



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:29 am BST

PDB ID : 1W8X
Title : Structural analysis of PRD1
Authors : Abrescia, N.G.A.; Cockburn, J.J.B.; Grimes, J.M.; Sutton, G.C.; Diprose, J.M.; Butcher, S.J.; Fuller, S.D.; San Martin, C.; Burnett, R.M.; Stuart, D.I.; Bamford, D.H.; Bamford, J.K.H.
Deposited on : 2004-10-01
Resolution : 4.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

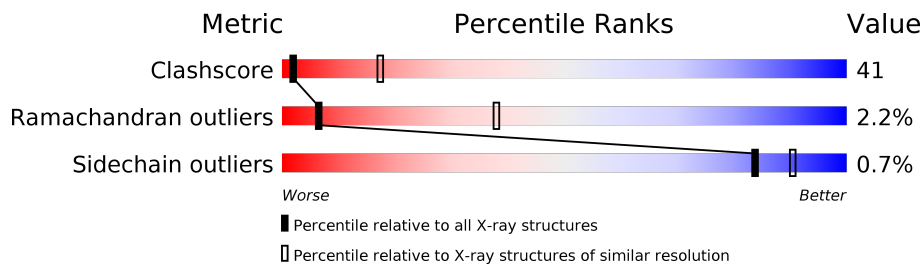
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 1044 (4.60-3.80) |
| Ramachandran outliers | 138981 | 1000 (4.60-3.80) |
| Sidechain outliers | 138945 | 1007 (4.62-3.78) |




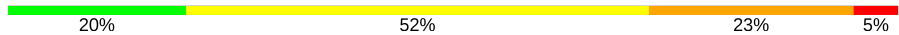
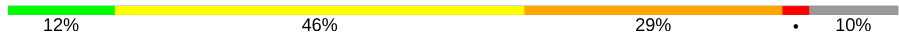
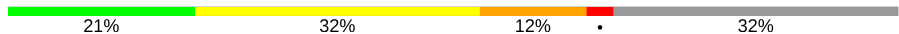
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 395 | |
| 1 | B | 395 | |
| 1 | C | 395 | |
| 1 | D | 395 | |
| 1 | E | 395 | |
| 1 | F | 395 | |
| 1 | G | 395 | |
| 1 | H | 395 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | I | 395 |  72% 20% . . . |
| 1 | J | 395 |  74% 18% 6% .. |
| 1 | K | 395 |  73% 19% . . . |
| 1 | L | 395 |  67% 24% . . . |
| 2 | M | 83 |  20% 52% 23% 5% |
| 3 | N | 126 |  12% 46% 29% . 10% |
| 4 | P | 117 |  21% 32% 12% . 32% |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 38116 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 MAJOR CAPSID PROTEIN (PROTEIN P3).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 380 | Total 2956 | C 1873 | N 503 | O 573 | S 7 | 0 | 0 | 0 |
| 1 | B | 392 | Total 3045 | C 1929 | N 517 | O 592 | S 7 | 0 | 0 | 0 |
| 1 | C | 385 | Total 2999 | C 1901 | N 510 | O 581 | S 7 | 0 | 0 | 0 |
| 1 | D | 392 | Total 3045 | C 1929 | N 517 | O 592 | S 7 | 0 | 0 | 0 |
| 1 | E | 378 | Total 2944 | C 1868 | N 500 | O 569 | S 7 | 0 | 0 | 0 |
| 1 | F | 388 | Total 3009 | C 1908 | N 510 | O 584 | S 7 | 0 | 0 | 0 |
| 1 | G | 375 | Total 2926 | C 1857 | N 496 | O 566 | S 7 | 0 | 0 | 0 |
| 1 | H | 392 | Total 3045 | C 1929 | N 517 | O 592 | S 7 | 0 | 0 | 0 |
| 1 | I | 392 | Total 3045 | C 1929 | N 517 | O 592 | S 7 | 0 | 0 | 0 |
| 1 | J | 390 | Total 3027 | C 1919 | N 514 | O 587 | S 7 | 0 | 0 | 0 |
| 1 | K | 384 | Total 2992 | C 1897 | N 509 | O 579 | S 7 | 0 | 0 | 0 |
| 1 | L | 379 | Total 2953 | C 1873 | N 502 | O 571 | S 7 | 0 | 0 | 0 |

- Molecule 2 is a protein called PROTEIN P30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | M | 83 | Total 638 | C 408 | N 113 | O 114 | S 3 | 0 | 0 | 0 |

- Molecule 3 is a protein called PROTEIN P31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | N | 114 | 872 | 552 | 147 | 169 | 4 | 0 | 0 | 0 |

- Molecule 4 is a protein called PROTEIN P16.

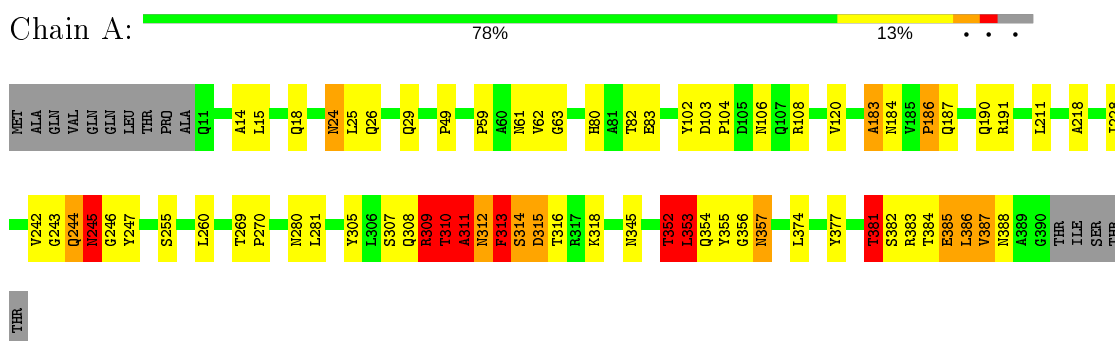
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | P | 80 | 620 | 401 | 103 | 114 | 2 | 0 | 0 | 1 |

3 Residue-property plots

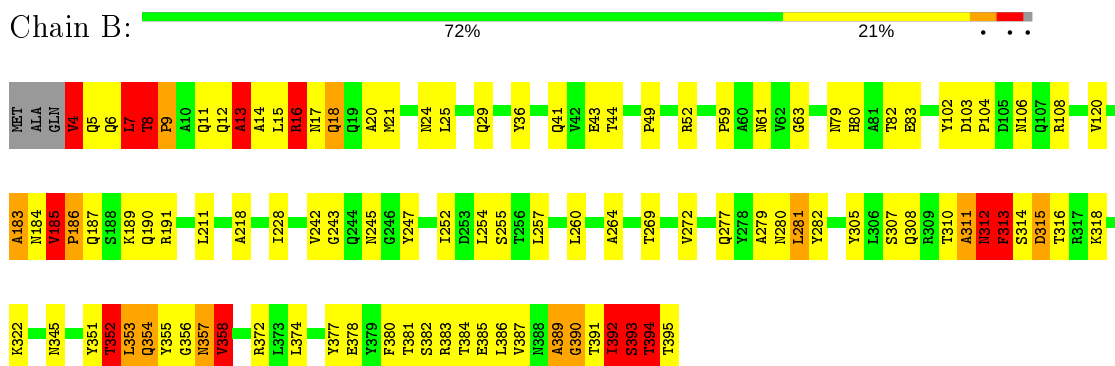
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

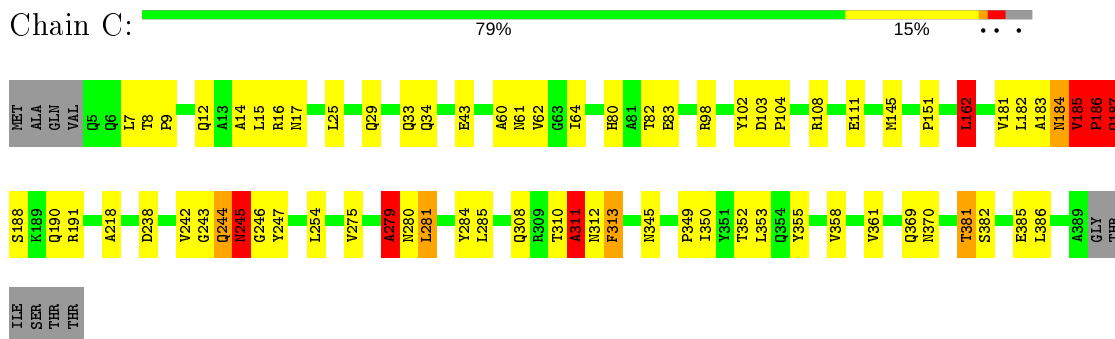
- Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)



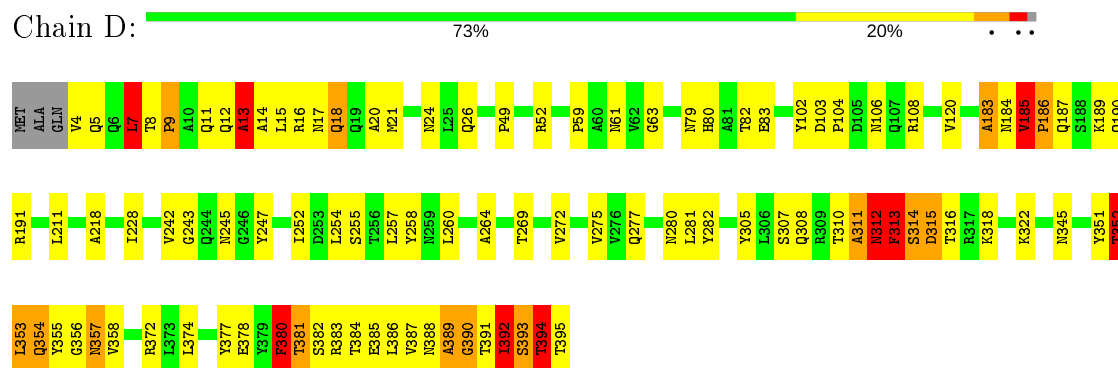
- Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)



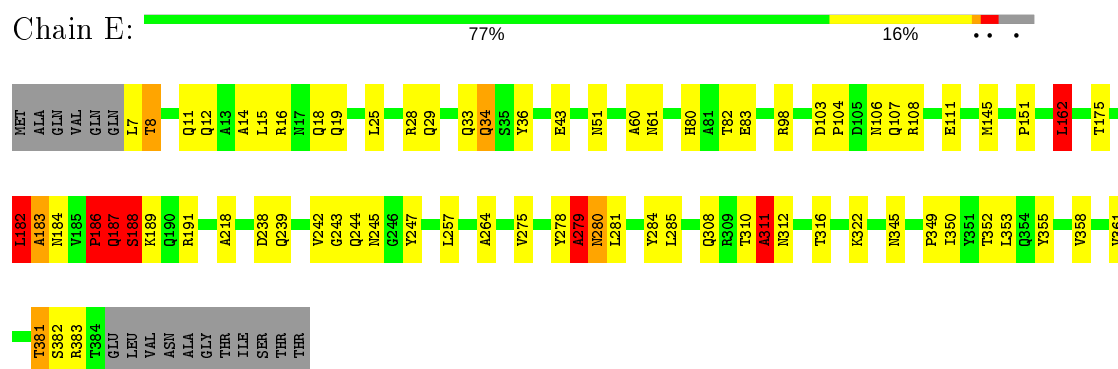
- Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)



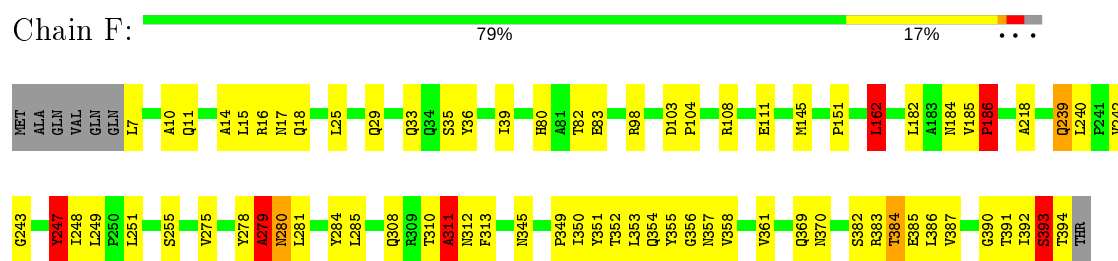
- Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)



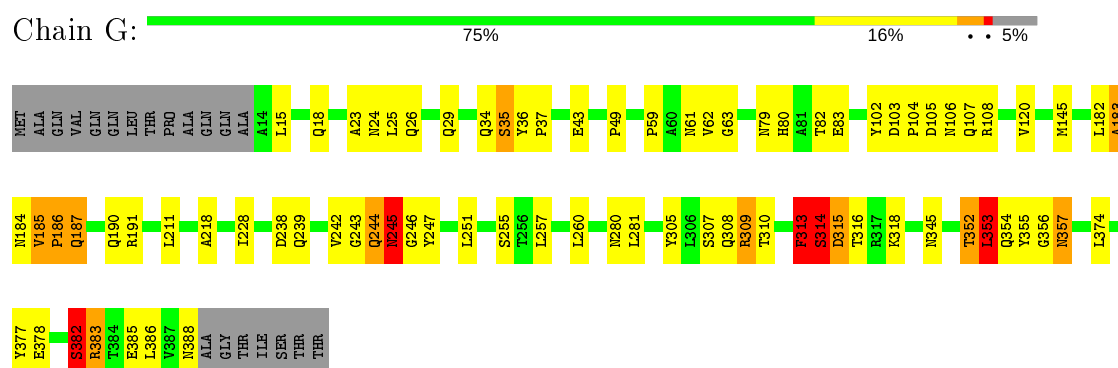
- Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)



- Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)

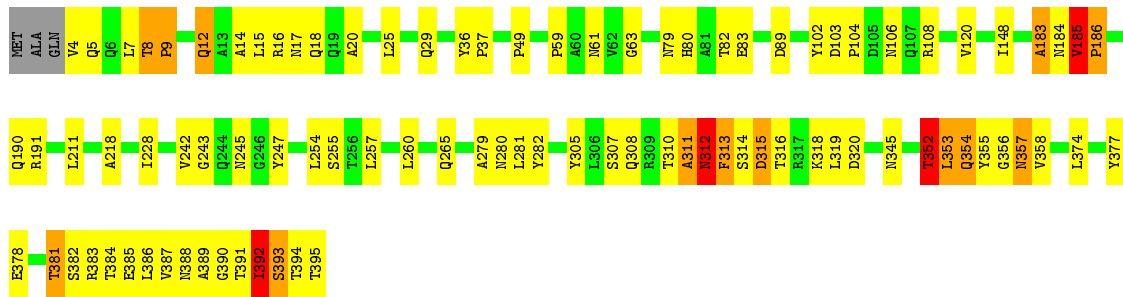


- Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)



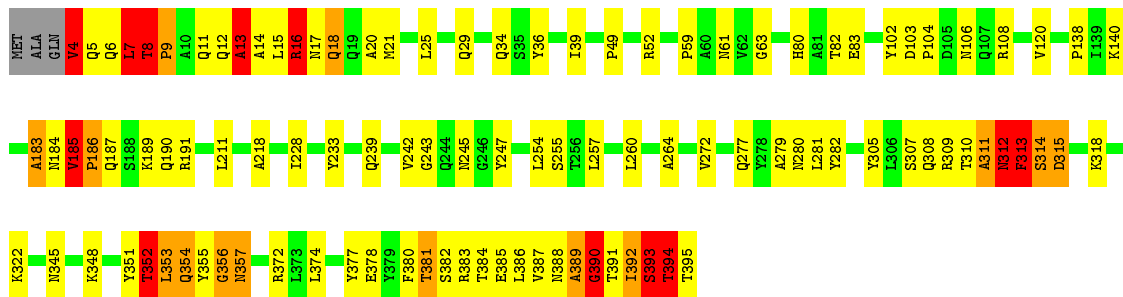
• Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)

