | TYR |
| 1 | D | 177 | GLN |
| 1 | D | 179 | ALA |
| 1 | D | 245 | SER |
| 1 | D | 278 | LYS |
| 1 | D | 303 | ASP |
| 1 | D | 305 | GLN |
| 1 | D | 352 | GLU |
| 1 | D | 466 | ARG |
| 1 | E | 151 | TYR |
| 1 | E | 221 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 225 | CYS |
| 1 | E | 357 | ASN |
| 1 | F | 41 | ARG |
| 1 | F | 144 | ARG |
| 1 | F | 178 | VAL |
| 1 | F | 182 | PRO |
| 1 | F | 218 | SER |
| 1 | F | 245 | SER |
| 1 | F | 352 | GLU |
| 1 | G | 138 | ASN |
| 1 | G | 168 | HIS |
| 1 | G | 179 | ALA |
| 1 | G | 184 | ASP |
| 1 | G | 218 | SER |
| 1 | G | 221 | PRO |
| 1 | G | 241 | PRO |
| 1 | G | 242 | TYR |
| 1 | G | 298 | SER |
| 1 | G | 303 | ASP |
| 1 | G | 316 | ALA |
| 1 | H | 25 | ASP |
| 1 | H | 151 | TYR |
| 1 | H | 221 | PRO |
| 1 | H | 235 | ILE |
| 1 | H | 245 | SER |
| 1 | H | 351 | SER |
| 1 | H | 391 | ILE |
| 1 | H | 458 | ASP |
| 1 | H | 460 | ASP |
| 1 | H | 466 | ARG |
| 1 | I | 41 | ARG |
| 1 | I | 84 | GLY |
| 1 | I | 201 | VAL |
| 1 | I | 234 | TYR |
| 1 | J | 41 | ARG |
| 1 | J | 140 | GLY |
| 1 | J | 151 | TYR |
| 1 | J | 177 | GLN |
| 1 | J | 216 | ASN |
| 1 | J | 225 | CYS |
| 1 | J | 245 | SER |
| 1 | J | 293 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 299 | MET |
| 1 | J | 316 | ALA |
| 1 | J | 352 | GLU |
| 1 | J | 466 | ARG |
| 1 | K | 84 | GLY |
| 1 | K | 178 | VAL |
| 1 | K | 184 | ASP |
| 1 | K | 216 | ASN |
| 1 | K | 221 | PRO |
| 1 | K | 282 | SER |
| 1 | K | 352 | GLU |
| 1 | K | 460 | ASP |
| 1 | L | 178 | VAL |
| 1 | L | 218 | SER |
| 1 | L | 278 | LYS |
| 1 | L | 303 | ASP |
| 1 | M | 57 | ASN |
| 1 | M | 90 | PHE |
| 1 | M | 178 | VAL |
| 1 | M | 218 | SER |
| 1 | M | 293 | PRO |
| 1 | N | 41 | ARG |
| 1 | N | 93 | PRO |
| 1 | N | 124 | ASN |
| 1 | N | 138 | ASN |
| 1 | N | 179 | ALA |
| 1 | N | 216 | ASN |
| 1 | N | 349 | SER |
| 1 | N | 352 | GLU |
| 1 | O | 41 | ARG |
| 1 | O | 81 | ASN |
| 1 | O | 82 | LYS |
| 1 | O | 124 | ASN |
| 1 | O | 179 | ALA |
| 1 | O | 184 | ASP |
| 1 | O | 391 | ILE |
| 1 | A | 93 | PRO |
| 1 | A | 124 | ASN |
| 1 | A | 141 | VAL |
| 1 | A | 185 | CYS |
| 1 | A | 221 | PRO |
| 1 | A | 239 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 241 | PRO |
| 1 | A | 293 | PRO |
| 1 | A | 351 | SER |
| 1 | A | 466 | ARG |
| 1 | B | 242 | TYR |
| 1 | C | 93 | PRO |
| 1 | C | 218 | SER |
| 1 | C | 221 | PRO |
| 1 | C | 234 | TYR |
| 1 | C | 235 | ILE |
| 1 | D | 235 | ILE |
| 1 | D | 391 | ILE |
| 1 | D | 400 | GLU |
| 1 | D | 401 | ASP |
| 1 | E | 138 | ASN |
| 1 | E | 177 | GLN |
| 1 | E | 218 | SER |
| 1 | E | 273 | ASP |
| 1 | E | 466 | ARG |
| 1 | F | 23 | SER |
| 1 | F | 184 | ASP |
| 1 | F | 199 | ASP |
| 1 | F | 221 | PRO |
| 1 | F | 293 | PRO |
| 1 | G | 41 | ARG |
| 1 | G | 182 | PRO |
| 1 | H | 41 | ARG |
| 1 | H | 173 | SER |
| 1 | H | 182 | PRO |
| 1 | H | 216 | ASN |
| 1 | H | 278 | LYS |
| 1 | H | 293 | PRO |
| 1 | H | 352 | GLU |
| 1 | H | 400 | GLU |
| 1 | H | 447 | TRP |
| 1 | I | 124 | ASN |
| 1 | I | 168 | HIS |
| 1 | I | 178 | VAL |
| 1 | I | 182 | PRO |
| 1 | I | 241 | PRO |
| 1 | I | 293 | PRO |
| 1 | I | 298 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 351 | SER |
| 1 | J | 131 | ASN |
| 1 | J | 221 | PRO |
| 1 | J | 222 | LEU |
| 1 | K | 182 | PRO |
| 1 | K | 281 | GLY |
| 1 | K | 324 | CYS |
| 1 | K | 351 | SER |
| 1 | L | 41 | ARG |
| 1 | L | 184 | ASP |
| 1 | L | 221 | PRO |
| 1 | L | 288 | SER |
| 1 | L | 298 | SER |
| 1 | M | 185 | CYS |
| 1 | M | 299 | MET |
| 1 | M | 340 | THR |
| 1 | M | 391 | ILE |
| 1 | N | 26 | GLU |
| 1 | N | 144 | ARG |
| 1 | N | 176 | THR |
| 1 | N | 182 | PRO |
| 1 | N | 221 | PRO |
| 1 | N | 241 | PRO |
| 1 | N | 390 | TYR |
| 1 | O | 303 | ASP |
| 1 | O | 322 | GLY |
| 1 | O | 470 | LEU |
| 1 | A | 41 | ARG |
| 1 | A | 139 | ALA |
| 1 | A | 142 | ASP |
| 1 | A | 201 | VAL |
| 1 | A | 249 | TYR |
| 1 | B | 337 | THR |
| 1 | B | 357 | ASN |
| 1 | C | 182 | PRO |
| 1 | C | 340 | THR |
| 1 | D | 26 | GLU |
| 1 | D | 93 | PRO |
| 1 | D | 182 | PRO |
| 1 | E | 179 | ALA |
| 1 | E | 245 | SER |
| 1 | F | 25 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 63 | PRO |
| 1 | F | 299 | MET |
| 1 | F | 349 | SER |
| 1 | G | 211 | THR |
| 1 | G | 293 | PRO |
| 1 | G | 325 | TRP |
| 1 | G | 351 | SER |
| 1 | H | 93 | PRO |
| 1 | H | 176 | THR |
| 1 | I | 185 | CYS |
| 1 | I | 316 | ALA |
| 1 | I | 352 | GLU |
| 1 | I | 397 | THR |
| 1 | J | 173 | SER |
| 1 | J | 398 | ILE |
| 1 | K | 41 | ARG |
| 1 | K | 138 | ASN |
| 1 | K | 293 | PRO |
| 1 | K | 316 | ALA |
| 1 | L | 93 | PRO |
| 1 | L | 177 | GLN |
| 1 | L | 185 | CYS |
| 1 | L | 352 | GLU |
| 1 | L | 357 | ASN |
| 1 | M | 144 | ARG |
| 1 | M | 239 | SER |
| 1 | M | 241 | PRO |
| 1 | M | 400 | GLU |
| 1 | N | 184 | ASP |
| 1 | N | 235 | ILE |