Chain H:  76% 19%



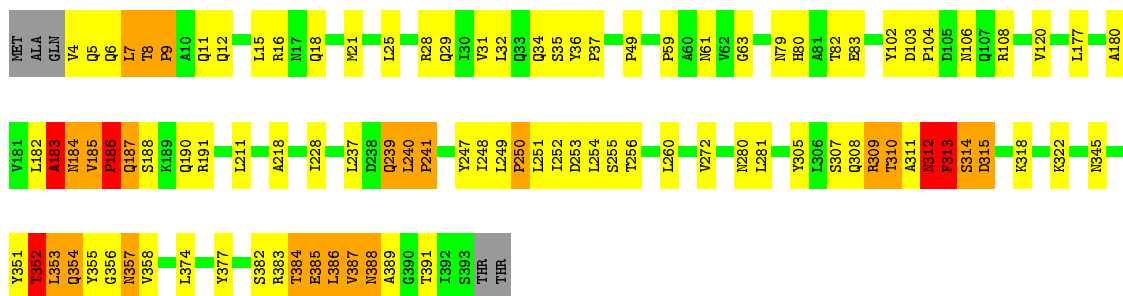
• Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)

Chain I:  72% 20%



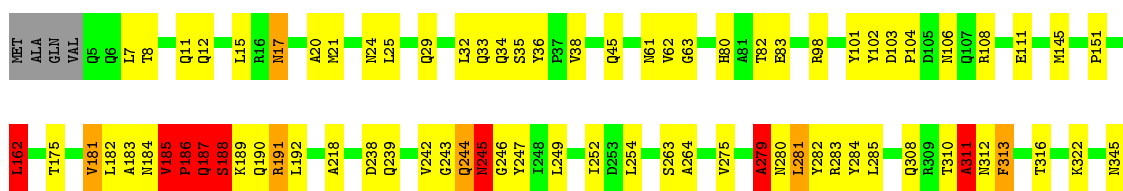
• Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)

Chain J:  74% 18% 6%



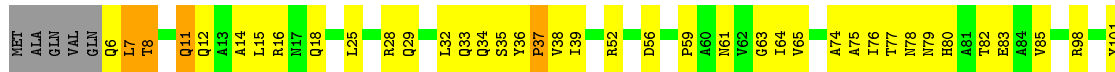
• Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)

Chain K:  73% 19%

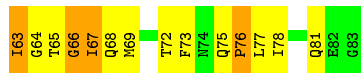
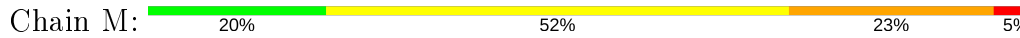




● Molecule 1: MAJOR CAPSID PROTEIN (PROTEIN P3)



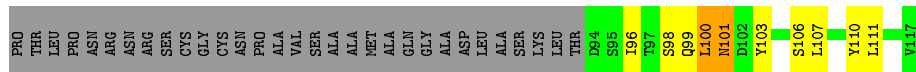
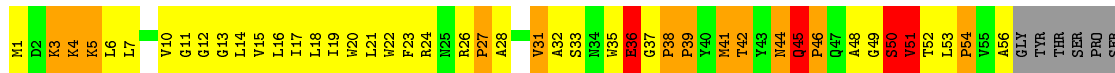
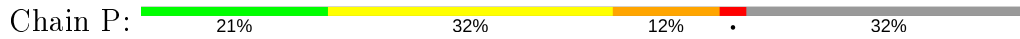
● Molecule 2: PROTEIN P30



● Molecule 3: PROTEIN P31



● Molecule 4: PROTEIN P16



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 903.00Å 920.60Å 926.20Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 100.00 – 4.20 | Depositor |
| % Data completeness (in resolution range) | (Not available) (100.00-4.20) | Depositor |
| R_{merge} | 0.33 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | X-PLOR | Depositor |
| R, R_{free} | (Not available) , (Not available) | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| Total number of atoms | 38116 | wwPDB-VP |
| Average B, all atoms (Å ²) | 20.0 | wwPDB-VP |

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 | 1.32 | 17/3021 (0.6%) | 1.47 | 28/4128 (0.7%) |
| 1 | B | 1.71 | 32/3110 (1.0%) | 1.89 | 50/4250 (1.2%) |
| 1 | C | 1.08 | 12/3064 (0.4%) | 1.15 | 26/4186 (0.6%) |
| 1 | D | 1.38 | 26/3111 (0.8%) | 1.63 | 37/4253 (0.9%) |
| 1 | E | 0.77 | 9/3011 (0.3%) | 1.18 | 20/4117 (0.5%) |
| 1 | F | 1.34 | 15/3074 (0.5%) | 1.56 | 22/4201 (0.5%) |
| 1 | G | 1.16 | 15/2991 (0.5%) | 1.33 | 23/4087 (0.6%) |
| 1 | H | 1.32 | 21/3112 (0.7%) | 1.23 | 25/4256 (0.6%) |
| 1 | I | 1.55 | 30/3110 (1.0%) | 1.87 | 48/4250 (1.1%) |
| 1 | J | 1.25 | 32/3092 (1.0%) | 1.13 | 20/4225 (0.5%) |
| 1 | K | 1.19 | 15/3058 (0.5%) | 1.49 | 37/4179 (0.9%) |
| 1 | L | 1.25 | 10/3018 (0.3%) | 1.17 | 28/4123 (0.7%) |
| 2 | M | 2.88 | 42/657 (6.4%) | 2.16 | 27/898 (3.0%) |
| 3 | N | 3.68 | 54/892 (6.1%) | 2.82 | 46/1209 (3.8%) |
| 4 | P | 2.89 | 37/637 (5.8%) | 1.83 | 19/871 (2.2%) |
| All | All | 1.48 | 367/38958 (0.9%) | 1.52 | 456/53233 (0.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 7 |
| 1 | B | 0 | 13 |
| 1 | C | 0 | 7 |
| 1 | D | 0 | 10 |
| 1 | E | 0 | 5 |
| 1 | F | 0 | 6 |
| 1 | G | 0 | 5 |
| 1 | H | 0 | 5 |
| 1 | I | 0 | 10 |
| 1 | J | 0 | 5 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | K | 0 | 10 |
| 1 | L | 0 | 5 |
| 3 | N | 0 | 3 |
| All | All | 0 | 91 |

All (367) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3 | N | 111 | SER | C-O | -43.65 | 0.40 | 1.23 |
| 1 | F | 391 | THR | C-O | -43.51 | 0.40 | 1.23 |
| 3 | N | 27 | VAL | C-O | -41.51 | 0.44 | 1.23 |
| 3 | N | 26 | SER | C-O | -36.70 | 0.53 | 1.23 |
| 1 | A | 313 | PHE | C-N | -35.91 | 0.51 | 1.34 |
| 1 | L | 312 | ASN | C-O | -34.83 | 0.57 | 1.23 |
| 4 | P | 32 | ALA | C-O | -33.88 | 0.58 | 1.23 |
| 1 | B | 358 | VAL | CA-CB | -33.23 | 0.84 | 1.54 |
| 1 | L | 150 | ALA | C-N | 31.57 | 1.94 | 1.34 |
| 1 | K | 186 | PRO | C-N | -30.73 | 0.63 | 1.34 |
| 2 | M | 64 | GLY | C-O | -29.82 | 0.76 | 1.23 |
| 1 | F | 186 | PRO | C-N | -28.84 | 0.67 | 1.34 |
| 4 | P | 31 | VAL | C-O | -28.50 | 0.69 | 1.23 |
| 1 | B | 4 | VAL | CA-CB | 28.35 | 2.14 | 1.54 |
| 1 | I | 4 | VAL | CA-CB | 28.34 | 2.14 | 1.54 |
| 1 | G | 245 | ASN | C-O | -28.21 | 0.69 | 1.23 |
| 1 | A | 245 | ASN | C-O | -28.20 | 0.69 | 1.23 |
| 1 | A | 24 | ASN | C-N | 28.08 | 1.98 | 1.34 |
| 1 | C | 245 | ASN | C-O | -27.64 | 0.70 | 1.23 |
| 1 | K | 245 | ASN | C-O | -27.58 | 0.70 | 1.23 |
| 1 | B | 185 | VAL | C-O | -27.44 | 0.71 | 1.23 |
| 1 | D | 185 | VAL | C-O | -27.44 | 0.71 | 1.23 |
| 1 | H | 185 | VAL | C-O | -27.43 | 0.71 | 1.23 |
| 1 | I | 185 | VAL | C-O | -27.42 | 0.71 | 1.23 |
| 1 | G | 313 | PHE | C-N | -27.14 | 0.71 | 1.34 |
| 1 | L | 381 | THR | C-N | 27.07 | 1.96 | 1.34 |
| 1 | C | 186 | PRO | C-N | -27.03 | 0.71 | 1.34 |
| 1 | D | 313 | PHE | C-O | -25.42 | 0.75 | 1.23 |
| 1 | B | 313 | PHE | C-O | -25.41 | 0.75 | 1.23 |
| 1 | H | 313 | PHE | C-O | -25.36 | 0.75 | 1.23 |
| 1 | F | 239 | GLN | C-N | -24.86 | 0.76 | 1.34 |
| 1 | I | 313 | PHE | C-O | -23.90 | 0.78 | 1.23 |
| 3 | N | 57 | CYS | C-O | -23.56 | 0.78 | 1.23 |
| 1 | J | 313 | PHE | C-O | -23.52 | 0.78 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | H | 381 | THR | C-N | 21.65 | 1.83 | 1.34 |
| 3 | N | 54 | GLY | C-O | -21.02 | 0.90 | 1.23 |
| 1 | B | 7 | LEU | C-N | -20.91 | 0.85 | 1.34 |
| 1 | D | 7 | LEU | C-N | -20.91 | 0.85 | 1.34 |
| 1 | I | 7 | LEU | C-N | -20.88 | 0.86 | 1.34 |
| 1 | J | 184 | ASN | C-O | -20.07 | 0.85 | 1.23 |
| 1 | K | 243 | GLY | C-N | -19.86 | 0.88 | 1.34 |
| 1 | C | 243 | GLY | C-N | -19.78 | 0.88 | 1.34 |
| 1 | K | 191 | ARG | C-N | 19.47 | 1.78 | 1.34 |
| 1 | I | 311 | ALA | C-N | -18.98 | 0.90 | 1.34 |
| 1 | B | 313 | PHE | C-N | -18.76 | 0.90 | 1.34 |
| 1 | D | 313 | PHE | C-N | -18.73 | 0.91 | 1.34 |
| 1 | H | 313 | PHE | C-N | -18.72 | 0.91 | 1.34 |
| 1 | D | 311 | ALA | C-N | -18.67 | 0.91 | 1.34 |
| 1 | H | 311 | ALA | C-N | -18.65 | 0.91 | 1.34 |
| 1 | B | 311 | ALA | C-N | -18.63 | 0.91 | 1.34 |
| 1 | G | 35 | SER | C-N | 18.61 | 1.76 | 1.34 |
| 1 | I | 8 | THR | C-N | 18.54 | 1.69 | 1.34 |
| 1 | B | 8 | THR | C-N | 18.50 | 1.69 | 1.34 |
| 1 | A | 243 | GLY | C-N | -18.44 | 0.91 | 1.34 |
| 1 | G | 243 | GLY | C-N | -18.41 | 0.91 | 1.34 |
| 1 | K | 380 | PHE | C-N | -18.24 | 0.92 | 1.34 |
| 1 | B | 389 | ALA | C-O | -17.85 | 0.89 | 1.23 |
| 1 | D | 389 | ALA | C-O | -17.84 | 0.89 | 1.23 |
| 1 | H | 389 | ALA | C-O | -17.82 | 0.89 | 1.23 |
| 3 | N | 17 | GLY | C-O | -17.80 | 0.95 | 1.23 |
| 1 | I | 389 | ALA | C-O | -17.79 | 0.89 | 1.23 |
| 1 | A | 381 | THR | C-N | -17.63 | 0.93 | 1.34 |
| 1 | L | 312 | ASN | C-N | -17.29 | 0.94 | 1.34 |
| 1 | J | 256 | THR | C-N | -16.99 | 0.94 | 1.34 |
| 1 | E | 381 | THR | C-N | 16.70 | 1.72 | 1.34 |
| 1 | B | 16 | ARG | C-N | -16.69 | 0.95 | 1.34 |
| 1 | I | 16 | ARG | C-N | -16.68 | 0.95 | 1.34 |
| 1 | B | 358 | VAL | N-CA | 16.31 | 1.78 | 1.46 |
| 1 | I | 392 | ILE | C-N | 16.28 | 1.71 | 1.34 |
| 1 | L | 257 | LEU | C-N | 16.19 | 1.71 | 1.34 |
| 2 | M | 11 | GLY | C-O | -15.87 | 0.98 | 1.23 |
| 1 | G | 382 | SER | C-N | 15.66 | 1.70 | 1.34 |
| 1 | B | 185 | VAL | C-N | -15.60 | 1.04 | 1.34 |
| 1 | D | 185 | VAL | C-N | -15.60 | 1.04 | 1.34 |
| 1 | E | 311 | ALA | C-N | -15.59 | 0.98 | 1.34 |
| 1 | F | 311 | ALA | C-N | -15.59 | 0.98 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | H | 185 | VAL | C-N | -15.57 | 1.04 | 1.34 |
| 1 | I | 185 | VAL | C-N | -15.56 | 1.04 | 1.34 |
| 1 | I | 313 | PHE | C-N | -15.39 | 0.98 | 1.34 |
| 3 | N | 16 | ASN | C-N | 15.32 | 1.60 | 1.33 |
| 1 | J | 384 | THR | C-N | 15.21 | 1.69 | 1.34 |
| 1 | B | 358 | VAL | CA-C | 15.20 | 1.92 | 1.52 |
| 1 | B | 352 | THR | C-N | -15.07 | 0.99 | 1.34 |
| 1 | J | 352 | THR | C-N | -15.05 | 0.99 | 1.34 |
| 1 | H | 352 | THR | C-N | -15.03 | 0.99 | 1.34 |
| 1 | D | 352 | THR | C-N | -15.01 | 0.99 | 1.34 |
| 1 | I | 352 | THR | C-N | -14.97 | 0.99 | 1.34 |
| 3 | N | 111 | SER | C-N | -14.81 | 0.99 | 1.34 |
| 4 | P | 5 | LYS | C-O | -14.67 | 0.95 | 1.23 |
| 1 | B | 394 | THR | C-N | -14.59 | 1.00 | 1.34 |
| 1 | D | 394 | THR | C-N | -14.57 | 1.00 | 1.34 |
| 1 | I | 394 | THR | C-N | -14.55 | 1.00 | 1.34 |
| 3 | N | 55 | VAL | C-N | 14.15 | 1.66 | 1.34 |
| 2 | M | 46 | PRO | N-CA | -14.06 | 1.23 | 1.47 |
| 3 | N | 57 | CYS | C-N | -13.42 | 1.03 | 1.34 |
| 1 | F | 247 | TYR | C-N | -13.39 | 1.03 | 1.34 |
| 1 | G | 183 | ALA | C-N | -13.38 | 1.03 | 1.34 |
| 1 | A | 183 | ALA | C-N | -13.35 | 1.03 | 1.34 |
| 3 | N | 65 | ASN | C-O | -13.01 | 0.98 | 1.23 |
| 1 | C | 382 | SER | C-O | -12.74 | 0.99 | 1.23 |
| 2 | M | 46 | PRO | C-O | -12.70 | 0.97 | 1.23 |
| 3 | N | 56 | GLN | N-CA | -12.68 | 1.21 | 1.46 |
| 1 | F | 390 | GLY | CA-C | -12.60 | 1.31 | 1.51 |
| 2 | M | 66 | GLY | CA-C | -12.55 | 1.31 | 1.51 |
| 3 | N | 110 | LYS | C-O | -12.43 | 0.99 | 1.23 |
| 1 | B | 4 | VAL | N-CA | 12.36 | 1.71 | 1.46 |
| 1 | I | 4 | VAL | N-CA | 12.36 | 1.71 | 1.46 |
| 4 | P | 45 | GLN | C-N | 12.31 | 1.57 | 1.34 |
| 1 | I | 245 | ASN | C-N | -12.26 | 1.10 | 1.33 |
| 1 | J | 9 | PRO | C-O | -12.18 | 0.98 | 1.23 |
| 1 | D | 245 | ASN | C-N | -12.15 | 1.11 | 1.33 |
| 1 | H | 245 | ASN | C-N | -12.13 | 1.11 | 1.33 |
| 1 | B | 245 | ASN | C-N | -12.13 | 1.11 | 1.33 |
| 1 | J | 187 | GLN | C-N | 12.03 | 1.61 | 1.34 |
| 3 | N | 68 | ALA | N-CA | -11.89 | 1.22 | 1.46 |
| 1 | F | 393 | SER | C-O | -11.88 | 1.00 | 1.23 |
| 1 | C | 244 | GLN | C-O | -11.79 | 1.00 | 1.23 |
| 1 | K | 244 | GLN | C-O | -11.72 | 1.01 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3 | N | 18 | CYS | C-O | -11.70 | 1.01 | 1.23 |
| 2 | M | 6 | GLN | C-O | -11.68 | 1.01 | 1.23 |
| 1 | J | 313 | PHE | C-N | -11.66 | 1.07 | 1.34 |
| 1 | G | 244 | GLN | C-O | -11.65 | 1.01 | 1.23 |
| 4 | P | 49 | GLY | C-O | -11.65 | 1.05 | 1.23 |
| 1 | B | 392 | ILE | C-N | 11.64 | 1.60 | 1.34 |
| 1 | A | 244 | GLN | C-O | -11.61 | 1.01 | 1.23 |
| 3 | N | 44 | THR | N-CA | -11.56 | 1.23 | 1.46 |
| 1 | B | 357 | ASN | C-N | -11.56 | 1.07 | 1.34 |
| 3 | N | 61 | ASP | C-O | -11.44 | 1.01 | 1.23 |
| 1 | J | 250 | PRO | C-N | -11.39 | 1.07 | 1.34 |
| 2 | M | 9 | TYR | C-N | 11.35 | 1.60 | 1.34 |
| 1 | E | 187 | GLN | N-CA | -11.33 | 1.23 | 1.46 |
| 1 | J | 388 | ASN | C-O | -11.31 | 1.01 | 1.23 |
| 2 | M | 12 | PRO | C-O | -11.28 | 1.00 | 1.23 |
| 1 | D | 392 | ILE | C-N | -11.26 | 1.08 | 1.34 |
| 1 | D | 18 | GLN | C-O | -11.25 | 1.01 | 1.23 |
| 1 | I | 18 | GLN | C-O | -11.23 | 1.02 | 1.23 |
| 1 | H | 18 | GLN | C-O | -11.21 | 1.02 | 1.23 |
| 1 | B | 18 | GLN | C-O | -11.21 | 1.02 | 1.23 |
| 3 | N | 31 | PHE | C-O | -11.14 | 1.02 | 1.23 |
| 4 | P | 4 | LYS | N-CA | -10.95 | 1.24 | 1.46 |
| 1 | C | 187 | GLN | C-O | -10.90 | 1.02 | 1.23 |
| 3 | N | 17 | GLY | C-N | -10.90 | 1.08 | 1.34 |
| 2 | M | 49 | GLN | N-CA | -10.83 | 1.24 | 1.46 |
| 2 | M | 24 | MET | C-N | 10.79 | 1.54 | 1.34 |
| 1 | A | 356 | GLY | C-N | -10.73 | 1.09 | 1.34 |
| 1 | G | 356 | GLY | C-N | -10.73 | 1.09 | 1.34 |
| 2 | M | 15 | ILE | C-O | -10.66 | 1.03 | 1.23 |
| 2 | M | 64 | GLY | C-N | -10.53 | 1.09 | 1.34 |
| 4 | P | 41 | MET | C-O | -10.52 | 1.03 | 1.23 |
| 1 | E | 279 | ALA | C-N | -10.49 | 1.09 | 1.34 |
| 1 | F | 279 | ALA | C-N | -10.49 | 1.09 | 1.34 |
| 3 | N | 19 | ASP | C-O | -10.48 | 1.03 | 1.23 |
| 4 | P | 99 | GLN | C-O | -10.47 | 1.03 | 1.23 |
| 1 | I | 389 | ALA | C-N | -10.39 | 1.14 | 1.33 |
| 1 | D | 389 | ALA | C-N | -10.38 | 1.14 | 1.33 |
| 1 | H | 389 | ALA | C-N | -10.37 | 1.14 | 1.33 |
| 3 | N | 109 | LYS | C-O | -10.36 | 1.03 | 1.23 |
| 1 | B | 389 | ALA | C-N | -10.35 | 1.14 | 1.33 |
| 2 | M | 64 | GLY | CA-C | -10.33 | 1.35 | 1.51 |
| 3 | N | 65 | ASN | C-N | -10.28 | 1.10 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | F | 391 | THR | CA-C | -10.18 | 1.26 | 1.52 |
| 3 | N | 27 | VAL | CA-CB | 10.16 | 1.76 | 1.54 |
| 3 | N | 112 | VAL | C-N | 10.16 | 1.53 | 1.34 |
| 1 | D | 354 | GLN | C-O | -10.14 | 1.04 | 1.23 |
| 1 | H | 354 | GLN | C-O | -10.14 | 1.04 | 1.23 |
| 1 | B | 354 | GLN | C-O | -10.13 | 1.04 | 1.23 |
| 1 | I | 354 | GLN | C-O | -10.12 | 1.04 | 1.23 |
| 1 | J | 354 | GLN | C-O | -10.12 | 1.04 | 1.23 |
| 1 | H | 392 | ILE | C-N | 10.11 | 1.57 | 1.34 |
| 2 | M | 24 | MET | CA-C | -10.08 | 1.26 | 1.52 |
| 3 | N | 26 | SER | CA-CB | 10.05 | 1.68 | 1.52 |
| 4 | P | 36 | GLU | CA-C | -9.98 | 1.27 | 1.52 |
| 2 | M | 46 | PRO | C-N | -9.90 | 1.11 | 1.34 |
| 1 | B | 381 | THR | C-N | 9.70 | 1.56 | 1.34 |
| 1 | I | 381 | THR | C-N | 9.70 | 1.56 | 1.34 |
| 1 | K | 17 | ASN | C-N | 9.69 | 1.56 | 1.34 |
| 1 | D | 381 | THR | C-N | 9.68 | 1.56 | 1.34 |
| 3 | N | 17 | GLY | N-CA | -9.67 | 1.31 | 1.46 |
| 1 | L | 382 | SER | C-O | -9.55 | 1.05 | 1.23 |
| 3 | N | 22 | GLU | C-O | -9.54 | 1.05 | 1.23 |
| 1 | J | 184 | ASN | N-CA | -9.51 | 1.27 | 1.46 |