| 1 | N | 468 | PHE |
| 1 | O | 63 | PRO |
| 1 | O | 138 | ASN |
| 1 | O | 245 | SER |
| 1 | A | 182 | PRO |
| 1 | B | 63 | PRO |
| 1 | B | 124 | ASN |
| 1 | B | 138 | ASN |
| 1 | C | 26 | GLU |
| 1 | C | 185 | CYS |
| 1 | C | 208 | MET |
| 1 | C | 293 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 168 | HIS |
| 1 | D | 173 | SER |
| 1 | E | 86 | PRO |
| 1 | E | 233 | ASP |
| 1 | E | 293 | PRO |
| 1 | E | 458 | ASP |
| 1 | F | 185 | CYS |
| 1 | F | 208 | MET |
| 1 | F | 303 | ASP |
| 1 | G | 63 | PRO |
| 1 | G | 82 | LYS |
| 1 | H | 218 | SER |
| 1 | H | 276 | TYR |
| 1 | H | 303 | ASP |
| 1 | I | 151 | TYR |
| 1 | I | 221 | PRO |
| 1 | I | 288 | SER |
| 1 | J | 303 | ASP |
| 1 | K | 185 | CYS |
| 1 | K | 241 | PRO |
| 1 | L | 241 | PRO |
| 1 | M | 235 | ILE |
| 1 | M | 316 | ALA |
| 1 | N | 398 | ILE |
| 1 | O | 93 | PRO |
| 1 | O | 235 | ILE |
| 1 | O | 293 | PRO |
| 1 | A | 173 | SER |
| 1 | A | 357 | ASN |
| 1 | B | 81 | ASN |
| 1 | B | 245 | SER |
| 1 | B | 387 | VAL |
| 1 | C | 323 | ILE |
| 1 | C | 351 | SER |
| 1 | E | 182 | PRO |
| 1 | E | 322 | GLY |
| 1 | F | 357 | ASN |
| 1 | G | 93 | PRO |
| 1 | G | 151 | TYR |
| 1 | G | 387 | VAL |
| 1 | H | 63 | PRO |
| 1 | H | 390 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 93 | PRO |
| 1 | J | 201 | VAL |
| 1 | J | 458 | ASP |
| 1 | L | 142 | ASP |
| 1 | L | 243 | GLY |
| 1 | L | 391 | ILE |
| 1 | O | 185 | CYS |
| 1 | O | 388 | MET |
| 1 | C | 63 | PRO |
| 1 | E | 178 | VAL |
| 1 | F | 267 | VAL |
| 1 | J | 45 | VAL |
| 1 | J | 281 | GLY |
| 1 | K | 93 | PRO |
| 1 | L | 267 | VAL |
| 1 | L | 322 | GLY |
| 1 | O | 387 | VAL |
| 1 | E | 93 | PRO |
| 1 | G | 297 | GLY |
| 1 | I | 297 | GLY |
| 1 | O | 201 | VAL |
| 1 | A | 281 | GLY |
| 1 | B | 281 | GLY |
| 1 | E | 235 | ILE |
| 1 | G | 185 | CYS |
| 1 | G | 398 | ILE |
| 1 | H | 241 | PRO |
| 1 | D | 84 | GLY |
| 1 | D | 107 | VAL |
| 1 | D | 221 | PRO |
| 1 | E | 241 | PRO |
| 1 | J | 195 | ILE |
| 1 | N | 178 | VAL |
| 1 | B | 293 | PRO |
| 1 | D | 63 | PRO |
| 1 | D | 86 | PRO |
| 1 | J | 182 | PRO |
| 1 | K | 235 | ILE |
| 1 | O | 182 | PRO |
| 1 | O | 241 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 367/368 (100%) | 304 (83%) | 63 (17%) | 2 13 |
| 1 | B | 367/368 (100%) | 302 (82%) | 65 (18%) | 2 12 |
| 1 | C | 367/368 (100%) | 300 (82%) | 67 (18%) | 1 10 |
| 1 | D | 367/368 (100%) | 308 (84%) | 59 (16%) | 2 15 |
| 1 | E | 367/368 (100%) | 299 (82%) | 68 (18%) | 1 10 |
| 1 | F | 367/368 (100%) | 305 (83%) | 62 (17%) | 2 13 |
| 1 | G | 367/368 (100%) | 303 (83%) | 64 (17%) | 2 12 |
| 1 | H | 367/368 (100%) | 302 (82%) | 65 (18%) | 2 12 |
| 1 | I | 367/368 (100%) | 310 (84%) | 57 (16%) | 2 17 |
| 1 | J | 367/368 (100%) | 311 (85%) | 56 (15%) | 2 17 |
| 1 | K | 367/368 (100%) | 300 (82%) | 67 (18%) | 1 10 |
| 1 | L | 367/368 (100%) | 312 (85%) | 55 (15%) | 3 18 |
| 1 | M | 367/368 (100%) | 305 (83%) | 62 (17%) | 2 13 |
| 1 | N | 367/368 (100%) | 296 (81%) | 71 (19%) | 1 9 |
| 1 | O | 367/368 (100%) | 307 (84%) | 60 (16%) | 2 15 |
| All | All | 5505/5520 (100%) | 4564 (83%) | 941 (17%) | 2 13 |

All (941) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 32 | ASN |
| 1 | A | 43 | LEU |
| 1 | A | 54 | LYS |
| 1 | A | 58 | ASN |
| 1 | A | 61 | LEU |
| 1 | A | 63 | PRO |
| 1 | A | 64 | LYS |
| 1 | A | 66 | SER |
| 1 | A | 91 | TYR |
| 1 | A | 95 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 97 | ARG |
| 1 | A | 129 | THR |
| 1 | A | 135 | TYR |
| 1 | A | 145 | GLU |
| 1 | A | 149 | MET |
| 1 | A | 156 | LEU |
| 1 | A | 173 | SER |
| 1 | A | 176 | THR |
| 1 | A | 180 | VAL |
| 1 | A | 182 | PRO |
| 1 | A | 184 | ASP |
| 1 | A | 188 | LEU |
| 1 | A | 190 | LEU |
| 1 | A | 193 | THR |
| 1 | A | 197 | ASP |
| 1 | A | 219 | GLU |
| 1 | A | 220 | VAL |
| 1 | A | 222 | LEU |
| 1 | A | 224 | ILE |
| 1 | A | 229 | CYS |
| 1 | A | 244 | ASP |
| 1 | A | 246 | LEU |
| 1 | A | 247 | PHE |
| 1 | A | 250 | LEU |
| 1 | A | 252 | ARG |
| 1 | A | 255 | MET |
| 1 | A | 257 | VAL |
| 1 | A | 258 | ARG |
| 1 | A | 262 | ASN |
| 1 | A | 274 | ASP |
| 1 | A | 277 | ILE |
| 1 | A | 280 | SER |
| 1 | A | 286 | LEU |
| 1 | A | 291 | TYR |
| 1 | A | 295 | PRO |
| 1 | A | 296 | SER |
| 1 | A | 308 | ASN |
| 1 | A | 315 | ARG |
| 1 | A | 317 | GLN |
| 1 | A | 329 | LEU |
| 1 | A | 337 | THR |
| 1 | A | 341 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 344 | LEU |
| 1 | A | 352 | GLU |
| 1 | A | 353 | THR |
| 1 | A | 357 | ASN |
| 1 | A | 388 | MET |
| 1 | A | 395 | ASN |
| 1 | A | 442 | LYS |
| 1 | A | 443 | LYS |
| 1 | A | 464 | LEU |
| 1 | A | 470 | LEU |
| 1 | A | 472 | LEU |
| 1 | B | 23 | SER |
| 1 | B | 31 | THR |
| 1 | B | 32 | ASN |
| 1 | B | 52 | ILE |
| 1 | B | 54 | LYS |
| 1 | B | 56 | ASN |
| 1 | B | 66 | SER |