| 3 | N | 27 | VAL | C-N | -9.44 | 1.12 | 1.34 |
| 3 | N | 76 | THR | C-N | 9.38 | 1.50 | 1.33 |
| 1 | L | 311 | ALA | C-N | -9.31 | 1.12 | 1.34 |
| 1 | A | 314 | SER | N-CA | -9.29 | 1.27 | 1.46 |
| 2 | M | 69 | MET | C-O | -9.26 | 1.05 | 1.23 |
| 1 | D | 357 | ASN | C-O | -9.23 | 1.05 | 1.23 |
| 1 | I | 357 | ASN | C-O | -9.22 | 1.05 | 1.23 |
| 1 | C | 311 | ALA | C-N | -9.21 | 1.12 | 1.34 |
| 4 | P | 31 | VAL | C-N | -9.20 | 1.12 | 1.34 |
| 1 | J | 357 | ASN | C-O | -9.20 | 1.05 | 1.23 |
| 1 | K | 311 | ALA | C-N | -9.19 | 1.12 | 1.34 |
| 4 | P | 36 | GLU | C-O | -9.18 | 1.05 | 1.23 |
| 1 | H | 357 | ASN | C-O | -9.17 | 1.05 | 1.23 |
| 1 | G | 314 | SER | C-N | 9.16 | 1.55 | 1.34 |
| 3 | N | 65 | ASN | N-CA | -9.14 | 1.28 | 1.46 |
| 4 | P | 54 | PRO | C-O | -9.14 | 1.04 | 1.23 |
| 1 | A | 353 | LEU | N-CA | -9.11 | 1.28 | 1.46 |
| 4 | P | 48 | ALA | C-O | -9.10 | 1.06 | 1.23 |
| 1 | G | 353 | LEU | N-CA | -9.08 | 1.28 | 1.46 |
| 4 | P | 32 | ALA | N-CA | -9.06 | 1.28 | 1.46 |
| 1 | L | 161 | GLU | C-N | -9.05 | 1.13 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | M | 67 | ILE | C-O | -9.03 | 1.06 | 1.23 |
| 1 | J | 356 | GLY | C-N | -8.88 | 1.13 | 1.34 |
| 1 | B | 357 | ASN | C-O | -8.88 | 1.06 | 1.23 |
| 1 | H | 356 | GLY | C-N | -8.88 | 1.13 | 1.34 |
| 4 | P | 48 | ALA | C-N | 8.88 | 1.49 | 1.33 |
| 4 | P | 33 | SER | C-O | -8.85 | 1.06 | 1.23 |
| 1 | D | 356 | GLY | C-N | -8.83 | 1.13 | 1.34 |
| 1 | I | 356 | GLY | C-N | -8.82 | 1.13 | 1.34 |
| 1 | B | 390 | GLY | C-O | -8.81 | 1.09 | 1.23 |
| 1 | I | 390 | GLY | C-O | -8.79 | 1.09 | 1.23 |
| 1 | H | 390 | GLY | C-O | -8.79 | 1.09 | 1.23 |
| 1 | D | 390 | GLY | C-O | -8.78 | 1.09 | 1.23 |
| 1 | B | 390 | GLY | C-N | 8.73 | 1.54 | 1.34 |
| 1 | I | 390 | GLY | C-N | 8.73 | 1.54 | 1.34 |
| 1 | D | 390 | GLY | C-N | 8.72 | 1.54 | 1.34 |
| 4 | P | 42 | THR | C-O | -8.67 | 1.06 | 1.23 |
| 1 | D | 12 | GLN | C-O | -8.63 | 1.06 | 1.23 |
| 1 | J | 186 | PRO | CA-C | -8.61 | 1.35 | 1.52 |
| 1 | H | 12 | GLN | C-O | -8.59 | 1.07 | 1.23 |
| 1 | B | 12 | GLN | C-O | -8.59 | 1.07 | 1.23 |
| 1 | I | 12 | GLN | C-O | -8.55 | 1.07 | 1.23 |
| 3 | N | 44 | THR | C-O | -8.53 | 1.07 | 1.23 |
| 2 | M | 21 | THR | C-N | 8.48 | 1.53 | 1.34 |
| 4 | P | 98 | SER | C-O | -8.40 | 1.07 | 1.23 |
| 1 | L | 245 | ASN | C-N | 8.35 | 1.48 | 1.33 |
| 1 | C | 16 | ARG | C-N | 8.34 | 1.53 | 1.34 |
| 2 | M | 67 | ILE | N-CA | -8.26 | 1.29 | 1.46 |
| 1 | J | 18 | GLN | C-O | -8.22 | 1.07 | 1.23 |
| 2 | M | 10 | ALA | N-CA | -8.18 | 1.29 | 1.46 |
| 1 | J | 385 | GLU | N-CA | -8.16 | 1.30 | 1.46 |
| 3 | N | 73 | VAL | C-O | -8.13 | 1.07 | 1.23 |
| 1 | K | 382 | SER | CA-C | -8.05 | 1.32 | 1.52 |
| 1 | H | 9 | PRO | C-O | -8.03 | 1.07 | 1.23 |
| 1 | C | 187 | GLN | C-N | 8.03 | 1.52 | 1.34 |
| 1 | B | 9 | PRO | C-O | -8.02 | 1.07 | 1.23 |
| 1 | I | 9 | PRO | C-O | -8.01 | 1.07 | 1.23 |
| 1 | D | 9 | PRO | C-O | -7.99 | 1.07 | 1.23 |
| 2 | M | 41 | ALA | C-O | -7.98 | 1.08 | 1.23 |
| 1 | G | 309 | ARG | C-N | 7.95 | 1.52 | 1.34 |
| 4 | P | 32 | ALA | C-N | -7.91 | 1.15 | 1.34 |
| 1 | J | 389 | ALA | C-O | -7.88 | 1.08 | 1.23 |
| 1 | J | 188 | SER | N-CA | 7.88 | 1.62 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | N | 27 | VAL | N-CA | -7.88 | 1.30 | 1.46 |
| 1 | A | 314 | SER | CA-C | -7.84 | 1.32 | 1.52 |
| 4 | P | 32 | ALA | CA-CB | 7.83 | 1.69 | 1.52 |
| 1 | F | 391 | THR | C-N | -7.80 | 1.16 | 1.34 |
| 3 | N | 67 | GLY | C-N | 7.76 | 1.51 | 1.34 |
| 2 | M | 11 | GLY | C-N | -7.75 | 1.19 | 1.34 |
| 2 | M | 41 | ALA | C-N | -7.67 | 1.16 | 1.34 |
| 1 | F | 390 | GLY | C-O | -7.52 | 1.11 | 1.23 |
| 3 | N | 43 | LEU | C-O | -7.51 | 1.09 | 1.23 |
| 3 | N | 28 | ARG | CA-CB | 7.49 | 1.70 | 1.53 |
| 1 | J | 183 | ALA | C-N | 7.47 | 1.51 | 1.34 |
| 4 | P | 49 | GLY | CA-C | -7.44 | 1.40 | 1.51 |
| 1 | A | 387 | VAL | C-O | -7.34 | 1.09 | 1.23 |
| 1 | D | 380 | PHE | C-N | -7.33 | 1.17 | 1.34 |
| 2 | M | 17 | GLY | C-O | -7.33 | 1.11 | 1.23 |
| 1 | J | 184 | ASN | C-N | -7.32 | 1.17 | 1.34 |
| 1 | B | 393 | SER | C-N | 7.25 | 1.50 | 1.34 |
| 1 | H | 393 | SER | C-N | 7.24 | 1.50 | 1.34 |
| 1 | I | 393 | SER | C-N | 7.24 | 1.50 | 1.34 |
| 1 | E | 187 | GLN | C-O | -7.22 | 1.09 | 1.23 |
| 1 | D | 393 | SER | C-N | 7.22 | 1.50 | 1.34 |
| 1 | H | 357 | ASN | C-N | -7.20 | 1.17 | 1.34 |
| 1 | J | 357 | ASN | C-N | -7.20 | 1.17 | 1.34 |
| 1 | D | 357 | ASN | C-N | -7.18 | 1.17 | 1.34 |
| 1 | I | 357 | ASN | C-N | -7.18 | 1.17 | 1.34 |
| 1 | F | 391 | THR | CA-CB | 7.17 | 1.72 | 1.53 |
| 1 | B | 4 | VAL | CA-C | 7.16 | 1.71 | 1.52 |
| 3 | N | 97 | ARG | C-O | -7.15 | 1.09 | 1.23 |
| 1 | I | 4 | VAL | CA-C | 7.14 | 1.71 | 1.52 |
| 3 | N | 66 | ASP | C-O | -7.05 | 1.09 | 1.23 |
| 3 | N | 33 | ALA | C-O | -6.99 | 1.10 | 1.23 |
| 3 | N | 66 | ASP | C-N | -6.95 | 1.20 | 1.33 |
| 3 | N | 26 | SER | CA-C | -6.91 | 1.34 | 1.52 |
| 1 | E | 244 | GLN | N-CA | -6.90 | 1.32 | 1.46 |
| 1 | B | 281 | LEU | N-CA | 6.85 | 1.60 | 1.46 |
| 3 | N | 22 | GLU | C-N | 6.85 | 1.45 | 1.33 |
| 4 | P | 33 | SER | C-N | -6.82 | 1.18 | 1.34 |
| 3 | N | 79 | ARG | C-N | 6.75 | 1.49 | 1.34 |
| 4 | P | 4 | LYS | C-O | -6.72 | 1.10 | 1.23 |
| 4 | P | 4 | LYS | C-N | -6.68 | 1.18 | 1.34 |
| 1 | F | 387 | VAL | C-N | 6.67 | 1.49 | 1.34 |
| 1 | F | 384 | THR | C-O | -6.63 | 1.10 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | P | 38 | PRO | C-O | -6.61 | 1.10 | 1.23 |
| 2 | M | 7 | PHE | C-N | -6.56 | 1.21 | 1.34 |
| 1 | K | 187 | GLN | C-O | -6.50 | 1.10 | 1.23 |
| 1 | A | 309 | ARG | C-N | 6.48 | 1.49 | 1.34 |
| 1 | J | 12 | GLN | C-O | -6.45 | 1.11 | 1.23 |
| 4 | P | 42 | THR | C-N | 6.43 | 1.48 | 1.34 |
| 4 | P | 32 | ALA | CA-C | -6.40 | 1.36 | 1.52 |
| 1 | K | 381 | THR | C-O | -6.39 | 1.11 | 1.23 |
| 1 | A | 187 | GLN | C-O | -6.37 | 1.11 | 1.23 |
| 4 | P | 31 | VAL | CA-C | -6.37 | 1.36 | 1.52 |
| 2 | M | 65 | THR | N-CA | -6.36 | 1.33 | 1.46 |
| 1 | F | 393 | SER | C-N | -6.35 | 1.19 | 1.34 |
| 1 | D | 26 | GLN | C-N | -6.34 | 1.19 | 1.34 |
| 1 | G | 187 | GLN | C-O | -6.33 | 1.11 | 1.23 |
| 2 | M | 54 | ALA | C-O | -6.28 | 1.11 | 1.23 |
| 2 | M | 7 | PHE | N-CA | -6.26 | 1.33 | 1.46 |
| 4 | P | 100 | LEU | C-O | -6.26 | 1.11 | 1.23 |
| 4 | P | 49 | GLY | N-CA | -6.25 | 1.36 | 1.46 |
| 1 | G | 245 | ASN | C-N | 6.24 | 1.44 | 1.33 |
| 1 | A | 245 | ASN | C-N | 6.19 | 1.44 | 1.33 |
| 4 | P | 27 | PRO | C-N | 6.17 | 1.48 | 1.34 |
| 2 | M | 51 | PRO | C-O | -6.16 | 1.10 | 1.23 |
| 1 | C | 279 | ALA | C-N | -6.16 | 1.19 | 1.34 |
| 1 | K | 279 | ALA | C-N | -6.13 | 1.20 | 1.34 |
| 2 | M | 47 | PHE | C-O | -6.13 | 1.11 | 1.23 |
| 1 | J | 386 | LEU | N-CA | 6.13 | 1.58 | 1.46 |
| 1 | J | 312 | ASN | C-O | -6.12 | 1.11 | 1.23 |
| 3 | N | 27 | VAL | CA-C | -6.11 | 1.37 | 1.52 |
| 3 | N | 18 | CYS | C-N | -6.10 | 1.20 | 1.34 |
| 1 | C | 185 | VAL | N-CA | -6.08 | 1.34 | 1.46 |
| 2 | M | 67 | ILE | C-N | -6.04 | 1.20 | 1.34 |
| 2 | M | 22 | GLU | N-CA | -6.03 | 1.34 | 1.46 |
| 3 | N | 86 | LYS | N-CA | -6.00 | 1.34 | 1.46 |
| 1 | J | 387 | VAL | C-N | 5.98 | 1.47 | 1.34 |
| 3 | N | 44 | THR | CA-CB | 5.96 | 1.68 | 1.53 |
| 3 | N | 54 | GLY | C-N | -5.94 | 1.20 | 1.34 |
| 2 | M | 65 | THR | CA-CB | 5.89 | 1.68 | 1.53 |
| 2 | M | 12 | PRO | CA-C | -5.86 | 1.41 | 1.52 |
| 3 | N | 19 | ASP | CA-C | -5.85 | 1.37 | 1.52 |
| 1 | E | 183 | ALA | N-CA | -5.82 | 1.34 | 1.46 |
| 1 | E | 34 | GLN | C-N | -5.81 | 1.20 | 1.34 |
| 1 | J | 7 | LEU | C-O | -5.81 | 1.12 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | P | 51 | VAL | C-O | -5.81 | 1.12 | 1.23 |
| 4 | P | 50 | SER | N-CA | -5.81 | 1.34 | 1.46 |
| 1 | D | 183 | ALA | C-N | -5.75 | 1.20 | 1.34 |
| 1 | I | 183 | ALA | C-N | -5.75 | 1.20 | 1.34 |
| 1 | K | 187 | GLN | C-N | -5.75 | 1.20 | 1.34 |
| 2 | M | 36 | ALA | CA-CB | 5.74 | 1.64 | 1.52 |
| 1 | B | 183 | ALA | C-N | -5.73 | 1.20 | 1.34 |
| 1 | H | 183 | ALA | C-N | -5.71 | 1.21 | 1.34 |
| 3 | N | 25 | GLN | C-N | 5.70 | 1.47 | 1.34 |
| 4 | P | 50 | SER | CA-CB | 5.68 | 1.61 | 1.52 |
| 2 | M | 46 | PRO | N-CD | 5.65 | 1.55 | 1.47 |
| 1 | J | 310 | THR | N-CA | -5.64 | 1.35 | 1.46 |
| 1 | J | 384 | THR | N-CA | 5.60 | 1.57 | 1.46 |
| 4 | P | 50 | SER | C-O | -5.59 | 1.12 | 1.23 |
| 1 | K | 383 | ARG | C-O | -5.56 | 1.12 | 1.23 |
| 3 | N | 81 | LYS | C-O | -5.44 | 1.13 | 1.23 |
| 1 | G | 383 | ARG | C-O | -5.43 | 1.13 | 1.23 |
| 1 | I | 309 | ARG | C-N | 5.43 | 1.46 | 1.34 |
| 1 | C | 381 | THR | C-N | 5.42 | 1.46 | 1.34 |
| 1 | A | 386 | LEU | C-O | -5.41 | 1.13 | 1.23 |
| 1 | L | 313 | PHE | C-N | 5.40 | 1.46 | 1.34 |
| 1 | J | 385 | GLU | CA-C | 5.38 | 1.67 | 1.52 |
| 1 | K | 385 | GLU | C-O | -5.36 | 1.13 | 1.23 |
| 3 | N | 34 | VAL | C-O | -5.34 | 1.13 | 1.23 |
| 3 | N | 81 | LYS | C-N | -5.33 | 1.21 | 1.34 |
| 1 | J | 8 | THR | C-N | 5.32 | 1.44 | 1.34 |
| 3 | N | 84 | ALA | C-N | -5.32 | 1.23 | 1.33 |
| 2 | M | 4 | ASN | C-O | -5.28 | 1.13 | 1.23 |
| 2 | M | 58 | GLN | C-O | -5.26 | 1.13 | 1.23 |
| 4 | P | 44 | ASN | C-O | -5.18 | 1.13 | 1.23 |
| 2 | M | 65 | THR | CA-C | -5.13 | 1.39 | 1.52 |
| 4 | P | 100 | LEU | C-N | -5.10 | 1.22 | 1.34 |
| 2 | M | 47 | PHE | CA-C | -5.08 | 1.39 | 1.52 |
| 1 | J | 185 | VAL | N-CA | -5.06 | 1.36 | 1.46 |
| 1 | E | 245 | ASN | C-N | -5.05 | 1.24 | 1.33 |
| 1 | G | 357 | ASN | C-N | -5.05 | 1.22 | 1.34 |
| 2 | M | 36 | ALA | C-N | -5.03 | 1.24 | 1.33 |
| 2 | M | 18 | PRO | C-N | 5.02 | 1.45 | 1.34 |
| 1 | A | 357 | ASN | C-N | -5.02 | 1.22 | 1.34 |

All (456) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | A | 24 | ASN | O-C-N | -53.44 | 37.20 | 122.70 |
| 1 | F | 247 | TYR | O-C-N | -45.14 | 50.48 | 122.70 |
| 1 | G | 313 | PHE | O-C-N | -44.62 | 51.31 | 122.70 |
| 1 | B | 16 | ARG | O-C-N | -42.15 | 55.26 | 122.70 |
| 1 | I | 16 | ARG | O-C-N | -42.14 | 55.28 | 122.70 |
| 3 | N | 5 | ASN | C-N-CD | -41.75 | 28.75 | 120.60 |
| 1 | I | 7 | LEU | O-C-N | -38.43 | 61.21 | 122.70 |
| 1 | D | 7 | LEU | O-C-N | -38.42 | 61.22 | 122.70 |
| 1 | B | 7 | LEU | O-C-N | -38.40 | 61.26 | 122.70 |
| 1 | K | 380 | PHE | O-C-N | -36.95 | 63.58 | 122.70 |
| 1 | D | 394 | THR | O-C-N | -36.40 | 64.46 | 122.70 |
| 1 | B | 394 | THR | O-C-N | -36.37 | 64.50 | 122.70 |
| 1 | I | 394 | THR | O-C-N | -36.37 | 64.51 | 122.70 |
| 2 | M | 11 | GLY | C-N-CD | -34.88 | 43.86 | 120.60 |
| 1 | F | 186 | PRO | O-C-N | -31.58 | 72.17 | 122.70 |
| 1 | K | 187 | GLN | O-C-N | -31.41 | 72.45 | 122.70 |
| 1 | E | 186 | PRO | O-C-N | -31.31 | 72.60 | 122.70 |
| 1 | I | 313 | PHE | O-C-N | -29.87 | 74.91 | 122.70 |
| 1 | F | 391 | THR | CA-C-O | -28.70 | 59.84 | 120.10 |
| 1 | F | 239 | GLN | O-C-N | 26.55 | 165.17 | 122.70 |
| 1 | H | 185 | VAL | C-N-CD | -25.41 | 64.69 | 120.60 |
| 1 | B | 185 | VAL | C-N-CD | -25.41 | 64.70 | 120.60 |
| 1 | D | 185 | VAL | C-N-CD | -25.39 | 64.73 | 120.60 |
| 1 | I | 185 | VAL | C-N-CD | -25.39 | 64.73 | 120.60 |
| 1 | L | 312 | ASN | O-C-N | -25.27 | 82.28 | 122.70 |
| 1 | B | 7 | LEU | CA-C-N | 24.87 | 171.91 | 117.20 |
| 1 | I | 7 | LEU | CA-C-N | 24.83 | 171.83 | 117.20 |
| 3 | N | 111 | SER | O-C-N | -24.82 | 82.99 | 122.70 |
| 1 | D | 7 | LEU | CA-C-N | 24.81 | 171.79 | 117.20 |
| 1 | H | 313 | PHE | O-C-N | -24.07 | 84.20 | 122.70 |
| 1 | D | 313 | PHE | O-C-N | -24.04 | 84.23 | 122.70 |
| 1 | B | 313 | PHE | O-C-N | -24.01 | 84.28 | 122.70 |
| 1 | G | 314 | SER | O-C-N | -23.39 | 85.28 | 122.70 |
| 1 | I | 16 | ARG | CA-C-N | 23.01 | 167.82 | 117.20 |
| 1 | B | 16 | ARG | CA-C-N | 22.97 | 167.73 | 117.20 |
| 1 | K | 380 | PHE | CA-C-N | 22.89 | 167.56 | 117.20 |
| 1 | F | 186 | PRO | CA-C-N | 22.33 | 166.32 | 117.20 |
| 1 | F | 239 | GLN | C-N-CA | -22.16 | 66.29 | 121.70 |
| 1 | E | 381 | THR | O-C-N | 21.82 | 157.62 | 122.70 |
| 1 | G | 352 | THR | O-C-N | -21.49 | 88.31 | 122.70 |
| 1 | I | 16 | ARG | C-N-CA | 21.48 | 175.41 | 121.70 |
| 1 | A | 352 | THR | O-C-N | -21.48 | 88.33 | 122.70 |
| 1 | B | 16 | ARG | C-N-CA | 21.47 | 175.36 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | K | 187 | GLN | CA-C-N | 20.56 | 162.44 | 117.20 |
| 1 | A | 314 | SER | CA-C-N | -20.23 | 72.69 | 117.20 |
| 1 | E | 186 | PRO | CA-C-N | 20.12 | 161.48 | 117.20 |
| 1 | F | 239 | GLN | CA-C-N | -20.04 | 73.12 | 117.20 |
| 1 | C | 186 | PRO | O-C-N | -19.91 | 90.85 | 122.70 |
| 1 | I | 313 | PHE | CA-C-N | 19.83 | 160.83 | 117.20 |
| 1 | A | 313 | PHE | O-C-N | -19.82 | 90.98 | 122.70 |
| 3 | N | 27 | VAL | CA-C-N | 19.37 | 159.82 | 117.20 |
| 1 | F | 391 | THR | CA-C-N | 19.25 | 159.55 | 117.20 |
| 1 | D | 392 | ILE | O-C-N | -18.80 | 92.62 | 122.70 |
| 1 | K | 245 | ASN | O-C-N | -18.33 | 92.03 | 123.20 |
| 1 | C | 245 | ASN | O-C-N | -18.31 | 92.08 | 123.20 |
| 1 | J | 313 | PHE | O-C-N | -18.16 | 93.64 | 122.70 |
| 1 | B | 7 | LEU | C-N-CA | 17.98 | 166.65 | 121.70 |
| 1 | I | 7 | LEU | C-N-CA | 17.96 | 166.59 | 121.70 |
| 1 | D | 7 | LEU | C-N-CA | 17.92 | 166.50 | 121.70 |
| 3 | N | 26 | SER | C-N-CA | 17.72 | 166.00 | 121.70 |
| 1 | D | 313 | PHE | CA-C-N | 17.68 | 156.09 | 117.20 |
| 1 | B | 313 | PHE | CA-C-N | 17.67 | 156.07 | 117.20 |
| 1 | H | 313 | PHE | CA-C-N | 17.67 | 156.07 | 117.20 |
| 1 | I | 352 | THR | O-C-N | -17.43 | 94.81 | 122.70 |
| 1 | H | 352 | THR | O-C-N | -17.41 | 94.84 | 122.70 |
| 1 | J | 352 | THR | O-C-N | -17.37 | 94.90 | 122.70 |
| 1 | D | 352 | THR | O-C-N | -17.37 | 94.91 | 122.70 |
| 1 | B | 352 | THR | O-C-N | -17.36 | 94.93 | 122.70 |
| 1 | K | 245 | ASN | CA-C-N | 17.22 | 150.65 | 116.20 |
| 1 | C | 245 | ASN | CA-C-N | 17.21 | 150.61 | 116.20 |
| 3 | N | 111 | SER | C-N-CA | 16.91 | 163.98 | 121.70 |
| 1 | B | 392 | ILE | O-C-N | -16.82 | 95.79 | 122.70 |
| 1 | K | 187 | GLN | C-N-CA | 16.46 | 162.86 | 121.70 |
| 1 | E | 381 | THR | CA-C-N | -16.28 | 81.38 | 117.20 |
| 3 | N | 111 | SER | CA-C-N | 16.18 | 152.81 | 117.20 |
| 1 | L | 312 | ASN | CA-C-N | 16.06 | 152.52 | 117.20 |
| 1 | B | 381 | THR | O-C-N | 15.82 | 148.01 | 122.70 |
| 1 | D | 381 | THR | O-C-N | 15.80 | 147.98 | 122.70 |
| 1 | I | 381 | THR | O-C-N | 15.79 | 147.97 | 122.70 |
| 1 | B | 311 | ALA | O-C-N | -15.74 | 97.51 | 122.70 |
| 1 | H | 311 | ALA | O-C-N | -15.73 | 97.53 | 122.70 |
| 1 | A | 352 | THR | C-N-CA | 15.73 | 161.02 | 121.70 |
| 1 | D | 311 | ALA | O-C-N | -15.72 | 97.55 | 122.70 |
| 1 | G | 352 | THR | C-N-CA | 15.72 | 160.99 | 121.70 |
| 1 | G | 382 | SER | CA-C-N | -15.67 | 82.72 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | G | 352 | THR | CA-C-N | 15.54 | 151.38 | 117.20 |
| 1 | A | 352 | THR | CA-C-N | 15.52 | 151.34 | 117.20 |
| 1 | B | 4 | VAL | CB-CA-C | -15.41 | 82.11 | 111.40 |
| 1 | I | 4 | VAL | CB-CA-C | -15.41 | 82.11 | 111.40 |
| 1 | J | 250 | PRO | O-C-N | -15.28 | 98.25 | 122.70 |
| 1 | A | 311 | ALA | O-C-N | -14.91 | 98.85 | 122.70 |
| 1 | B | 4 | VAL | N-CA-CB | -14.84 | 78.85 | 111.50 |
| 3 | N | 26 | SER | CA-C-N | 14.84 | 149.85 | 117.20 |
| 1 | I | 4 | VAL | N-CA-CB | -14.84 | 78.86 | 111.50 |
| 1 | F | 186 | PRO | C-N-CA | 14.69 | 158.43 | 121.70 |
| 3 | N | 90 | PHE | C-N-CD | -14.65 | 88.36 | 120.60 |
| 3 | N | 57 | CYS | O-C-N | -14.63 | 99.28 | 122.70 |
| 1 | L | 161 | GLU | O-C-N | -14.52 | 99.47 | 122.70 |
| 1 | H | 381 | THR | O-C-N | 14.20 | 145.43 | 122.70 |
| 1 | A | 314 | SER | O-C-N | 13.79 | 144.76 | 122.70 |
| 1 | E | 186 | PRO | C-N-CA | 13.77 | 156.13 | 121.70 |
| 1 | H | 352 | THR | C-N-CA | 13.68 | 155.90 | 121.70 |
| 1 | D | 352 | THR | C-N-CA | 13.67 | 155.88 | 121.70 |
| 1 | J | 352 | THR | C-N-CA | 13.66 | 155.85 | 121.70 |
| 1 | B | 352 | THR | C-N-CA | 13.65 | 155.83 | 121.70 |
| 1 | I | 352 | THR | C-N-CA | 13.64 | 155.80 | 121.70 |
| 1 | D | 380 | PHE | O-C-N | -13.63 | 100.89 | 122.70 |
| 1 | L | 312 | ASN | C-N-CA | 13.62 | 155.75 | 121.70 |
| 1 | D | 392 | ILE | CA-C-N | 13.62 | 147.15 | 117.20 |
| 3 | N | 27 | VAL | O-C-N | -13.45 | 101.18 | 122.70 |
| 1 | C | 184 | ASN | C-N-CA | -13.34 | 88.36 | 121.70 |
| 1 | K | 279 | ALA | O-C-N | -13.30 | 101.42 | 122.70 |
| 1 | C | 279 | ALA | O-C-N | -13.20 | 101.57 | 122.70 |
| 3 | N | 17 | GLY | O-C-N | -13.13 | 101.69 | 122.70 |
| 1 | D | 390 | GLY | O-C-N | -13.09 | 101.76 | 122.70 |
| 1 | I | 390 | GLY | O-C-N | -13.08 | 101.78 | 122.70 |
| 1 | B | 390 | GLY | O-C-N | -13.06 | 101.80 | 122.70 |
| 1 | A | 24 | ASN | CA-C-N | -13.05 | 88.49 | 117.20 |
| 1 | F | 279 | ALA | C-N-CA | 12.83 | 153.77 | 121.70 |
| 1 | E | 279 | ALA | C-N-CA | 12.82 | 153.75 | 121.70 |
| 3 | N | 27 | VAL | N-CA-C | 12.80 | 145.57 | 111.00 |
| 4 | P | 31 | VAL | CA-C-N | 12.80 | 145.36 | 117.20 |
| 1 | K | 186 | PRO | O-C-N | -12.69 | 102.40 | 122.70 |
| 1 | I | 380 | PHE | O-C-N | 12.65 | 142.94 | 122.70 |
| 1 | B | 380 | PHE | O-C-N | 12.63 | 142.91 | 122.70 |
| 4 | P | 45 | GLN | C-N-CD | -12.58 | 92.93 | 120.60 |
| 3 | N | 94 | VAL | C-N-CD | -12.47 | 93.17 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | B | 358 | VAL | N-CA-CB | 12.45 | 138.90 | 111.50 |
| 1 | C | 186 | PRO | CA-N-CD | -12.45 | 94.07 | 111.50 |
| 1 | B | 311 | ALA | C-N-CA | 12.37 | 152.63 | 121.70 |
| 1 | H | 311 | ALA | C-N-CA | 12.37 | 152.62 | 121.70 |
| 1 | D | 311 | ALA | C-N-CA | 12.36 | 152.61 | 121.70 |
| 1 | B | 381 | THR | CA-C-N | -12.36 | 90.02 | 117.20 |
| 1 | D | 381 | THR | CA-C-N | -12.34 | 90.05 | 117.20 |
| 1 | I | 381 | THR | CA-C-N | -12.34 | 90.06 | 117.20 |
| 1 | F | 247 | TYR | C-N-CA | 12.20 | 152.21 | 121.70 |
| 1 | A | 381 | THR | O-C-N | -11.93 | 103.62 | 122.70 |
| 1 | L | 150 | ALA | O-C-N | 11.90 | 143.71 | 121.10 |
| 4 | P | 32 | ALA | C-N-CA | 11.85 | 151.32 | 121.70 |
| 4 | P | 31 | VAL | C-N-CA | 11.81 | 151.23 | 121.70 |
| 1 | F | 391 | THR | C-N-CA | 11.79 | 151.19 | 121.70 |
| 1 | H | 352 | THR | CA-C-N | 11.68 | 142.89 | 117.20 |
| 1 | B | 352 | THR | CA-C-N | 11.67 | 142.87 | 117.20 |
| 1 | D | 352 | THR | CA-C-N | 11.65 | 142.84 | 117.20 |
| 1 | J | 352 | THR | CA-C-N | 11.65 | 142.83 | 117.20 |
| 1 | I | 352 | THR | CA-C-N | 11.64 | 142.81 | 117.20 |
| 1 | H | 381 | THR | CA-C-N | -11.60 | 91.69 | 117.20 |
| 1 | J | 185 | VAL | C-N-CD | -11.58 | 95.13 | 120.60 |
| 1 | I | 313 | PHE | C-N-CA | 11.54 | 150.54 | 121.70 |
| 3 | N | 27 | VAL | C-N-CA | 11.43 | 150.28 | 121.70 |
| 1 | K | 311 | ALA | O-C-N | -11.34 | 104.55 | 122.70 |
| 1 | C | 243 | GLY | O-C-N | -11.28 | 104.65 | 122.70 |
| 1 | I | 392 | ILE | C-N-CA | -11.28 | 93.50 | 121.70 |
| 1 | A | 313 | PHE | C-N-CA | 11.27 | 149.87 | 121.70 |
| 1 | C | 311 | ALA | O-C-N | -11.25 | 104.70 | 122.70 |
| 1 | K | 243 | GLY | O-C-N | -11.25 | 104.70 | 122.70 |
| 1 | L | 177 | LEU | C-N-CA | -11.25 | 93.58 | 121.70 |
| 1 | K | 380 | PHE | C-N-CA | 11.22 | 149.76 | 121.70 |
| 1 | F | 391 | THR | O-C-N | 11.19 | 140.61 | 122.70 |
| 3 | N | 28 | ARG | N-CA-C | 11.11 | 141.00 | 111.00 |
| 1 | K | 188 | SER | C-N-CA | 11.09 | 149.42 | 121.70 |
| 1 | B | 8 | THR | O-C-N | 11.01 | 142.01 | 121.10 |
| 1 | I | 8 | THR | O-C-N | 11.00 | 142.01 | 121.10 |
| 1 | H | 311 | ALA | CA-C-N | 10.81 | 140.99 | 117.20 |
| 1 | I | 311 | ALA | O-C-N | -10.81 | 105.40 | 122.70 |
| 1 | B | 311 | ALA | CA-C-N | 10.81 | 140.97 | 117.20 |
| 1 | D | 311 | ALA | CA-C-N | 10.79 | 140.94 | 117.20 |
| 4 | P | 32 | ALA | CA-C-N | 10.77 | 140.90 | 117.20 |
| 1 | G | 185 | VAL | C-N-CD | -10.73 | 97.00 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | A | 314 | SER | CA-C-O | 10.69 | 142.54 | 120.10 |
| 3 | N | 26 | SER | CA-C-O | -10.67 | 97.70 | 120.10 |
| 3 | N | 40 | LYS | O-C-N | -10.65 | 105.66 | 122.70 |
| 1 | I | 4 | VAL | CA-CB-CG1 | 10.63 | 126.84 | 110.90 |
| 1 | B | 4 | VAL | CA-CB-CG1 | 10.62 | 126.83 | 110.90 |
| 1 | I | 185 | VAL | O-C-N | -10.62 | 100.93 | 121.10 |
| 1 | H | 185 | VAL | O-C-N | -10.62 | 100.93 | 121.10 |
| 1 | B | 185 | VAL | O-C-N | -10.61 | 100.95 | 121.10 |
| 4 | P | 31 | VAL | O-C-N | -10.59 | 105.75 | 122.70 |
| 1 | D | 185 | VAL | O-C-N | -10.57 | 101.01 | 121.10 |
| 1 | C | 186 | PRO | CA-C-N | 10.50 | 140.29 | 117.20 |
| 1 | F | 311 | ALA | O-C-N | -10.43 | 106.01 | 122.70 |
| 1 | E | 311 | ALA | O-C-N | -10.41 | 106.04 | 122.70 |
| 2 | M | 64 | GLY | CA-C-N | 10.38 | 140.05 | 117.20 |
| 3 | N | 25 | GLN | O-C-N | -10.21 | 106.36 | 122.70 |
| 1 | C | 243 | GLY | C-N-CA | 10.17 | 147.13 | 121.70 |
| 1 | K | 243 | GLY | C-N-CA | 10.17 | 147.12 | 121.70 |
| 1 | C | 381 | THR | CA-C-N | -10.16 | 94.85 | 117.20 |
| 4 | P | 36 | GLU | CA-C-N | 10.15 | 136.51 | 116.20 |
| 3 | N | 27 | VAL | CA-C-O | -10.14 | 98.80 | 120.10 |
| 1 | B | 358 | VAL | N-CA-C | -10.10 | 83.72 | 111.00 |
| 1 | K | 186 | PRO | CA-C-N | 10.10 | 139.42 | 117.20 |
| 1 | G | 35 | SER | O-C-N | 9.91 | 138.55 | 122.70 |
| 4 | P | 36 | GLU | O-C-N | -9.89 | 106.38 | 123.20 |
| 1 | C | 245 | ASN | C-N-CA | 9.83 | 142.94 | 122.30 |
| 1 | K | 245 | ASN | C-N-CA | 9.82 | 142.92 | 122.30 |
| 1 | A | 313 | PHE | CA-C-N | 9.80 | 138.77 | 117.20 |
| 1 | J | 313 | PHE | CA-C-N | 9.80 | 138.76 | 117.20 |
| 1 | C | 279 | ALA | C-N-CA | 9.79 | 146.19 | 121.70 |
| 1 | K | 279 | ALA | C-N-CA | 9.78 | 146.15 | 121.70 |
| 1 | G | 313 | PHE | CA-C-N | 9.68 | 138.50 | 117.20 |
| 3 | N | 43 | LEU | O-C-N | -9.66 | 107.23 | 122.70 |
| 1 | L | 381 | THR | CA-C-N | -9.62 | 96.03 | 117.20 |
| 1 | L | 177 | LEU | CA-C-N | -9.57 | 96.15 | 117.20 |
| 3 | N | 12 | THR | C-N-CD | -9.53 | 99.63 | 120.60 |
| 1 | L | 177 | LEU | O-C-N | 9.45 | 137.83 | 122.70 |
| 3 | N | 26 | SER | N-CA-C | 9.26 | 136.01 | 111.00 |
| 4 | P | 32 | ALA | N-CA-C | 9.24 | 135.96 | 111.00 |
| 1 | L | 243 | GLY | O-C-N | -9.24 | 107.91 | 122.70 |
| 1 | I | 380 | PHE | CA-C-N | -9.22 | 96.92 | 117.20 |
| 1 | B | 380 | PHE | CA-C-N | -9.21 | 96.94 | 117.20 |
| 1 | K | 186 | PRO | CA-N-CD | -9.18 | 98.65 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | M | 41 | ALA | O-C-N | -9.15 | 108.06 | 122.70 |
| 1 | A | 243 | GLY | C-N-CA | 9.13 | 144.52 | 121.70 |
| 1 | G | 243 | GLY | C-N-CA | 9.12 | 144.49 | 121.70 |
| 1 | K | 185 | VAL | C-N-CD | -8.85 | 101.13 | 120.60 |
| 3 | N | 17 | GLY | CA-C-N | 8.85 | 136.67 | 117.20 |
| 1 | A | 245 | ASN | CA-C-N | 8.81 | 133.81 | 116.20 |
| 1 | G | 245 | ASN | CA-C-N | 8.79 | 133.78 | 116.20 |
| 1 | H | 392 | ILE | O-C-N | -8.77 | 108.66 | 122.70 |
| 2 | M | 64 | GLY | O-C-N | -8.77 | 108.67 | 122.70 |
| 1 | I | 389 | ALA | CA-C-N | 8.76 | 133.73 | 116.20 |
| 1 | D | 389 | ALA | CA-C-N | 8.74 | 133.68 | 116.20 |
| 1 | F | 279 | ALA | O-C-N | -8.74 | 108.71 | 122.70 |
| 1 | H | 389 | ALA | CA-C-N | 8.74 | 133.68 | 116.20 |
| 1 | E | 279 | ALA | O-C-N | -8.72 | 108.74 | 122.70 |
| 1 | B | 389 | ALA | CA-C-N | 8.72 | 133.64 | 116.20 |