| 1 | B | 91 | TYR |
| 1 | B | 95 | THR |
| 1 | B | 97 | ARG |
| 1 | B | 113 | LEU |
| 1 | B | 122 | LEU |
| 1 | B | 127 | ASP |
| 1 | B | 135 | TYR |
| 1 | B | 145 | GLU |
| 1 | B | 149 | MET |
| 1 | B | 153 | GLN |
| 1 | B | 167 | GLU |
| 1 | B | 174 | PRO |
| 1 | B | 182 | PRO |
| 1 | B | 184 | ASP |
| 1 | B | 187 | PRO |
| 1 | B | 188 | LEU |
| 1 | B | 193 | THR |
| 1 | B | 197 | ASP |
| 1 | B | 218 | SER |
| 1 | B | 222 | LEU |
| 1 | B | 244 | ASP |
| 1 | B | 246 | LEU |
| 1 | B | 247 | PHE |
| 1 | B | 250 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 252 | ARG |
| 1 | B | 255 | MET |
| 1 | B | 257 | VAL |
| 1 | B | 262 | ASN |
| 1 | B | 273 | ASP |
| 1 | B | 274 | ASP |
| 1 | B | 282 | SER |
| 1 | B | 288 | SER |
| 1 | B | 292 | PHE |
| 1 | B | 293 | PRO |
| 1 | B | 294 | THR |
| 1 | B | 295 | PRO |
| 1 | B | 301 | THR |
| 1 | B | 315 | ARG |
| 1 | B | 317 | GLN |
| 1 | B | 329 | LEU |
| 1 | B | 332 | THR |
| 1 | B | 341 | ASN |
| 1 | B | 342 | MET |
| 1 | B | 343 | SER |
| 1 | B | 344 | LEU |
| 1 | B | 352 | GLU |
| 1 | B | 353 | THR |
| 1 | B | 357 | ASN |
| 1 | B | 358 | THR |
| 1 | B | 386 | ASP |
| 1 | B | 395 | ASN |
| 1 | B | 402 | TRP |
| 1 | B | 442 | LYS |
| 1 | B | 443 | LYS |
| 1 | B | 461 | GLN |
| 1 | B | 464 | LEU |
| 1 | B | 470 | LEU |
| 1 | B | 472 | LEU |
| 1 | C | 23 | SER |
| 1 | C | 31 | THR |
| 1 | C | 32 | ASN |
| 1 | C | 43 | LEU |
| 1 | C | 51 | PRO |
| 1 | C | 54 | LYS |
| 1 | C | 57 | ASN |
| 1 | C | 63 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 66 | SER |
| 1 | C | 71 | ARG |
| 1 | C | 91 | TYR |
| 1 | C | 95 | THR |
| 1 | C | 97 | ARG |
| 1 | C | 129 | THR |
| 1 | C | 143 | ASN |
| 1 | C | 145 | GLU |
| 1 | C | 148 | SER |
| 1 | C | 149 | MET |
| 1 | C | 155 | GLN |
| 1 | C | 157 | CYS |
| 1 | C | 175 | CYS |
| 1 | C | 177 | GLN |
| 1 | C | 180 | VAL |
| 1 | C | 184 | ASP |
| 1 | C | 187 | PRO |
| 1 | C | 188 | LEU |
| 1 | C | 190 | LEU |
| 1 | C | 193 | THR |
| 1 | C | 212 | THR |
| 1 | C | 213 | LEU |
| 1 | C | 219 | GLU |
| 1 | C | 220 | VAL |
| 1 | C | 223 | ASP |
| 1 | C | 224 | ILE |
| 1 | C | 225 | CYS |
| 1 | C | 228 | ILE |
| 1 | C | 244 | ASP |
| 1 | C | 247 | PHE |
| 1 | C | 250 | LEU |
| 1 | C | 252 | ARG |
| 1 | C | 255 | MET |
| 1 | C | 258 | ARG |
| 1 | C | 262 | ASN |
| 1 | C | 274 | ASP |
| 1 | C | 280 | SER |
| 1 | C | 282 | SER |
| 1 | C | 292 | PHE |
| 1 | C | 293 | PRO |
| 1 | C | 294 | THR |
| 1 | C | 302 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 315 | ARG |
| 1 | C | 317 | GLN |
| 1 | C | 329 | LEU |
| 1 | C | 332 | THR |
| 1 | C | 336 | THR |
| 1 | C | 338 | ARG |
| 1 | C | 340 | THR |
| 1 | C | 341 | ASN |
| 1 | C | 344 | LEU |
| 1 | C | 352 | GLU |
| 1 | C | 374 | PHE |
| 1 | C | 442 | LYS |
| 1 | C | 443 | LYS |
| 1 | C | 449 | VAL |
| 1 | C | 464 | LEU |
| 1 | C | 470 | LEU |
| 1 | C | 472 | LEU |
| 1 | D | 23 | SER |
| 1 | D | 32 | ASN |
| 1 | D | 53 | LYS |
| 1 | D | 54 | LYS |
| 1 | D | 56 | ASN |
| 1 | D | 68 | LEU |
| 1 | D | 71 | ARG |
| 1 | D | 91 | TYR |
| 1 | D | 97 | ARG |
| 1 | D | 129 | THR |
| 1 | D | 135 | TYR |
| 1 | D | 145 | GLU |
| 1 | D | 149 | MET |
| 1 | D | 154 | THR |
| 1 | D | 155 | GLN |
| 1 | D | 163 | PRO |
| 1 | D | 175 | CYS |
| 1 | D | 180 | VAL |
| 1 | D | 182 | PRO |
| 1 | D | 184 | ASP |
| 1 | D | 188 | LEU |
| 1 | D | 193 | THR |
| 1 | D | 224 | ILE |
| 1 | D | 227 | SER |
| 1 | D | 246 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 247 | PHE |
| 1 | D | 250 | LEU |
| 1 | D | 255 | MET |
| 1 | D | 257 | VAL |
| 1 | D | 262 | ASN |
| 1 | D | 273 | ASP |
| 1 | D | 274 | ASP |
| 1 | D | 282 | SER |
| 1 | D | 292 | PHE |
| 1 | D | 295 | PRO |
| 1 | D | 308 | ASN |
| 1 | D | 315 | ARG |
| 1 | D | 317 | GLN |
| 1 | D | 329 | LEU |
| 1 | D | 332 | THR |
| 1 | D | 336 | THR |
| 1 | D | 338 | ARG |
| 1 | D | 341 | ASN |
| 1 | D | 342 | MET |
| 1 | D | 344 | LEU |
| 1 | D | 352 | GLU |
| 1 | D | 353 | THR |
| 1 | D | 357 | ASN |
| 1 | D | 358 | THR |
| 1 | D | 361 | LYS |
| 1 | D | 365 | ARG |
| 1 | D | 372 | LEU |
| 1 | D | 384 | THR |
| 1 | D | 395 | ASN |
| 1 | D | 443 | LYS |
| 1 | D | 459 | LEU |
| 1 | D | 460 | ASP |
| 1 | D | 464 | LEU |
| 1 | D | 470 | LEU |
| 1 | E | 23 | SER |
| 1 | E | 32 | ASN |
| 1 | E | 49 | TYR |
| 1 | E | 54 | LYS |
| 1 | E | 57 | ASN |
| 1 | E | 66 | SER |
| 1 | E | 71 | ARG |
| 1 | E | 91 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 97 | ARG |
| 1 | E | 117 | ILE |
| 1 | E | 122 | LEU |
| 1 | E | 127 | ASP |
| 1 | E | 129 | THR |
| 1 | E | 135 | TYR |
| 1 | E | 145 | GLU |
| 1 | E | 149 | MET |
| 1 | E | 153 | GLN |
| 1 | E | 154 | THR |
| 1 | E | 163 | PRO |
| 1 | E | 167 | GLU |
| 1 | E | 174 | PRO |
| 1 | E | 175 | CYS |
| 1 | E | 180 | VAL |
| 1 | E | 182 | PRO |
| 1 | E | 184 | ASP |
| 1 | E | 187 | PRO |
| 1 | E | 188 | LEU |
| 1 | E | 193 | THR |
| 1 | E | 197 | ASP |
| 1 | E | 212 | THR |
| 1 | E | 219 | GLU |
| 1 | E | 227 | SER |
| 1 | E | 229 | CYS |
| 1 | E | 239 | SER |
| 1 | E | 246 | LEU |
| 1 | E | 247 | PHE |
| 1 | E | 250 | LEU |
| 1 | E | 252 | ARG |
| 1 | E | 255 | MET |
| 1 | E | 257 | VAL |
| 1 | E | 262 | ASN |
| 1 | E | 273 | ASP |
| 1 | E | 277 | ILE |
| 1 | E | 280 | SER |
| 1 | E | 294 | THR |
| 1 | E | 295 | PRO |
| 1 | E | 301 | THR |
| 1 | E | 315 | ARG |
| 1 | E | 317 | GLN |
| 1 | E | 329 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 332 | THR |
| 1 | E | 336 | THR |
| 1 | E | 337 | THR |
| 1 | E | 341 | ASN |
| 1 | E | 344 | LEU |
| 1 | E | 345 | CYS |
| 1 | E | 352 | GLU |
| 1 | E | 357 | ASN |
| 1 | E | 358 | THR |
| 1 | E | 386 | ASP |
| 1 | E | 395 | ASN |
| 1 | E | 443 | LYS |
| 1 | E | 445 | THR |
| 1 | E | 449 | VAL |
| 1 | E | 460 | ASP |
| 1 | E | 464 | LEU |
| 1 | E | 470 | LEU |
| 1 | E | 472 | LEU |
| 1 | F | 32 | ASN |
| 1 | F | 54 | LYS |
| 1 | F | 58 | ASN |
| 1 | F | 66 | SER |
| 1 | F | 72 | VAL |
| 1 | F | 91 | TYR |
| 1 | F | 97 | ARG |
| 1 | F | 122 | LEU |
| 1 | F | 127 | ASP |
| 1 | F | 129 | THR |
| 1 | F | 145 | GLU |
| 1 | F | 148 | SER |
| 1 | F | 149 | MET |
| 1 | F | 153 | GLN |
| 1 | F | 154 | THR |
| 1 | F | 167 | GLU |
| 1 | F | 173 | SER |
| 1 | F | 174 | PRO |
| 1 | F | 176 | THR |
| 1 | F | 180 | VAL |
| 1 | F | 182 | PRO |
| 1 | F | 184 | ASP |
| 1 | F | 187 | PRO |
| 1 | F | 188 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 193 | THR |
| 1 | F | 222 | LEU |
| 1 | F | 224 | ILE |
| 1 | F | 225 | CYS |
| 1 | F | 229 | CYS |
| 1 | F | 246 | LEU |
| 1 | F | 247 | PHE |
| 1 | F | 250 | LEU |
| 1 | F | 252 | ARG |
| 1 | F | 255 | MET |
| 1 | F | 257 | VAL |
| 1 | F | 260 | LEU |
| 1 | F | 262 | ASN |
| 1 | F | 274 | ASP |
| 1 | F | 277 | ILE |
| 1 | F | 294 | THR |
| 1 | F | 310 | PRO |
| 1 | F | 315 | ARG |
| 1 | F | 317 | GLN |
| 1 | F | 320 | ASN |
| 1 | F | 329 | LEU |
| 1 | F | 332 | THR |
| 1 | F | 336 | THR |
| 1 | F | 341 | ASN |
| 1 | F | 343 | SER |
| 1 | F | 344 | LEU |
| 1 | F | 353 | THR |
| 1 | F | 358 | THR |
| 1 | F | 365 | ARG |
| 1 | F | 384 | THR |
| 1 | F | 386 | ASP |
| 1 | F | 388 | MET |
| 1 | F | 395 | ASN |
| 1 | F | 396 | SER |
| 1 | F | 443 | LYS |
| 1 | F | 464 | LEU |
| 1 | F | 470 | LEU |
| 1 | F | 472 | LEU |
| 1 | G | 23 | SER |
| 1 | G | 32 | ASN |
| 1 | G | 52 | ILE |
| 1 | G | 54 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 57 | ASN |
| 1 | G | 61 | LEU |
| 1 | G | 66 | SER |
| 1 | G | 71 | ARG |
| 1 | G | 77 | LEU |
| 1 | G | 91 | TYR |
| 1 | G | 97 | ARG |
| 1 | G | 102 | CYS |
| 1 | G | 122 | LEU |
| 1 | G | 129 | THR |
| 1 | G | 135 | TYR |
| 1 | G | 145 | GLU |
| 1 | G | 149 | MET |
| 1 | G | 153 | GLN |
| 1 | G | 180 | VAL |
| 1 | G | 184 | ASP |
| 1 | G | 187 | PRO |
| 1 | G | 188 | LEU |
| 1 | G | 193 | THR |
| 1 | G | 219 | GLU |
| 1 | G | 223 | ASP |
| 1 | G | 224 | ILE |
| 1 | G | 225 | CYS |
| 1 | G | 228 | ILE |
| 1 | G | 229 | CYS |
| 1 | G | 244 | ASP |
| 1 | G | 247 | PHE |
| 1 | G | 250 | LEU |
| 1 | G | 252 | ARG |
| 1 | G | 255 | MET |
| 1 | G | 258 | ARG |
| 1 | G | 262 | ASN |
| 1 | G | 272 | PRO |
| 1 | G | 274 | ASP |
| 1 | G | 280 | SER |
| 1 | G | 282 | SER |
| 1 | G | 286 | LEU |
| 1 | G | 292 | PHE |
| 1 | G | 293 | PRO |
| 1 | G | 299 | MET |
| 1 | G | 303 | ASP |
| 1 | G | 315 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 317 | GLN |
| 1 | G | 329 | LEU |
| 1 | G | 332 | THR |
| 1 | G | 341 | ASN |
| 1 | G | 343 | SER |
| 1 | G | 344 | LEU |
| 1 | G | 345 | CYS |
| 1 | G | 348 | ILE |
| 1 | G | 352 | GLU |
| 1 | G | 353 | THR |
| 1 | G | 391 | ILE |
| 1 | G | 395 | ASN |
| 1 | G | 442 | LYS |
| 1 | G | 443 | LYS |
| 1 | G | 461 | GLN |
| 1 | G | 463 | PRO |
| 1 | G | 464 | LEU |
| 1 | G | 472 | LEU |
| 1 | H | 31 | THR |
| 1 | H | 32 | ASN |
| 1 | H | 54 | LYS |
| 1 | H | 56 | ASN |
| 1 | H | 59 | LYS |
| 1 | H | 66 | SER |
| 1 | H | 68 | LEU |
| 1 | H | 71 | ARG |
| 1 | H | 91 | TYR |
| 1 | H | 97 | ARG |
| 1 | H | 112 | PRO |
| 1 | H | 129 | THR |
| 1 | H | 135 | TYR |
| 1 | H | 145 | GLU |
| 1 | H | 149 | MET |
| 1 | H | 153 | GLN |
| 1 | H | 174 | PRO |
| 1 | H | 175 | CYS |
| 1 | H | 180 | VAL |
| 1 | H | 182 | PRO |
| 1 | H | 184 | ASP |
| 1 | H | 186 | PRO |
| 1 | H | 187 | PRO |
| 1 | H | 188 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 193 | THR |
| 1 | H | 217 | LYS |
| 1 | H | 218 | SER |
| 1 | H | 222 | LEU |
| 1 | H | 227 | SER |
| 1 | H | 232 | PRO |
| 1 | H | 246 | LEU |
| 1 | H | 247 | PHE |
| 1 | H | 250 | LEU |
| 1 | H | 252 | ARG |
| 1 | H | 255 | MET |
| 1 | H | 257 | VAL |
| 1 | H | 258 | ARG |
| 1 | H | 262 | ASN |
| 1 | H | 274 | ASP |