| 1 | K | 185 | VAL | CB-CA-C | -8.70 | 94.87 | 111.40 |
| 1 | J | 187 | GLN | O-C-N | -8.62 | 108.90 | 122.70 |
| 1 | L | 150 | ALA | C-N-CD | 8.60 | 146.46 | 128.40 |
| 1 | L | 279 | ALA | C-N-CA | 8.53 | 143.03 | 121.70 |
| 4 | P | 36 | GLU | C-N-CA | 8.47 | 140.08 | 122.30 |
| 1 | K | 244 | GLN | O-C-N | -8.46 | 109.16 | 122.70 |
| 1 | I | 311 | ALA | C-N-CA | 8.44 | 142.79 | 121.70 |
| 2 | M | 36 | ALA | C-N-CA | 8.43 | 139.99 | 122.30 |
| 1 | C | 244 | GLN | O-C-N | -8.42 | 109.22 | 122.70 |
| 2 | M | 46 | PRO | O-C-N | -8.38 | 109.30 | 122.70 |
| 1 | J | 250 | PRO | CA-C-N | 8.36 | 135.60 | 117.20 |
| 3 | N | 25 | GLN | CA-C-N | 8.36 | 135.60 | 117.20 |
| 3 | N | 19 | ASP | O-C-N | -8.34 | 109.36 | 122.70 |
| 1 | D | 313 | PHE | C-N-CA | 8.30 | 142.45 | 121.70 |
| 1 | H | 313 | PHE | C-N-CA | 8.28 | 142.41 | 121.70 |
| 1 | B | 313 | PHE | C-N-CA | 8.28 | 142.39 | 121.70 |
| 1 | L | 381 | THR | O-C-N | -8.26 | 109.49 | 122.70 |
| 1 | K | 17 | ASN | O-C-N | 8.19 | 135.81 | 122.70 |
| 1 | I | 245 | ASN | O-C-N | 8.13 | 137.03 | 123.20 |
| 1 | B | 245 | ASN | O-C-N | 8.12 | 137.00 | 123.20 |
| 1 | D | 245 | ASN | O-C-N | 8.12 | 137.00 | 123.20 |
| 1 | H | 245 | ASN | O-C-N | 8.10 | 136.97 | 123.20 |
| 1 | D | 380 | PHE | C-N-CA | 8.09 | 141.93 | 121.70 |
| 1 | L | 236 | TYR | CA-C-N | -8.07 | 99.44 | 117.20 |
| 1 | J | 310 | THR | CA-C-N | -8.01 | 99.58 | 117.20 |
| 1 | E | 187 | GLN | CA-C-N | -7.97 | 99.67 | 117.20 |
| 1 | E | 182 | LEU | CA-C-N | -7.94 | 99.72 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 381 | THR | C-N-CA | -7.93 | 101.88 | 121.70 |
| 1 | I | 381 | THR | C-N-CA | -7.91 | 101.91 | 121.70 |
| 1 | D | 381 | THR | C-N-CA | -7.90 | 101.95 | 121.70 |
| 1 | A | 243 | GLY | O-C-N | -7.87 | 110.11 | 122.70 |
| 1 | G | 243 | GLY | O-C-N | -7.85 | 110.14 | 122.70 |
| 1 | H | 389 | ALA | O-C-N | -7.85 | 109.86 | 123.20 |
| 1 | I | 389 | ALA | O-C-N | -7.85 | 109.86 | 123.20 |
| 1 | I | 380 | PHE | C-N-CA | -7.83 | 102.12 | 121.70 |
| 1 | B | 389 | ALA | O-C-N | -7.82 | 109.90 | 123.20 |
| 1 | D | 389 | ALA | O-C-N | -7.82 | 109.91 | 123.20 |
| 1 | B | 380 | PHE | C-N-CA | -7.82 | 102.15 | 121.70 |
| 3 | N | 28 | ARG | O-C-N | -7.81 | 109.92 | 123.20 |
| 2 | M | 36 | ALA | N-CA-C | 7.77 | 131.98 | 111.00 |
| 1 | K | 244 | GLN | CA-C-N | 7.76 | 134.27 | 117.20 |
| 1 | C | 244 | GLN | CA-C-N | 7.72 | 134.19 | 117.20 |
| 1 | L | 150 | ALA | CA-C-N | -7.67 | 95.64 | 117.10 |
| 1 | J | 184 | ASN | O-C-N | -7.66 | 110.44 | 122.70 |
| 1 | K | 243 | GLY | CA-C-N | 7.65 | 134.03 | 117.20 |
| 1 | H | 392 | ILE | CA-C-N | -7.61 | 100.45 | 117.20 |
| 1 | C | 243 | GLY | CA-C-N | 7.59 | 133.90 | 117.20 |
| 1 | D | 380 | PHE | CA-C-N | 7.58 | 133.87 | 117.20 |
| 3 | N | 109 | LYS | C-N-CA | 7.54 | 140.54 | 121.70 |
| 1 | G | 35 | SER | CA-C-N | -7.51 | 100.69 | 117.20 |
| 1 | I | 185 | VAL | CA-C-N | 7.48 | 138.04 | 117.10 |
| 1 | B | 185 | VAL | CA-C-N | 7.47 | 138.03 | 117.10 |
| 1 | H | 185 | VAL | CA-C-N | 7.47 | 138.02 | 117.10 |
| 1 | D | 185 | VAL | CA-C-N | 7.46 | 138.00 | 117.10 |
| 4 | P | 32 | ALA | O-C-N | -7.45 | 110.78 | 122.70 |
| 1 | I | 8 | THR | C-N-CD | 7.44 | 144.03 | 128.40 |
| 1 | B | 392 | ILE | C-N-CA | -7.44 | 103.10 | 121.70 |
| 1 | J | 184 | ASN | CA-C-N | 7.43 | 133.54 | 117.20 |
| 1 | B | 8 | THR | C-N-CD | 7.43 | 144.00 | 128.40 |
| 1 | J | 309 | ARG | C-N-CA | -7.43 | 103.13 | 121.70 |
| 1 | L | 257 | LEU | CA-C-N | -7.39 | 100.93 | 117.20 |
| 1 | B | 394 | THR | CA-C-N | 7.35 | 133.38 | 117.20 |
| 1 | K | 244 | GLN | C-N-CA | 7.34 | 140.05 | 121.70 |
| 1 | D | 394 | THR | CA-C-N | 7.32 | 133.31 | 117.20 |
| 1 | K | 17 | ASN | CA-C-N | -7.31 | 101.11 | 117.20 |
| 1 | C | 244 | GLN | C-N-CA | 7.30 | 139.96 | 121.70 |
| 1 | E | 186 | PRO | CA-N-CD | -7.28 | 101.31 | 111.50 |
| 1 | I | 394 | THR | CA-C-N | 7.28 | 133.21 | 117.20 |
| 1 | E | 187 | GLN | O-C-N | 7.24 | 134.28 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | K | 191 | ARG | C-N-CA | -7.17 | 103.76 | 121.70 |
| 1 | I | 311 | ALA | CA-C-N | 7.17 | 132.98 | 117.20 |
| 1 | J | 250 | PRO | C-N-CA | 7.16 | 139.60 | 121.70 |
| 1 | A | 244 | GLN | O-C-N | -7.11 | 111.32 | 122.70 |
| 3 | N | 54 | GLY | O-C-N | -7.11 | 111.33 | 122.70 |
| 4 | P | 5 | LYS | O-C-N | -7.10 | 111.34 | 122.70 |
| 1 | G | 244 | GLN | O-C-N | -7.09 | 111.35 | 122.70 |
| 2 | M | 39 | GLN | O-C-N | -7.07 | 111.38 | 122.70 |
| 3 | N | 57 | CYS | C-N-CA | 7.03 | 139.27 | 121.70 |
| 1 | I | 4 | VAL | N-CA-C | -6.95 | 92.23 | 111.00 |
| 1 | B | 4 | VAL | N-CA-C | -6.95 | 92.25 | 111.00 |
| 1 | K | 185 | VAL | N-CA-C | 6.93 | 129.72 | 111.00 |
| 1 | K | 186 | PRO | C-N-CA | 6.93 | 139.03 | 121.70 |
| 1 | J | 184 | ASN | C-N-CA | 6.93 | 139.02 | 121.70 |
| 1 | F | 391 | THR | N-CA-C | 6.92 | 129.69 | 111.00 |
| 1 | I | 8 | THR | CA-C-N | -6.89 | 97.80 | 117.10 |
| 1 | B | 8 | THR | CA-C-N | -6.88 | 97.84 | 117.10 |
| 1 | F | 393 | SER | CA-C-O | 6.87 | 134.52 | 120.10 |
| 1 | G | 245 | ASN | O-C-N | -6.86 | 111.55 | 123.20 |
| 1 | A | 245 | ASN | O-C-N | -6.85 | 111.55 | 123.20 |
| 1 | A | 310 | THR | N-CA-CB | 6.83 | 123.28 | 110.30 |
| 1 | C | 279 | ALA | CA-C-N | 6.80 | 132.16 | 117.20 |
| 1 | G | 35 | SER | C-N-CA | -6.79 | 104.73 | 121.70 |
| 3 | N | 31 | PHE | O-C-N | -6.76 | 111.88 | 122.70 |
| 1 | B | 358 | VAL | CB-CA-C | 6.75 | 124.23 | 111.40 |
| 3 | N | 40 | LYS | C-N-CA | 6.75 | 138.59 | 121.70 |
| 4 | P | 5 | LYS | CA-C-N | 6.75 | 132.05 | 117.20 |
| 1 | K | 279 | ALA | CA-C-N | 6.75 | 132.04 | 117.20 |
| 1 | A | 244 | GLN | C-N-CA | 6.68 | 138.40 | 121.70 |
| 1 | G | 244 | GLN | C-N-CA | 6.66 | 138.35 | 121.70 |
| 1 | C | 381 | THR | O-C-N | 6.65 | 133.34 | 122.70 |
| 1 | B | 4 | VAL | C-N-CA | -6.65 | 105.07 | 121.70 |
| 1 | I | 4 | VAL | C-N-CA | -6.64 | 105.09 | 121.70 |
| 1 | L | 313 | PHE | O-C-N | 6.61 | 133.27 | 122.70 |
| 4 | P | 101 | ASN | O-C-N | -6.57 | 112.19 | 122.70 |
| 1 | A | 244 | GLN | CA-C-N | 6.53 | 131.57 | 117.20 |
| 1 | I | 312 | ASN | O-C-N | -6.52 | 112.28 | 122.70 |
| 1 | G | 244 | GLN | CA-C-N | 6.51 | 131.52 | 117.20 |
| 3 | N | 23 | GLY | C-N-CD | -6.50 | 106.31 | 120.60 |
| 3 | N | 57 | CYS | CA-C-N | 6.50 | 131.49 | 117.20 |
| 1 | J | 187 | GLN | CA-C-N | 6.48 | 131.45 | 117.20 |
| 2 | M | 64 | GLY | C-N-CA | 6.46 | 137.85 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | M | 39 | GLN | CA-C-N | 6.46 | 131.40 | 117.20 |
| 1 | A | 314 | SER | N-CA-C | 6.40 | 128.29 | 111.00 |
| 1 | K | 181 | VAL | C-N-CA | 6.40 | 137.71 | 121.70 |
| 3 | N | 26 | SER | O-C-N | -6.40 | 112.45 | 122.70 |
| 1 | I | 245 | ASN | CA-C-N | -6.38 | 103.45 | 116.20 |
| 1 | D | 245 | ASN | CA-C-N | -6.37 | 103.46 | 116.20 |
| 1 | B | 245 | ASN | CA-C-N | -6.36 | 103.47 | 116.20 |
| 1 | H | 245 | ASN | CA-C-N | -6.36 | 103.48 | 116.20 |
| 2 | M | 66 | GLY | CA-C-N | 6.36 | 131.19 | 117.20 |
| 1 | I | 13 | ALA | C-N-CA | -6.36 | 105.81 | 121.70 |
| 1 | G | 314 | SER | C-N-CA | -6.35 | 105.83 | 121.70 |
| 1 | B | 13 | ALA | C-N-CA | -6.34 | 105.84 | 121.70 |
| 1 | F | 393 | SER | CA-C-N | -6.32 | 103.31 | 117.20 |
| 1 | D | 13 | ALA | C-N-CA | -6.31 | 105.92 | 121.70 |
| 3 | N | 40 | LYS | CA-C-N | 6.30 | 131.06 | 117.20 |
| 3 | N | 110 | LYS | C-N-CA | 6.29 | 137.42 | 121.70 |
| 1 | L | 243 | GLY | CA-C-N | 6.28 | 131.02 | 117.20 |
| 1 | G | 382 | SER | O-C-N | -6.25 | 112.70 | 122.70 |
| 1 | J | 18 | GLN | O-C-N | 6.25 | 132.70 | 122.70 |
| 2 | M | 41 | ALA | CA-C-N | 6.24 | 130.92 | 117.20 |
| 1 | D | 312 | ASN | O-C-N | -6.22 | 112.75 | 122.70 |
| 1 | B | 312 | ASN | O-C-N | -6.21 | 112.76 | 122.70 |
| 1 | H | 312 | ASN | O-C-N | -6.20 | 112.78 | 122.70 |
| 1 | L | 236 | TYR | O-C-N | 6.17 | 132.57 | 122.70 |
| 1 | L | 280 | ASN | C-N-CA | 6.15 | 137.08 | 121.70 |
| 1 | H | 381 | THR | C-N-CA | -6.14 | 106.35 | 121.70 |
| 1 | L | 313 | PHE | CA-C-N | -6.11 | 103.76 | 117.20 |
| 1 | A | 311 | ALA | CA-C-N | 6.10 | 130.62 | 117.20 |
| 1 | C | 185 | VAL | CA-C-N | -6.09 | 100.06 | 117.10 |
| 1 | A | 186 | PRO | N-CA-CB | 6.03 | 110.53 | 103.30 |
| 1 | F | 243 | GLY | O-C-N | -6.01 | 113.08 | 122.70 |
| 1 | K | 191 | ARG | CA-C-N | -6.00 | 104.00 | 117.20 |
| 3 | N | 110 | LYS | N-CA-C | 6.00 | 127.20 | 111.00 |
| 3 | N | 25 | GLN | C-N-CA | 5.99 | 136.68 | 121.70 |
| 1 | L | 236 | TYR | CA-CB-CG | 5.99 | 124.78 | 113.40 |
| 1 | K | 162 | LEU | CA-CB-CG | 5.96 | 129.01 | 115.30 |
| 1 | J | 310 | THR | O-C-N | 5.95 | 132.22 | 122.70 |
| 3 | N | 61 | ASP | O-C-N | -5.95 | 113.19 | 122.70 |
| 1 | F | 162 | LEU | CA-CB-CG | 5.93 | 128.95 | 115.30 |
| 1 | L | 161 | GLU | CA-C-N | 5.93 | 130.25 | 117.20 |
| 1 | C | 162 | LEU | CA-CB-CG | 5.92 | 128.91 | 115.30 |
| 1 | L | 162 | LEU | CA-CB-CG | 5.92 | 128.91 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | E | 162 | LEU | CA-CB-CG | 5.91 | 128.90 | 115.30 |
| 1 | I | 389 | ALA | C-N-CA | 5.91 | 134.70 | 122.30 |
| 1 | A | 311 | ALA | C-N-CA | 5.90 | 136.45 | 121.70 |
| 3 | N | 65 | ASN | CA-C-N | 5.88 | 130.12 | 117.20 |
| 1 | H | 389 | ALA | C-N-CA | 5.87 | 134.63 | 122.30 |
| 1 | J | 256 | THR | O-C-N | -5.87 | 113.31 | 122.70 |
| 1 | D | 389 | ALA | C-N-CA | 5.85 | 134.59 | 122.30 |
| 1 | I | 309 | ARG | C-N-CA | 5.85 | 136.34 | 121.70 |
| 1 | B | 389 | ALA | C-N-CA | 5.84 | 134.57 | 122.30 |
| 1 | J | 8 | THR | CA-C-O | 5.82 | 132.32 | 120.10 |
| 1 | C | 311 | ALA | CA-C-N | 5.79 | 129.94 | 117.20 |
| 2 | M | 76 | PRO | CA-C-N | -5.79 | 104.47 | 117.20 |
| 1 | K | 311 | ALA | CA-C-N | 5.78 | 129.92 | 117.20 |
| 1 | B | 394 | THR | C-N-CA | 5.75 | 136.08 | 121.70 |
| 1 | D | 394 | THR | C-N-CA | 5.75 | 136.07 | 121.70 |
| 1 | I | 243 | GLY | O-C-N | -5.71 | 113.56 | 122.70 |
| 3 | N | 65 | ASN | O-C-N | -5.71 | 113.57 | 122.70 |
| 1 | H | 243 | GLY | O-C-N | -5.70 | 113.58 | 122.70 |
| 1 | I | 394 | THR | C-N-CA | 5.70 | 135.94 | 121.70 |
| 1 | B | 243 | GLY | O-C-N | -5.68 | 113.61 | 122.70 |
| 3 | N | 54 | GLY | CA-C-N | 5.68 | 129.70 | 117.20 |
| 1 | D | 243 | GLY | O-C-N | -5.68 | 113.62 | 122.70 |
| 4 | P | 32 | ALA | CA-C-O | -5.61 | 108.31 | 120.10 |
| 4 | P | 38 | PRO | C-N-CD | -5.59 | 108.29 | 120.60 |
| 1 | E | 244 | GLN | CA-C-O | -5.56 | 108.42 | 120.10 |
| 1 | K | 185 | VAL | CA-C-N | -5.55 | 101.55 | 117.10 |
| 1 | C | 185 | VAL | N-CA-C | -5.55 | 96.02 | 111.00 |
| 1 | C | 186 | PRO | N-CA-C | 5.54 | 126.51 | 112.10 |
| 1 | C | 185 | VAL | O-C-N | 5.54 | 131.62 | 121.10 |
| 2 | M | 60 | TYR | C-N-CA | 5.50 | 135.46 | 121.70 |
| 1 | K | 383 | ARG | C-N-CA | 5.50 | 135.44 | 121.70 |
| 2 | M | 76 | PRO | CA-C-O | 5.50 | 133.39 | 120.20 |
| 1 | E | 188 | SER | CA-C-N | -5.49 | 105.12 | 117.20 |
| 3 | N | 18 | CYS | CA-C-N | 5.49 | 129.28 | 117.20 |
| 1 | A | 310 | THR | N-CA-C | -5.48 | 96.20 | 111.00 |
| 1 | G | 313 | PHE | C-N-CA | 5.46 | 135.35 | 121.70 |
| 2 | M | 16 | PRO | O-C-N | -5.44 | 113.95 | 123.20 |
| 1 | H | 185 | VAL | C-N-CA | 5.44 | 144.84 | 122.00 |
| 1 | I | 185 | VAL | C-N-CA | 5.44 | 144.84 | 122.00 |
| 1 | B | 185 | VAL | C-N-CA | 5.43 | 144.82 | 122.00 |
| 1 | L | 279 | ALA | O-C-N | -5.43 | 114.01 | 122.70 |
| 1 | C | 313 | PHE | O-C-N | 5.43 | 131.38 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | D | 185 | VAL | C-N-CA | 5.42 | 144.78 | 122.00 |
| 1 | F | 279 | ALA | CA-C-N | 5.42 | 129.12 | 117.20 |
| 2 | M | 46 | PRO | CA-C-N | 5.41 | 129.10 | 117.20 |
| 2 | M | 67 | ILE | O-C-N | -5.40 | 114.06 | 122.70 |
| 1 | E | 279 | ALA | CA-C-N | 5.40 | 129.07 | 117.20 |
| 1 | K | 313 | PHE | O-C-N | 5.39 | 131.32 | 122.70 |
| 4 | P | 31 | VAL | CA-C-O | -5.38 | 108.79 | 120.10 |
| 3 | N | 64 | GLU | O-C-N | -5.38 | 114.09 | 122.70 |
| 1 | L | 161 | GLU | C-N-CA | 5.37 | 135.13 | 121.70 |
| 3 | N | 61 | ASP | CA-C-N | 5.33 | 128.93 | 117.20 |
| 4 | P | 98 | SER | O-C-N | -5.30 | 114.22 | 122.70 |
| 1 | E | 311 | ALA | CA-C-N | 5.29 | 128.84 | 117.20 |
| 1 | F | 311 | ALA | CA-C-N | 5.27 | 128.80 | 117.20 |
| 1 | L | 237 | LEU | N-CA-C | -5.25 | 96.82 | 111.00 |
| 2 | M | 48 | LEU | CA-C-N | 5.25 | 128.75 | 117.20 |
| 1 | E | 243 | GLY | O-C-N | -5.23 | 114.33 | 122.70 |
| 2 | M | 15 | ILE | C-N-CD | -5.23 | 109.09 | 120.60 |
| 2 | M | 64 | GLY | CA-C-O | -5.20 | 111.24 | 120.60 |
| 1 | G | 314 | SER | CA-C-N | 5.19 | 128.61 | 117.20 |
| 4 | P | 3 | LYS | C-N-CA | -5.18 | 108.74 | 121.70 |
| 1 | L | 236 | TYR | N-CA-C | 5.18 | 124.98 | 111.00 |
| 1 | D | 26 | GLN | O-C-N | -5.17 | 114.42 | 122.70 |
| 1 | A | 310 | THR | CB-CA-C | -5.17 | 97.64 | 111.60 |
| 2 | M | 36 | ALA | N-CA-CB | -5.14 | 102.91 | 110.10 |
| 2 | M | 66 | GLY | O-C-N | -5.12 | 114.50 | 122.70 |
| 2 | M | 65 | THR | N-CA-C | 5.11 | 124.81 | 111.00 |
| 1 | A | 243 | GLY | CA-C-N | 5.11 | 128.44 | 117.20 |
| 2 | M | 63 | ILE | O-C-N | -5.10 | 114.53 | 123.20 |
| 2 | M | 13 | VAL | N-CA-C | -5.09 | 97.26 | 111.00 |
| 1 | G | 243 | GLY | CA-C-N | 5.08 | 128.38 | 117.20 |
| 1 | I | 312 | ASN | CA-C-N | 5.08 | 128.37 | 117.20 |
| 2 | M | 48 | LEU | O-C-N | -5.06 | 114.60 | 122.70 |
| 1 | E | 188 | SER | C-N-CA | 5.05 | 134.33 | 121.70 |
| 1 | E | 381 | THR | C-N-CA | -5.04 | 109.09 | 121.70 |
| 3 | N | 44 | THR | N-CA-C | 5.02 | 124.56 | 111.00 |