| 1 | H | 292 | PHE |
| 1 | H | 293 | PRO |
| 1 | H | 294 | THR |
| 1 | H | 300 | VAL |
| 1 | H | 303 | ASP |
| 1 | H | 308 | ASN |
| 1 | H | 310 | PRO |
| 1 | H | 315 | ARG |
| 1 | H | 317 | GLN |
| 1 | H | 329 | LEU |
| 1 | H | 332 | THR |
| 1 | H | 336 | THR |
| 1 | H | 341 | ASN |
| 1 | H | 344 | LEU |
| 1 | H | 353 | THR |
| 1 | H | 357 | ASN |
| 1 | H | 358 | THR |
| 1 | H | 380 | LYS |
| 1 | H | 384 | THR |
| 1 | H | 395 | ASN |
| 1 | H | 396 | SER |
| 1 | H | 399 | LEU |
| 1 | H | 402 | TRP |
| 1 | H | 443 | LYS |
| 1 | H | 460 | ASP |
| 1 | H | 470 | LEU |
| 1 | I | 21 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 32 | ASN |
| 1 | I | 54 | LYS |
| 1 | I | 57 | ASN |
| 1 | I | 66 | SER |
| 1 | I | 71 | ARG |
| 1 | I | 77 | LEU |
| 1 | I | 91 | TYR |
| 1 | I | 97 | ARG |
| 1 | I | 135 | TYR |
| 1 | I | 145 | GLU |
| 1 | I | 146 | CYS |
| 1 | I | 148 | SER |
| 1 | I | 149 | MET |
| 1 | I | 150 | ASP |
| 1 | I | 153 | GLN |
| 1 | I | 156 | LEU |
| 1 | I | 174 | PRO |
| 1 | I | 180 | VAL |
| 1 | I | 184 | ASP |
| 1 | I | 218 | SER |
| 1 | I | 220 | VAL |
| 1 | I | 221 | PRO |
| 1 | I | 224 | ILE |
| 1 | I | 244 | ASP |
| 1 | I | 247 | PHE |
| 1 | I | 250 | LEU |
| 1 | I | 252 | ARG |
| 1 | I | 256 | PHE |
| 1 | I | 257 | VAL |
| 1 | I | 260 | LEU |
| 1 | I | 262 | ASN |
| 1 | I | 274 | ASP |
| 1 | I | 277 | ILE |
| 1 | I | 291 | TYR |
| 1 | I | 292 | PHE |
| 1 | I | 295 | PRO |
| 1 | I | 303 | ASP |
| 1 | I | 315 | ARG |
| 1 | I | 317 | GLN |
| 1 | I | 329 | LEU |
| 1 | I | 332 | THR |
| 1 | I | 337 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 341 | ASN |
| 1 | I | 344 | LEU |
| 1 | I | 345 | CYS |
| 1 | I | 352 | GLU |
| 1 | I | 353 | THR |
| 1 | I | 357 | ASN |
| 1 | I | 358 | THR |
| 1 | I | 384 | THR |
| 1 | I | 395 | ASN |
| 1 | I | 438 | GLU |
| 1 | I | 443 | LYS |
| 1 | I | 460 | ASP |
| 1 | I | 464 | LEU |
| 1 | I | 470 | LEU |
| 1 | J | 32 | ASN |
| 1 | J | 54 | LYS |
| 1 | J | 57 | ASN |
| 1 | J | 66 | SER |
| 1 | J | 71 | ARG |
| 1 | J | 74 | ARG |
| 1 | J | 91 | TYR |
| 1 | J | 94 | ASP |
| 1 | J | 97 | ARG |
| 1 | J | 117 | ILE |
| 1 | J | 129 | THR |
| 1 | J | 145 | GLU |
| 1 | J | 149 | MET |
| 1 | J | 156 | LEU |
| 1 | J | 163 | PRO |
| 1 | J | 173 | SER |
| 1 | J | 180 | VAL |
| 1 | J | 182 | PRO |
| 1 | J | 184 | ASP |
| 1 | J | 187 | PRO |
| 1 | J | 190 | LEU |
| 1 | J | 193 | THR |
| 1 | J | 197 | ASP |
| 1 | J | 219 | GLU |
| 1 | J | 224 | ILE |
| 1 | J | 225 | CYS |
| 1 | J | 244 | ASP |
| 1 | J | 246 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 247 | PHE |
| 1 | J | 250 | LEU |
| 1 | J | 252 | ARG |
| 1 | J | 253 | GLU |
| 1 | J | 255 | MET |
| 1 | J | 257 | VAL |
| 1 | J | 258 | ARG |
| 1 | J | 262 | ASN |
| 1 | J | 273 | ASP |
| 1 | J | 290 | ASN |
| 1 | J | 291 | TYR |
| 1 | J | 295 | PRO |
| 1 | J | 303 | ASP |
| 1 | J | 308 | ASN |
| 1 | J | 315 | ARG |
| 1 | J | 317 | GLN |
| 1 | J | 329 | LEU |
| 1 | J | 332 | THR |
| 1 | J | 337 | THR |
| 1 | J | 341 | ASN |
| 1 | J | 344 | LEU |
| 1 | J | 345 | CYS |
| 1 | J | 353 | THR |
| 1 | J | 383 | LEU |
| 1 | J | 386 | ASP |
| 1 | J | 443 | LYS |
| 1 | J | 464 | LEU |
| 1 | J | 470 | LEU |
| 1 | K | 31 | THR |
| 1 | K | 32 | ASN |
| 1 | K | 54 | LYS |
| 1 | K | 57 | ASN |
| 1 | K | 66 | SER |
| 1 | K | 87 | ASP |
| 1 | K | 91 | TYR |
| 1 | K | 97 | ARG |
| 1 | K | 129 | THR |
| 1 | K | 135 | TYR |
| 1 | K | 145 | GLU |
| 1 | K | 149 | MET |
| 1 | K | 153 | GLN |
| 1 | K | 154 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 180 | VAL |
| 1 | K | 182 | PRO |
| 1 | K | 184 | ASP |
| 1 | K | 187 | PRO |
| 1 | K | 188 | LEU |
| 1 | K | 193 | THR |
| 1 | K | 212 | THR |
| 1 | K | 219 | GLU |
| 1 | K | 224 | ILE |
| 1 | K | 227 | SER |
| 1 | K | 228 | ILE |
| 1 | K | 232 | PRO |
| 1 | K | 240 | GLU |
| 1 | K | 245 | SER |
| 1 | K | 246 | LEU |
| 1 | K | 247 | PHE |
| 1 | K | 250 | LEU |
| 1 | K | 251 | ARG |
| 1 | K | 252 | ARG |
| 1 | K | 255 | MET |
| 1 | K | 257 | VAL |
| 1 | K | 258 | ARG |
| 1 | K | 262 | ASN |
| 1 | K | 273 | ASP |
| 1 | K | 274 | ASP |
| 1 | K | 283 | THR |
| 1 | K | 292 | PHE |
| 1 | K | 295 | PRO |
| 1 | K | 298 | SER |
| 1 | K | 308 | ASN |
| 1 | K | 315 | ARG |
| 1 | K | 317 | GLN |
| 1 | K | 329 | LEU |
| 1 | K | 330 | PHE |
| 1 | K | 332 | THR |
| 1 | K | 337 | THR |
| 1 | K | 338 | ARG |
| 1 | K | 341 | ASN |
| 1 | K | 342 | MET |
| 1 | K | 344 | LEU |
| 1 | K | 352 | GLU |
| 1 | K | 357 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 358 | THR |
| 1 | K | 395 | ASN |
| 1 | K | 399 | LEU |
| 1 | K | 402 | TRP |
| 1 | K | 442 | LYS |
| 1 | K | 443 | LYS |
| 1 | K | 445 | THR |
| 1 | K | 456 | SER |
| 1 | K | 461 | GLN |
| 1 | K | 464 | LEU |
| 1 | K | 470 | LEU |
| 1 | L | 23 | SER |
| 1 | L | 32 | ASN |
| 1 | L | 52 | ILE |
| 1 | L | 54 | LYS |
| 1 | L | 56 | ASN |
| 1 | L | 57 | ASN |
| 1 | L | 61 | LEU |
| 1 | L | 63 | PRO |
| 1 | L | 66 | SER |
| 1 | L | 71 | ARG |
| 1 | L | 91 | TYR |
| 1 | L | 95 | THR |
| 1 | L | 97 | ARG |
| 1 | L | 117 | ILE |
| 1 | L | 145 | GLU |
| 1 | L | 149 | MET |
| 1 | L | 154 | THR |
| 1 | L | 167 | GLU |
| 1 | L | 175 | CYS |
| 1 | L | 180 | VAL |
| 1 | L | 184 | ASP |
| 1 | L | 187 | PRO |
| 1 | L | 188 | LEU |
| 1 | L | 193 | THR |
| 1 | L | 228 | ILE |
| 1 | L | 229 | CYS |
| 1 | L | 247 | PHE |
| 1 | L | 250 | LEU |
| 1 | L | 252 | ARG |
| 1 | L | 255 | MET |
| 1 | L | 257 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L | 262 | ASN |
| 1 | L | 288 | SER |
| 1 | L | 291 | TYR |
| 1 | L | 292 | PHE |
| 1 | L | 293 | PRO |
| 1 | L | 299 | MET |
| 1 | L | 306 | ILE |
| 1 | L | 310 | PRO |
| 1 | L | 315 | ARG |
| 1 | L | 317 | GLN |
| 1 | L | 329 | LEU |
| 1 | L | 332 | THR |
| 1 | L | 337 | THR |
| 1 | L | 341 | ASN |
| 1 | L | 345 | CYS |
| 1 | L | 349 | SER |
| 1 | L | 352 | GLU |
| 1 | L | 353 | THR |
| 1 | L | 372 | LEU |
| 1 | L | 384 | THR |
| 1 | L | 388 | MET |
| 1 | L | 395 | ASN |
| 1 | L | 443 | LYS |
| 1 | L | 472 | LEU |
| 1 | M | 32 | ASN |
| 1 | M | 51 | PRO |
| 1 | M | 54 | LYS |
| 1 | M | 57 | ASN |
| 1 | M | 63 | PRO |
| 1 | M | 64 | LYS |
| 1 | M | 66 | SER |
| 1 | M | 71 | ARG |
| 1 | M | 91 | TYR |
| 1 | M | 97 | ARG |
| 1 | M | 117 | ILE |
| 1 | M | 129 | THR |
| 1 | M | 145 | GLU |
| 1 | M | 149 | MET |
| 1 | M | 156 | LEU |
| 1 | M | 157 | CYS |
| 1 | M | 173 | SER |
| 1 | M | 175 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 180 | VAL |
| 1 | M | 182 | PRO |
| 1 | M | 184 | ASP |
| 1 | M | 187 | PRO |
| 1 | M | 188 | LEU |
| 1 | M | 193 | THR |
| 1 | M | 219 | GLU |
| 1 | M | 222 | LEU |
| 1 | M | 223 | ASP |
| 1 | M | 224 | ILE |
| 1 | M | 225 | CYS |
| 1 | M | 244 | ASP |
| 1 | M | 247 | PHE |
| 1 | M | 250 | LEU |
| 1 | M | 252 | ARG |
| 1 | M | 254 | GLN |
| 1 | M | 255 | MET |
| 1 | M | 257 | VAL |
| 1 | M | 262 | ASN |
| 1 | M | 273 | ASP |
| 1 | M | 274 | ASP |
| 1 | M | 280 | SER |
| 1 | M | 290 | ASN |
| 1 | M | 293 | PRO |
| 1 | M | 303 | ASP |
| 1 | M | 308 | ASN |
| 1 | M | 315 | ARG |
| 1 | M | 317 | GLN |
| 1 | M | 329 | LEU |
| 1 | M | 332 | THR |
| 1 | M | 336 | THR |
| 1 | M | 338 | ARG |
| 1 | M | 341 | ASN |
| 1 | M | 344 | LEU |
| 1 | M | 345 | CYS |
| 1 | M | 352 | GLU |
| 1 | M | 353 | THR |
| 1 | M | 395 | ASN |
| 1 | M | 399 | LEU |
| 1 | M | 443 | LYS |
| 1 | M | 463 | PRO |
| 1 | M | 464 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 470 | LEU |
| 1 | M | 472 | LEU |
| 1 | N | 31 | THR |
| 1 | N | 32 | ASN |
| 1 | N | 43 | LEU |
| 1 | N | 52 | ILE |
| 1 | N | 54 | LYS |
| 1 | N | 56 | ASN |
| 1 | N | 57 | ASN |
| 1 | N | 66 | SER |
| 1 | N | 71 | ARG |
| 1 | N | 87 | ASP |
| 1 | N | 88 | THR |
| 1 | N | 91 | TYR |
| 1 | N | 97 | ARG |
| 1 | N | 115 | VAL |
| 1 | N | 122 | LEU |
| 1 | N | 129 | THR |
| 1 | N | 135 | TYR |
| 1 | N | 145 | GLU |
| 1 | N | 149 | MET |
| 1 | N | 153 | GLN |
| 1 | N | 154 | THR |
| 1 | N | 161 | CYS |
| 1 | N | 173 | SER |
| 1 | N | 174 | PRO |
| 1 | N | 176 | THR |
| 1 | N | 180 | VAL |
| 1 | N | 182 | PRO |
| 1 | N | 184 | ASP |
| 1 | N | 188 | LEU |
| 1 | N | 193 | THR |
| 1 | N | 225 | CYS |
| 1 | N | 227 | SER |
| 1 | N | 228 | ILE |
| 1 | N | 232 | PRO |
| 1 | N | 246 | LEU |
| 1 | N | 247 | PHE |
| 1 | N | 250 | LEU |
| 1 | N | 255 | MET |
| 1 | N | 257 | VAL |
| 1 | N | 262 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 274 | ASP |
| 1 | N | 277 | ILE |
| 1 | N | 292 | PHE |
| 1 | N | 293 | PRO |
| 1 | N | 294 | THR |
| 1 | N | 303 | ASP |
| 1 | N | 308 | ASN |
| 1 | N | 310 | PRO |
| 1 | N | 311 | TYR |
| 1 | N | 315 | ARG |
| 1 | N | 317 | GLN |
| 1 | N | 329 | LEU |
| 1 | N | 332 | THR |
| 1 | N | 336 | THR |
| 1 | N | 341 | ASN |
| 1 | N | 344 | LEU |
| 1 | N | 345 | CYS |
| 1 | N | 352 | GLU |
| 1 | N | 353 | THR |
| 1 | N | 357 | ASN |
| 1 | N | 365 | ARG |
| 1 | N | 384 | THR |
| 1 | N | 386 | ASP |
| 1 | N | 395 | ASN |
| 1 | N | 402 | TRP |
| 1 | N | 443 | LYS |
| 1 | N | 459 | LEU |
| 1 | N | 461 | GLN |
| 1 | N | 464 | LEU |
| 1 | N | 470 | LEU |
| 1 | N | 472 | LEU |
| 1 | O | 31 | THR |
| 1 | O | 32 | ASN |
| 1 | O | 52 | ILE |
| 1 | O | 54 | LYS |
| 1 | O | 56 | ASN |
| 1 | O | 66 | SER |
| 1 | O | 91 | TYR |
| 1 | O | 97 | ARG |
| 1 | O | 117 | ILE |
| 1 | O | 125 | LYS |
| 1 | O | 127 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 129 | THR |
| 1 | O | 135 | TYR |
| 1 | O | 145 | GLU |
| 1 | O | 148 | SER |
| 1 | O | 149 | MET |
| 1 | O | 167 | GLU |
| 1 | O | 173 | SER |
| 1 | O | 175 | CYS |
| 1 | O | 180 | VAL |
| 1 | O | 182 | PRO |
| 1 | O | 184 | ASP |
| 1 | O | 187 | PRO |