There are no chirality outliers.

All (91) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 245 | ASN | Mainchain |
| 1 | A | 309 | ARG | Mainchain |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|-------------------|
| 1 | A | 311 | ALA | Mainchain |
| 1 | A | 313 | PHE | Mainchain |
| 1 | A | 352 | THR | Peptide |
| 1 | A | 381 | THR | Mainchain,Peptide |
| 1 | B | 13 | ALA | Mainchain |
| 1 | B | 16 | ARG | Mainchain,Peptide |
| 1 | B | 313 | PHE | Mainchain,Peptide |
| 1 | B | 352 | THR | Mainchain,Peptide |
| 1 | B | 358 | VAL | Mainchain |
| 1 | B | 390 | GLY | Mainchain |
| 1 | B | 392 | ILE | Mainchain,Peptide |
| 1 | B | 394 | THR | Mainchain |
| 1 | B | 7 | LEU | Mainchain |
| 1 | C | 186 | PRO | Peptide |
| 1 | C | 245 | ASN | Mainchain |
| 1 | C | 279 | ALA | Mainchain,Peptide |
| 1 | C | 311 | ALA | Mainchain,Peptide |
| 1 | C | 381 | THR | Mainchain |
| 1 | D | 13 | ALA | Mainchain |
| 1 | D | 313 | PHE | Mainchain,Peptide |
| 1 | D | 352 | THR | Mainchain,Peptide |
| 1 | D | 380 | PHE | Mainchain |
| 1 | D | 390 | GLY | Mainchain |
| 1 | D | 392 | ILE | Mainchain |
| 1 | D | 394 | THR | Mainchain |
| 1 | D | 7 | LEU | Mainchain |
| 1 | E | 182 | LEU | Mainchain |
| 1 | E | 186 | PRO | Mainchain |
| 1 | E | 279 | ALA | Mainchain |
| 1 | E | 311 | ALA | Mainchain,Peptide |
| 1 | F | 186 | PRO | Mainchain,Peptide |
| 1 | F | 247 | TYR | Mainchain |
| 1 | F | 279 | ALA | Mainchain |
| 1 | F | 311 | ALA | Mainchain,Peptide |
| 1 | G | 245 | ASN | Mainchain |
| 1 | G | 313 | PHE | Mainchain |
| 1 | G | 314 | SER | Mainchain,Peptide |
| 1 | G | 352 | THR | Peptide |
| 1 | H | 313 | PHE | Mainchain,Peptide |
| 1 | H | 352 | THR | Mainchain,Peptide |
| 1 | H | 392 | ILE | Mainchain |
| 1 | I | 13 | ALA | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | I | 16 | ARG | Mainchain,Peptide |
| 1 | I | 313 | PHE | Mainchain,Peptide |
| 1 | I | 352 | THR | Mainchain,Peptide |
| 1 | I | 390 | GLY | Mainchain |
| 1 | I | 394 | THR | Mainchain |
| 1 | I | 7 | LEU | Mainchain |
| 1 | J | 183 | ALA | Mainchain |
| 1 | J | 250 | PRO | Mainchain |
| 1 | J | 313 | PHE | Mainchain |
| 1 | J | 352 | THR | Mainchain,Peptide |
| 1 | K | 181 | VAL | Peptide |
| 1 | K | 186 | PRO | Mainchain |
| 1 | K | 187 | GLN | Mainchain |
| 1 | K | 245 | ASN | Mainchain |
| 1 | K | 279 | ALA | Mainchain,Peptide |
| 1 | K | 311 | ALA | Mainchain,Peptide |
| 1 | K | 380 | PHE | Mainchain,Peptide |
| 1 | L | 11 | GLN | Mainchain |
| 1 | L | 161 | GLU | Mainchain |
| 1 | L | 177 | LEU | Mainchain |
| 1 | L | 279 | ALA | Mainchain,Peptide |
| 3 | N | 10 | THR | Mainchain |
| 3 | N | 111 | SER | Peptide |
| 3 | N | 52 | PHE | Mainchain |