| 1 | O | 188 | LEU |
| 1 | O | 193 | THR |
| 1 | O | 222 | LEU |
| 1 | O | 225 | CYS |
| 1 | O | 228 | ILE |
| 1 | O | 229 | CYS |
| 1 | O | 247 | PHE |
| 1 | O | 250 | LEU |
| 1 | O | 252 | ARG |
| 1 | O | 255 | MET |
| 1 | O | 257 | VAL |
| 1 | O | 262 | ASN |
| 1 | O | 273 | ASP |
| 1 | O | 274 | ASP |
| 1 | O | 280 | SER |
| 1 | O | 282 | SER |
| 1 | O | 292 | PHE |
| 1 | O | 294 | THR |
| 1 | O | 295 | PRO |
| 1 | O | 315 | ARG |
| 1 | O | 317 | GLN |
| 1 | O | 329 | LEU |
| 1 | O | 332 | THR |
| 1 | O | 338 | ARG |
| 1 | O | 341 | ASN |
| 1 | O | 344 | LEU |
| 1 | O | 345 | CYS |
| 1 | O | 352 | GLU |
| 1 | O | 357 | ASN |
| 1 | O | 395 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 441 | LEU |
| 1 | O | 442 | LYS |
| 1 | O | 443 | LYS |
| 1 | O | 461 | GLN |
| 1 | O | 464 | LEU |
| 1 | O | 470 | LEU |
| 1 | O | 472 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (238) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 57 | ASN |
| 1 | A | 69 | GLN |
| 1 | A | 92 | ASN |
| 1 | A | 143 | ASN |
| 1 | A | 153 | GLN |
| 1 | A | 168 | HIS |
| 1 | A | 259 | HIS |
| 1 | A | 262 | ASN |
| 1 | A | 290 | ASN |
| 1 | A | 317 | GLN |
| 1 | A | 319 | HIS |
| 1 | A | 327 | ASN |
| 1 | A | 328 | GLN |
| 1 | A | 366 | HIS |
| 1 | A | 377 | GLN |
| 1 | A | 395 | ASN |
| 1 | A | 403 | ASN |
| 1 | A | 450 | ASN |
| 1 | A | 461 | GLN |
| 1 | B | 57 | ASN |
| 1 | B | 69 | GLN |
| 1 | B | 92 | ASN |
| 1 | B | 153 | GLN |
| 1 | B | 192 | ASN |
| 1 | B | 259 | HIS |
| 1 | B | 262 | ASN |
| 1 | B | 290 | ASN |
| 1 | B | 317 | GLN |
| 1 | B | 373 | GLN |
| 1 | B | 377 | GLN |
| 1 | B | 403 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 461 | GLN |
| 1 | C | 57 | ASN |
| 1 | C | 69 | GLN |
| 1 | C | 92 | ASN |
| 1 | C | 153 | GLN |
| 1 | C | 168 | HIS |
| 1 | C | 259 | HIS |
| 1 | C | 262 | ASN |
| 1 | C | 290 | ASN |
| 1 | C | 314 | GLN |
| 1 | C | 317 | GLN |
| 1 | C | 327 | ASN |
| 1 | C | 328 | GLN |
| 1 | C | 377 | GLN |
| 1 | C | 403 | ASN |
| 1 | D | 57 | ASN |
| 1 | D | 69 | GLN |
| 1 | D | 92 | ASN |
| 1 | D | 143 | ASN |
| 1 | D | 153 | GLN |
| 1 | D | 168 | HIS |
| 1 | D | 259 | HIS |
| 1 | D | 262 | ASN |
| 1 | D | 290 | ASN |
| 1 | D | 317 | GLN |
| 1 | D | 341 | ASN |
| 1 | D | 377 | GLN |
| 1 | D | 395 | ASN |
| 1 | D | 403 | ASN |
| 1 | D | 461 | GLN |
| 1 | E | 57 | ASN |
| 1 | E | 69 | GLN |
| 1 | E | 92 | ASN |
| 1 | E | 153 | GLN |
| 1 | E | 168 | HIS |
| 1 | E | 259 | HIS |
| 1 | E | 262 | ASN |
| 1 | E | 290 | ASN |
| 1 | E | 317 | GLN |
| 1 | E | 319 | HIS |
| 1 | E | 377 | GLN |
| 1 | E | 395 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 403 | ASN |
| 1 | E | 461 | GLN |
| 1 | F | 57 | ASN |
| 1 | F | 69 | GLN |
| 1 | F | 92 | ASN |
| 1 | F | 138 | ASN |
| 1 | F | 153 | GLN |
| 1 | F | 155 | GLN |
| 1 | F | 181 | GLN |
| 1 | F | 254 | GLN |
| 1 | F | 259 | HIS |
| 1 | F | 262 | ASN |
| 1 | F | 290 | ASN |
| 1 | F | 317 | GLN |
| 1 | F | 319 | HIS |
| 1 | F | 377 | GLN |
| 1 | F | 395 | ASN |
| 1 | F | 450 | ASN |
| 1 | F | 461 | GLN |
| 1 | G | 57 | ASN |
| 1 | G | 69 | GLN |
| 1 | G | 92 | ASN |
| 1 | G | 138 | ASN |
| 1 | G | 153 | GLN |
| 1 | G | 168 | HIS |
| 1 | G | 181 | GLN |
| 1 | G | 254 | GLN |
| 1 | G | 259 | HIS |
| 1 | G | 262 | ASN |
| 1 | G | 290 | ASN |
| 1 | G | 317 | GLN |
| 1 | G | 319 | HIS |
| 1 | G | 327 | ASN |
| 1 | G | 328 | GLN |
| 1 | G | 341 | ASN |
| 1 | G | 373 | GLN |
| 1 | G | 377 | GLN |
| 1 | G | 395 | ASN |
| 1 | G | 403 | ASN |
| 1 | G | 450 | ASN |
| 1 | G | 461 | GLN |
| 1 | H | 57 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 69 | GLN |
| 1 | H | 92 | ASN |
| 1 | H | 138 | ASN |
| 1 | H | 153 | GLN |
| 1 | H | 259 | HIS |
| 1 | H | 262 | ASN |
| 1 | H | 290 | ASN |
| 1 | H | 317 | GLN |
| 1 | H | 327 | ASN |
| 1 | H | 377 | GLN |
| 1 | H | 395 | ASN |
| 1 | H | 403 | ASN |
| 1 | H | 461 | GLN |
| 1 | I | 57 | ASN |
| 1 | I | 69 | GLN |
| 1 | I | 92 | ASN |
| 1 | I | 138 | ASN |
| 1 | I | 153 | GLN |
| 1 | I | 168 | HIS |
| 1 | I | 259 | HIS |
| 1 | I | 262 | ASN |
| 1 | I | 290 | ASN |
| 1 | I | 327 | ASN |
| 1 | I | 403 | ASN |
| 1 | I | 461 | GLN |
| 1 | J | 57 | ASN |
| 1 | J | 69 | GLN |
| 1 | J | 138 | ASN |
| 1 | J | 153 | GLN |
| 1 | J | 168 | HIS |
| 1 | J | 192 | ASN |
| 1 | J | 254 | GLN |
| 1 | J | 259 | HIS |
| 1 | J | 262 | ASN |
| 1 | J | 305 | GLN |
| 1 | J | 317 | GLN |
| 1 | J | 319 | HIS |
| 1 | J | 327 | ASN |
| 1 | J | 341 | ASN |
| 1 | J | 395 | ASN |
| 1 | J | 403 | ASN |
| 1 | J | 461 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 57 | ASN |
| 1 | K | 69 | GLN |
| 1 | K | 92 | ASN |
| 1 | K | 138 | ASN |
| 1 | K | 153 | GLN |
| 1 | K | 155 | GLN |
| 1 | K | 168 | HIS |
| 1 | K | 192 | ASN |
| 1 | K | 259 | HIS |
| 1 | K | 262 | ASN |
| 1 | K | 317 | GLN |
| 1 | K | 319 | HIS |
| 1 | K | 341 | ASN |
| 1 | K | 395 | ASN |
| 1 | K | 403 | ASN |
| 1 | K | 450 | ASN |
| 1 | K | 461 | GLN |
| 1 | L | 32 | ASN |
| 1 | L | 57 | ASN |
| 1 | L | 69 | GLN |
| 1 | L | 92 | ASN |
| 1 | L | 138 | ASN |
| 1 | L | 153 | GLN |
| 1 | L | 192 | ASN |
| 1 | L | 262 | ASN |
| 1 | L | 290 | ASN |
| 1 | L | 305 | GLN |
| 1 | L | 317 | GLN |
| 1 | L | 341 | ASN |
| 1 | L | 403 | ASN |
| 1 | L | 461 | GLN |
| 1 | M | 57 | ASN |
| 1 | M | 69 | GLN |
| 1 | M | 92 | ASN |
| 1 | M | 138 | ASN |
| 1 | M | 181 | GLN |
| 1 | M | 192 | ASN |
| 1 | M | 259 | HIS |
| 1 | M | 262 | ASN |
| 1 | M | 290 | ASN |
| 1 | M | 317 | GLN |
| 1 | M | 319 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 328 | GLN |
| 1 | M | 341 | ASN |
| 1 | M | 395 | ASN |
| 1 | M | 403 | ASN |
| 1 | M | 461 | GLN |
| 1 | N | 32 | ASN |
| 1 | N | 57 | ASN |
| 1 | N | 69 | GLN |
| 1 | N | 92 | ASN |
| 1 | N | 96 | GLN |
| 1 | N | 138 | ASN |
| 1 | N | 153 | GLN |
| 1 | N | 168 | HIS |
| 1 | N | 181 | GLN |
| 1 | N | 254 | GLN |
| 1 | N | 259 | HIS |
| 1 | N | 262 | ASN |
| 1 | N | 290 | ASN |
| 1 | N | 317 | GLN |
| 1 | N | 377 | GLN |
| 1 | N | 395 | ASN |
| 1 | N | 403 | ASN |
| 1 | N | 461 | GLN |
| 1 | O | 57 | ASN |
| 1 | O | 69 | GLN |
| 1 | O | 92 | ASN |
| 1 | O | 138 | ASN |
| 1 | O | 153 | GLN |
| 1 | O | 168 | HIS |
| 1 | O | 181 | GLN |
| 1 | O | 262 | ASN |
| 1 | O | 305 | GLN |
| 1 | O | 317 | GLN |
| 1 | O | 319 | HIS |
| 1 | O | 341 | ASN |
| 1 | O | 377 | GLN |
| 1 | O | 395 | ASN |
| 1 | O | 403 | ASN |
| 1 | O | 450 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 419/424 (98%) | -0.52 | 2 (0%) | 91 | 85 | 40, 77, 111, 122 | 0 |
| 1 | B | 419/424 (98%) | -0.53 | 4 (0%) | 82 | 73 | 36, 76, 109, 131 | 0 |
| 1 | C | 419/424 (98%) | -0.48 | 3 (0%) | 87 | 81 | 44, 79, 110, 121 | 0 |
| 1 | D | 419/424 (98%) | -0.48 | 5 (1%) | 79 | 69 | 37, 78, 109, 130 | 0 |
| 1 | E | 419/424 (98%) | -0.45 | 11 (2%) | 56 | 43 | 41, 79, 114, 128 | 0 |
| 1 | F | 419/424 (98%) | -0.45 | 4 (0%) | 82 | 73 | 40, 80, 111, 131 | 0 |
| 1 | G | 419/424 (98%) | -0.42 | 3 (0%) | 87 | 81 | 46, 83, 112, 135 | 0 |
| 1 | H | 419/424 (98%) | -0.48 | 6 (1%) | 75 | 64 | 34, 78, 111, 136 | 0 |
| 1 | I | 419/424 (98%) | -0.42 | 6 (1%) | 75 | 64 | 48, 82, 113, 132 | 0 |
| 1 | J | 419/424 (98%) | -0.42 | 7 (1%) | 70 | 59 | 43, 79, 111, 134 | 0 |
| 1 | K | 419/424 (98%) | -0.53 | 1 (0%) | 95 | 93 | 35, 76, 109, 129 | 0 |
| 1 | L | 419/424 (98%) | -0.56 | 1 (0%) | 95 | 93 | 38, 73, 108, 137 | 0 |
| 1 | M | 419/424 (98%) | -0.54 | 1 (0%) | 95 | 93 | 43, 75, 108, 133 | 0 |
| 1 | N | 419/424 (98%) | -0.45 | 3 (0%) | 87 | 81 | 45, 80, 112, 128 | 0 |
| 1 | O | 419/424 (98%) | -0.42 | 5 (1%) | 79 | 69 | 45, 82, 112, 133 | 0 |
| All | All | 6285/6360 (98%) | -0.48 | 62 (0%) | 82 | 73 | 34, 78, 111, 137 | 0 |

All (62) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | L | 403 | ASN | 6.5 |
| 1 | H | 179 | ALA | 5.7 |
| 1 | O | 403 | ASN | 5.6 |
| 1 | I | 174 | PRO | 5.5 |
| 1 | O | 176 | THR | 5.0 |
| 1 | J | 438 | GLU | 4.6 |
| 1 | D | 174 | PRO | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 175 | CYS | 4.0 |
| 1 | G | 176 | THR | 3.8 |
| 1 | H | 58 | ASN | 3.7 |
| 1 | J | 55 | PRO | 3.7 |
| 1 | E | 56 | ASN | 3.7 |
| 1 | H | 178 | VAL | 3.6 |
| 1 | F | 176 | THR | 3.6 |
| 1 | H | 175 | CYS | 3.5 |
| 1 | D | 56 | ASN | 3.4 |
| 1 | B | 403 | ASN | 3.4 |
| 1 | D | 403 | ASN | 3.2 |
| 1 | E | 176 | THR | 3.2 |
| 1 | C | 175 | CYS | 3.2 |
| 1 | O | 439 | ASP | 3.1 |
| 1 | C | 176 | THR | 2.9 |
| 1 | F | 175 | CYS | 2.8 |
| 1 | I | 173 | SER | 2.8 |
| 1 | F | 174 | PRO | 2.8 |
| 1 | E | 174 | PRO | 2.7 |
| 1 | E | 173 | SER | 2.7 |
| 1 | F | 177 | GLN | 2.7 |
| 1 | C | 403 | ASN | 2.7 |
| 1 | B | 56 | ASN | 2.6 |
| 1 | J | 56 | ASN | 2.5 |
| 1 | E | 403 | ASN | 2.5 |
| 1 | H | 403 | ASN | 2.5 |
| 1 | B | 84 | GLY | 2.4 |
| 1 | O | 438 | GLU | 2.4 |
| 1 | D | 55 | PRO | 2.3 |
| 1 | J | 179 | ALA | 2.3 |
| 1 | J | 177 | GLN | 2.3 |
| 1 | E | 175 | CYS | 2.3 |
| 1 | H | 173 | SER | 2.3 |
| 1 | N | 114 | GLY | 2.3 |
| 1 | A | 401 | ASP | 2.3 |
| 1 | K | 403 | ASN | 2.3 |
| 1 | J | 173 | SER | 2.3 |
| 1 | A | 403 | ASN | 2.2 |
| 1 | E | 392 | HIS | 2.2 |
| 1 | M | 178 | VAL | 2.2 |
| 1 | O | 266 | THR | 2.2 |
| 1 | J | 439 | ASP | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | N | 401 | ASP | 2.2 |
| 1 | E | 93 | PRO | 2.1 |
| 1 | E | 133 | SER | 2.1 |
| 1 | I | 55 | PRO | 2.1 |
| 1 | E | 94 | ASP | 2.1 |
| 1 | I | 403 | ASN | 2.1 |
| 1 | I | 175 | CYS | 2.1 |
| 1 | N | 86 | PRO | 2.1 |
| 1 | G | 56 | ASN | 2.1 |
| 1 | G | 400 | GLU | 2.1 |
| 1 | B | 178 | VAL | 2.0 |
| 1 | I | 349 | SER | 2.0 |
| 1 | E | 55 | PRO | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.