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 | 2956 | 0 | 2851 | 116 | 0 |
| 1 | B | 3045 | 0 | 2937 | 307 | 0 |
| 1 | C | 2999 | 0 | 2903 | 129 | 0 |
| 1 | D | 3045 | 0 | 2939 | 334 | 0 |
| 1 | E | 2944 | 0 | 2846 | 212 | 0 |
| 1 | F | 3009 | 0 | 2912 | 268 | 0 |
| 1 | G | 2926 | 0 | 2832 | 196 | 0 |
| 1 | H | 3045 | 0 | 2951 | 197 | 0 |
| 1 | I | 3045 | 0 | 2931 | 337 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | J | 3027 | 0 | 2927 | 210 | 0 |
| 1 | K | 2992 | 0 | 2880 | 234 | 0 |
| 1 | L | 2953 | 0 | 2854 | 329 | 0 |
| 2 | M | 638 | 0 | 620 | 405 | 0 |
| 3 | N | 872 | 0 | 814 | 459 | 0 |
| 4 | P | 620 | 0 | 598 | 161 | 0 |
| All | All | 38116 | 0 | 36795 | 3092 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (3092) 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:J:16:ARG:HD3 | 1:J:21:MET:SD | 1.29 | 1.69 |
| 1:L:108:ARG:HH11 | 3:N:89:TYR:CB | 0.99 | 1.62 |
| 1:A:255:SER:HA | 1:A:383:ARG:CD | 1.30 | 1.60 |
| 1:E:189:LYS:HZ2 | 1:K:61:ASN:CB | 1.05 | 1.60 |
| 3:N:60:ILE:HD12 | 3:N:97:ARG:CD | 1.23 | 1.59 |
| 1:H:281:LEU:CD1 | 1:H:385:GLU:HB3 | 1.26 | 1.59 |
| 3:N:80:ILE:CG2 | 3:N:116:PHE:CA | 1.78 | 1.59 |
| 3:N:49:THR:CB | 3:N:112:VAL:HG11 | 1.25 | 1.58 |
| 1:D:187:GLN:HB2 | 2:M:9:TYR:CE1 | 1.35 | 1.58 |
| 1:G:15:LEU:CD2 | 1:G:18:GLN:HE21 | 1.17 | 1.58 |
| 3:N:80:ILE:HG21 | 3:N:116:PHE:CA | 1.28 | 1.58 |
| 3:N:27:VAL:CB | 3:N:27:VAL:CA | 1.76 | 1.58 |
| 1:J:384:THR:CG2 | 2:M:62:ALA:HB2 | 1.30 | 1.57 |
| 1:B:5:GLN:NE2 | 1:B:316:THR:CG2 | 1.68 | 1.57 |
| 1:B:108:ARG:NH2 | 1:D:314:SER:CA | 1.68 | 1.56 |
| 1:D:187:GLN:CD | 2:M:9:TYR:CD1 | 1.74 | 1.56 |
| 1:J:8:THR:CG2 | 1:J:9:PRO:HD2 | 1.13 | 1.55 |
| 1:C:8:THR:CG2 | 1:C:9:PRO:HD2 | 1.10 | 1.54 |
| 1:F:353:LEU:CD2 | 2:M:27:LEU:H | 1.15 | 1.53 |
| 1:B:358:VAL:HA | 1:B:358:VAL:CG2 | 1.39 | 1.53 |
| 1:B:281:LEU:CD1 | 1:B:385:GLU:HB3 | 1.38 | 1.51 |
| 1:I:5:GLN:CD | 1:I:310:THR:HG21 | 1.15 | 1.51 |
| 1:H:281:LEU:HD11 | 1:H:385:GLU:CB | 1.38 | 1.51 |
| 3:N:81:LYS:CD | 3:N:113:PRO:HG3 | 1.34 | 1.51 |
| 1:L:265:GLN:NE2 | 3:N:40:LYS:CE | 1.71 | 1.51 |
| 1:H:265:GLN:NE2 | 1:H:393:SER:HB2 | 1.24 | 1.50 |
| 1:I:4:VAL:CA | 1:I:4:VAL:N | 1.71 | 1.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:L:108:ARG:NH1 | 3:N:89:TYR:CA | 1.73 | 1.49 |
| 1:A:255:SER:CA | 1:A:383:ARG:HD2 | 1.02 | 1.49 |
| 1:F:239:GLN:CG | 2:M:45:MET:CE | 1.91 | 1.49 |
| 3:N:112:VAL:HG23 | 3:N:113:PRO:CD | 1.37 | 1.49 |
| 3:N:41:TYR:HA | 3:N:45:TYR:CD2 | 1.44 | 1.49 |
| 3:N:60:ILE:CD1 | 3:N:97:ARG:HH11 | 1.25 | 1.48 |
| 3:N:41:TYR:CA | 3:N:45:TYR:CD2 | 1.95 | 1.48 |
| 1:F:185:VAL:HG21 | 2:M:37:GLY:CA | 1.40 | 1.48 |
| 1:L:182:LEU:HD11 | 1:L:184:ASN:ND2 | 1.22 | 1.48 |
| 1:D:281:LEU:CD2 | 1:D:385:GLU:HB3 | 1.39 | 1.48 |
| 1:L:108:ARG:NH1 | 3:N:89:TYR:HA | 1.18 | 1.48 |
| 4:P:96:ILE:HD12 | 4:P:100:LEU:CD2 | 1.43 | 1.48 |
| 1:L:312:ASN:ND2 | 2:M:73:PHE:CZ | 1.81 | 1.47 |
| 3:N:64:GLU:CB | 3:N:93:LEU:HB2 | 1.39 | 1.47 |
| 1:E:182:LEU:CD2 | 1:E:184:ASN:ND2 | 1.74 | 1.47 |
| 1:H:281:LEU:CD1 | 1:H:385:GLU:CB | 1.88 | 1.46 |
| 1:F:239:GLN:CB | 2:M:45:MET:CE | 1.92 | 1.46 |
| 3:N:112:VAL:CG2 | 3:N:113:PRO:HD2 | 1.01 | 1.46 |
| 3:N:80:ILE:HG21 | 3:N:116:PHE:CB | 1.46 | 1.45 |
| 1:B:358:VAL:N | 1:B:358:VAL:CA | 1.79 | 1.45 |
| 3:N:49:THR:HB | 3:N:112:VAL:CG1 | 1.45 | 1.45 |
| 1:I:8:THR:C | 1:I:9:PRO:N | 1.69 | 1.45 |
| 1:G:382:SER:C | 1:G:383:ARG:N | 1.70 | 1.45 |
| 1:C:181:VAL:HG12 | 1:C:182:LEU:N | 1.27 | 1.44 |
| 3:N:60:ILE:CD1 | 3:N:97:ARG:HD2 | 1.47 | 1.44 |
| 1:D:5:GLN:NE2 | 1:E:36:TYR:CE2 | 1.80 | 1.44 |
| 1:D:282:TYR:CE2 | 1:D:386:LEU:HG | 1.52 | 1.44 |
| 3:N:61:ASP:HB2 | 3:N:75:GLU:CB | 1.30 | 1.44 |
| 1:J:384:THR:C | 1:J:385:GLU:N | 1.69 | 1.43 |
| 3:N:68:ALA:H | 3:N:87:GLN:CD | 1.20 | 1.43 |
| 1:B:108:ARG:CZ | 1:D:314:SER:CB | 1.96 | 1.43 |
| 1:B:8:THR:C | 1:B:9:PRO:N | 1.69 | 1.43 |
| 1:L:263:SER:OG | 3:N:40:LYS:CE | 1.66 | 1.43 |
| 1:G:239:GLN:HG3 | 1:I:4:VAL:CA | 1.47 | 1.43 |
| 3:N:49:THR:CG2 | 3:N:82:CYS:O | 1.65 | 1.43 |
| 1:D:108:ARG:NH2 | 1:I:314:SER:N | 1.64 | 1.42 |
| 3:N:49:THR:CG2 | 3:N:83:PRO:HA | 1.49 | 1.42 |
| 1:G:23:ALA:HB3 | 1:G:24:ASN:N | 1.20 | 1.42 |
| 3:N:28:ARG:NH1 | 3:N:37:GLU:HG2 | 1.31 | 1.42 |
| 1:G:185:VAL:CB | 2:M:4:ASN:HB2 | 1.50 | 1.42 |
| 1:I:392:ILE:C | 1:I:393:SER:N | 1.71 | 1.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:49:THR:CB | 3:N:112:VAL:CG1 | 1.96 | 1.41 |
| 1:B:108:ARG:NH2 | 1:D:314:SER:N | 1.66 | 1.41 |
| 1:E:189:LYS:NZ | 1:K:61:ASN:CB | 1.75 | 1.40 |
| 1:L:257:LEU:C | 1:L:258:TYR:N | 1.71 | 1.40 |
| 1:D:187:GLN:CD | 2:M:9:TYR:HD1 | 0.88 | 1.40 |
| 3:N:112:VAL:CG2 | 3:N:113:PRO:CD | 1.91 | 1.40 |
| 4:P:96:ILE:CD1 | 4:P:100:LEU:CD2 | 1.97 | 1.40 |
| 4:P:103:TYR:O | 4:P:107:LEU:CD1 | 1.68 | 1.40 |
| 1:D:372:ARG:NH1 | 1:I:272:VAL:CG2 | 1.83 | 1.40 |
| 2:M:45:MET:CB | 2:M:48:LEU:HD11 | 1.49 | 1.39 |
| 3:N:49:THR:HG23 | 3:N:83:PRO:CA | 1.52 | 1.39 |
| 1:B:277:GLN:CB | 1:B:394:THR:OG1 | 1.67 | 1.39 |
| 1:B:108:ARG:NH1 | 1:D:314:SER:CB | 1.86 | 1.39 |
| 3:N:28:ARG:NH1 | 3:N:37:GLU:CG | 1.84 | 1.39 |
| 1:E:381:THR:C | 1:E:382:SER:N | 1.72 | 1.38 |
| 1:H:392:ILE:HG22 | 1:H:393:SER:N | 1.38 | 1.38 |
| 1:G:35:SER:C | 1:G:36:TYR:N | 1.76 | 1.38 |
| 3:N:41:TYR:HB3 | 3:N:45:TYR:CB | 1.50 | 1.38 |
| 1:E:8:THR:HG21 | 1:E:11:GLN:CG | 1.54 | 1.38 |
| 3:N:79:ARG:NH2 | 3:N:104:HIS:HB2 | 1.37 | 1.38 |
| 1:D:281:LEU:CD2 | 1:D:385:GLU:CB | 1.99 | 1.37 |
| 1:L:11:GLN:O | 1:L:15:LEU:CD1 | 1.72 | 1.37 |
| 1:H:7:LEU:CD2 | 1:H:353:LEU:HD22 | 1.53 | 1.37 |
| 1:J:383:ARG:C | 2:M:60:TYR:CD1 | 1.98 | 1.37 |
| 3:N:66:ASP:C | 3:N:87:GLN:NE2 | 1.76 | 1.37 |
| 1:F:382:SER:CB | 1:F:383:ARG:N | 1.84 | 1.37 |
| 1:B:281:LEU:CD1 | 1:B:385:GLU:CB | 1.94 | 1.37 |
| 1:D:17:ASN:CB | 1:D:20:ALA:HB2 | 1.52 | 1.37 |
| 1:H:392:ILE:CG2 | 1:H:393:SER:H | 1.33 | 1.37 |
| 1:L:111:GLU:OE1 | 3:N:89:TYR:CB | 1.72 | 1.37 |
| 3:N:64:GLU:HB2 | 3:N:93:LEU:CB | 1.55 | 1.37 |
| 1:D:108:ARG:NH2 | 1:I:314:SER:CA | 1.81 | 1.36 |
| 1:I:17:ASN:CB | 1:I:20:ALA:HB2 | 1.52 | 1.36 |
| 1:F:239:GLN:CG | 2:M:45:MET:HE2 | 1.49 | 1.36 |
| 1:D:187:GLN:CB | 2:M:9:TYR:HE1 | 1.35 | 1.36 |
| 1:G:34:GLN:HE22 | 1:I:9:PRO:CB | 1.22 | 1.36 |
| 1:J:4:VAL:N | 1:K:239:GLN:CG | 1.88 | 1.36 |
| 4:P:107:LEU:O | 4:P:111:LEU:CD1 | 1.72 | 1.36 |
| 1:B:4:VAL:O | 1:B:313:PHE:CE1 | 1.77 | 1.36 |
| 1:F:353:LEU:HD22 | 2:M:27:LEU:N | 1.06 | 1.36 |
| 1:F:384:THR:O | 2:M:33:GLY:CA | 1.74 | 1.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:187:GLN:CG | 2:M:9:TYR:CD1 | 2.09 | 1.36 |
| 1:B:358:VAL:CG1 | 1:B:358:VAL:CA | 2.03 | 1.35 |
| 1:A:313:PHE:CE1 | 1:K:383:ARG:CA | 1.90 | 1.35 |
| 1:B:358:VAL:CG2 | 1:B:358:VAL:CA | 1.94 | 1.35 |
| 1:B:358:VAL:C | 1:B:358:VAL:CA | 1.92 | 1.35 |
| 1:B:44:THR:H | 1:K:191:ARG:CZ | 1.36 | 1.35 |
| 3:N:68:ALA:N | 3:N:87:GLN:NE2 | 1.70 | 1.35 |
| 1:C:8:THR:HG22 | 1:C:9:PRO:CD | 1.57 | 1.34 |
| 1:G:239:GLN:CG | 1:I:4:VAL:CA | 2.02 | 1.34 |
| 1:A:63:GLY:H | 1:A:184:ASN:ND2 | 1.25 | 1.34 |
| 1:B:108:ARG:CZ | 1:D:314:SER:HB2 | 1.50 | 1.34 |
| 1:B:281:LEU:HD11 | 1:B:385:GLU:CB | 1.31 | 1.34 |
| 3:N:81:LYS:HD3 | 3:N:113:PRO:CG | 1.57 | 1.34 |
| 4:P:96:ILE:CG2 | 4:P:100:LEU:HD13 | 1.57 | 1.34 |
| 1:D:389:ALA:HB2 | 1:I:354:GLN:NE2 | 1.42 | 1.34 |
| 1:B:108:ARG:CZ | 1:D:314:SER:CA | 2.06 | 1.34 |
| 1:F:312:ASN:OD1 | 2:M:21:THR:HB | 1.26 | 1.34 |
| 1:K:245:ASN:O | 1:K:246:GLY:N | 1.60 | 1.34 |
| 1:L:265:GLN:NE2 | 3:N:40:LYS:NZ | 1.75 | 1.33 |
| 3:N:80:ILE:CG2 | 3:N:116:PHE:HA | 0.87 | 1.33 |
| 1:J:8:THR:CG2 | 1:J:9:PRO:CD | 2.06 | 1.33 |
| 1:G:239:GLN:HG3 | 1:I:4:VAL:N | 1.41 | 1.33 |
| 1:L:108:ARG:NH1 | 3:N:89:TYR:CB | 1.84 | 1.33 |
| 1:G:15:LEU:HD22 | 1:G:18:GLN:NE2 | 1.01 | 1.33 |
| 1:L:312:ASN:CG | 2:M:73:PHE:CE2 | 2.00 | 1.33 |
| 3:N:67:GLY:N | 3:N:87:GLN:HE22 | 1.25 | 1.33 |
| 1:K:191:ARG:C | 1:K:192:LEU:N | 1.78 | 1.32 |
| 3:N:82:CYS:SG | 3:N:116:PHE:CE2 | 2.22 | 1.32 |
| 1:F:185:VAL:CG2 | 2:M:37:GLY:C | 1.98 | 1.32 |
| 1:G:382:SER:CB | 1:G:383:ARG:N | 1.93 | 1.32 |
| 1:A:255:SER:CA | 1:A:383:ARG:CD | 1.93 | 1.32 |
| 1:B:108:ARG:NH2 | 1:D:314:SER:HA | 1.25 | 1.32 |
| 1:L:78:ASN:O | 1:L:156:ALA:HA | 1.23 | 1.32 |
| 1:K:282:TYR:HA | 1:K:381:THR:CB | 1.60 | 1.31 |
| 3:N:41:TYR:HA | 3:N:45:TYR:CE2 | 1.65 | 1.31 |
| 4:P:37:GLY:C | 4:P:39:PRO:HD2 | 1.48 | 1.31 |
| 1:F:185:VAL:HG21 | 2:M:37:GLY:C | 1.51 | 1.31 |
| 1:H:381:THR:C | 1:H:382:SER:N | 1.83 | 1.31 |
| 1:G:251:LEU:CD1 | 1:G:388:ASN:OD1 | 1.76 | 1.31 |
| 1:G:63:GLY:H | 1:G:184:ASN:CG | 1.34 | 1.31 |
| 1:G:63:GLY:H | 1:G:184:ASN:ND2 | 1.25 | 1.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:41:TYR:CB | 3:N:45:TYR:CD2 | 2.11 | 1.31 |
| 1:C:8:THR:CG2 | 1:C:9:PRO:CD | 2.06 | 1.30 |
| 1:F:11:GLN:O | 1:F:15:LEU:HD13 | 1.25 | 1.30 |
| 1:A:255:SER:O | 1:A:383:ARG:CG | 1.78 | 1.30 |
| 1:G:185:VAL:HB | 2:M:4:ASN:CB | 1.61 | 1.30 |
| 1:C:245:ASN:O | 1:C:246:GLY:N | 1.60 | 1.29 |
| 1:I:5:GLN:OE1 | 1:I:310:THR:HG21 | 1.20 | 1.29 |
| 1:G:185:VAL:CG2 | 2:M:7:PHE:O | 1.79 | 1.29 |
| 4:P:12:GLY:O | 4:P:16:LEU:HD13 | 1.18 | 1.29 |
| 1:A:63:GLY:H | 1:A:184:ASN:CG | 1.34 | 1.29 |
| 1:E:189:LYS:NZ | 1:K:61:ASN:N | 1.79 | 1.29 |
| 1:L:280:ASN:OD1 | 1:L:352:THR:HG21 | 1.33 | 1.29 |
| 1:G:62:VAL:CA | 1:G:184:ASN:OD1 | 1.81 | 1.29 |
| 3:N:80:ILE:CD1 | 3:N:116:PHE:HB3 | 1.61 | 1.28 |
| 1:D:389:ALA:CB | 1:I:354:GLN:HE22 | 1.46 | 1.28 |
| 1:H:5:GLN:NE2 | 1:I:36:TYR:CD2 | 1.99 | 1.28 |
| 3:N:49:THR:CG2 | 3:N:112:VAL:HG11 | 1.63 | 1.28 |
| 1:B:108:ARG:NH1 | 1:D:314:SER:OG | 1.63 | 1.28 |
| 1:F:247:TYR:CE2 | 2:M:43:GLN:NE2 | 2.02 | 1.28 |
| 1:K:283:ARG:N | 1:K:381:THR:OG1 | 1.66 | 1.28 |
| 1:H:281:LEU:HD12 | 1:H:385:GLU:OE1 | 1.20 | 1.28 |
| 1:B:9:PRO:HG3 | 1:C:34:GLN:OE1 | 1.31 | 1.28 |
| 1:G:382:SER:CB | 1:G:383:ARG:H | 1.47 | 1.28 |
| 1:L:282:TYR:CE1 | 3:N:42:ASP:OD2 | 1.86 | 1.28 |
| 1:J:16:ARG:CD | 1:J:21:MET:SD | 2.22 | 1.27 |
| 1:F:311:ALA:CB | 2:M:23:THR:HB | 1.63 | 1.27 |
| 1:F:351:TYR:OH | 2:M:29:TYR:CE2 | 1.79 | 1.27 |
| 1:A:62:VAL:CA | 1:A:184:ASN:OD1 | 1.81 | 1.27 |
| 1:D:372:ARG:HH11 | 1:I:272:VAL:CG2 | 1.42 | 1.27 |
| 1:L:311:ALA:O | 2:M:73:PHE:HE2 | 1.02 | 1.27 |
| 3:N:91:PRO:C | 3:N:92:LEU:HD12 | 1.54 | 1.27 |
| 1:L:353:LEU:HA | 2:M:76:PRO:CG | 1.64 | 1.27 |
| 3:N:81:LYS:CD | 3:N:113:PRO:CG | 2.12 | 1.27 |
| 1:E:182:LEU:HD21 | 1:E:184:ASN:CG | 1.54 | 1.27 |
| 1:L:263:SER:CB | 3:N:40:LYS:HE2 | 1.64 | 1.27 |
| 1:C:104:PRO:HB3 | 1:C:188:SER:O | 1.34 | 1.27 |
| 1:D:17:ASN:HB3 | 1:D:20:ALA:CB | 1.63 | 1.27 |
| 1:D:9:PRO:HG3 | 1:E:34:GLN:OE1 | 1.22 | 1.27 |
| 4:P:52:THR:C | 4:P:53:LEU:HD12 | 1.53 | 1.27 |
| 1:G:245:ASN:CA | 1:G:245:ASN:O | 1.81 | 1.27 |
| 1:H:7:LEU:HD22 | 1:H:353:LEU:CD2 | 1.63 | 1.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:389:ALA:CB | 1:I:354:GLN:NE2 | 1.98 | 1.27 |
| 3:N:60:ILE:CD1 | 3:N:97:ARG:NH1 | 1.96 | 1.27 |
| 3:N:81:LYS:HB3 | 3:N:113:PRO:CG | 1.63 | 1.26 |
| 1:L:312:ASN:ND2 | 2:M:73:PHE:CE2 | 2.01 | 1.26 |
| 1:J:384:THR:HG22 | 2:M:62:ALA:CB | 1.64 | 1.26 |
| 1:J:383:ARG:C | 2:M:60:TYR:HD1 | 1.31 | 1.26 |
| 1:A:245:ASN:CA | 1:A:245:ASN:O | 1.82 | 1.26 |
| 1:B:4:VAL:CA | 1:B:4:VAL:CB | 2.14 | 1.26 |
| 3:N:49:THR:HG22 | 3:N:82:CYS:O | 1.10 | 1.26 |
| 1:I:17:ASN:HB3 | 1:I:20:ALA:CB | 1.63 | 1.26 |
| 1:K:282:TYR:CA | 1:K:381:THR:OG1 | 1.84 | 1.26 |
| 1:E:8:THR:CG2 | 1:E:11:GLN:HG3 | 1.65 | 1.25 |
| 1:I:5:GLN:CD | 1:I:310:THR:CG2 | 2.04 | 1.25 |
| 1:D:187:GLN:CB | 2:M:9:TYR:CE1 | 2.12 | 1.25 |
| 3:N:81:LYS:CB | 3:N:113:PRO:HG2 | 1.63 | 1.25 |
| 1:K:104:PRO:O | 1:K:188:SER:HB3 | 1.36 | 1.25 |
| 1:J:384:THR:CG2 | 2:M:62:ALA:CB | 2.13 | 1.25 |
| 1:E:189:LYS:HZ3 | 1:K:61:ASN:N | 1.29 | 1.25 |
| 1:L:353:LEU:O | 2:M:76:PRO:HD2 | 1.32 | 1.25 |
| 1:F:239:GLN:CB | 2:M:45:MET:HE1 | 1.52 | 1.25 |
| 1:D:187:GLN:CG | 2:M:9:TYR:HD1 | 1.44 | 1.25 |
| 3:N:65:ASN:ND2 | 3:N:71:ILE:HD12 | 1.51 | 1.25 |
| 2:M:14:PRO:C | 2:M:16:PRO:HD2 | 1.55 | 1.25 |
| 1:G:251:LEU:HD11 | 1:G:388:ASN:OD1 | 1.22 | 1.24 |
| 1:A:255:SER:O | 1:A:383:ARG:HG3 | 1.27 | 1.24 |
| 4:P:12:GLY:O | 4:P:16:LEU:CD1 | 1.84 | 1.24 |
| 1:F:382:SER:HB3 | 1:F:383:ARG:N | 0.92 | 1.24 |
| 1:K:245:ASN:O | 1:K:245:ASN:CA | 1.85 | 1.23 |
| 3:N:64:GLU:OE1 | 3:N:93:LEU:HB3 | 1.38 | 1.23 |
| 1:A:62:VAL:HA | 1:A:184:ASN:OD1 | 1.11 | 1.23 |
| 1:J:8:THR:HG22 | 1:J:9:PRO:CD | 1.67 | 1.23 |
| 1:D:17:ASN:CB | 1:D:20:ALA:CB | 2.15 | 1.23 |
| 1:G:62:VAL:HA | 1:G:184:ASN:OD1 | 1.11 | 1.23 |
| 1:I:5:GLN:OE1 | 1:I:310:THR:CG2 | 1.86 | 1.23 |
| 1:D:5:GLN:N | 1:E:239:GLN:NE2 | 1.85 | 1.23 |
| 1:E:189:LYS:NZ | 1:K:61:ASN:HB2 | 1.43 | 1.23 |
| 1:I:355:TYR:OH | 1:I:393:SER:O | 1.58 | 1.22 |
| 3:N:25:GLN:CB | 3:N:107:SER:OG | 1.86 | 1.22 |
| 1:C:245:ASN:O | 1:C:245:ASN:CA | 1.85 | 1.22 |
| 1:F:239:GLN:HG2 | 2:M:45:MET:CE | 1.54 | 1.22 |
| 1:F:239:GLN:HG2 | 2:M:45:MET:CG | 1.68 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:79:ARG:HH22 | 3:N:104:HIS:CB | 1.49 | 1.22 |
| 3:N:94:VAL:HG22 | 3:N:103:ARG:NH1 | 1.51 | 1.22 |
| 1:G:23:ALA:CB | 1:G:24:ASN:N | 2.02 | 1.22 |
| 1:F:185:VAL:CG1 | 2:M:38:ILE:H | 1.53 | 1.22 |
| 3:N:41:TYR:HB3 | 3:N:45:TYR:CG | 1.48 | 1.21 |
| 1:F:11:GLN:O | 1:F:15:LEU:CD1 | 1.87 | 1.21 |
| 1:I:281:LEU:HD11 | 1:I:385:GLU:CB | 1.61 | 1.21 |
| 1:A:313:PHE:CE1 | 1:K:383:ARG:HA | 1.41 | 1.21 |
| 1:L:75:ALA:HA | 1:L:160:GLY:O | 1.39 | 1.21 |
| 1:K:104:PRO:O | 1:K:188:SER:CB | 1.87 | 1.21 |
| 1:L:108:ARG:HH11 | 3:N:89:TYR:CA | 1.38 | 1.20 |
| 1:L:150:ALA:C | 1:L:151:PRO:N | 1.94 | 1.20 |
| 1:A:255:SER:C | 1:A:383:ARG:HD2 | 1.59 | 1.20 |
| 1:B:7:LEU:HD22 | 1:B:353:LEU:CD2 | 1.70 | 1.20 |
| 4:P:107:LEU:O | 4:P:111:LEU:HD13 | 1.07 | 1.20 |
| 2:M:41:ALA:O | 2:M:42:ARG:HG3 | 1.36 | 1.20 |
| 1:H:4:VAL:N | 1:I:239:GLN:CD | 1.93 | 1.20 |
| 1:F:35:SER:HB3 | 1:F:240:LEU:CD2 | 1.70 | 1.20 |
| 1:L:311:ALA:O | 2:M:73:PHE:CE2 | 1.95 | 1.19 |
| 1:D:187:GLN:NE2 | 2:M:9:TYR:HB3 | 1.57 | 1.19 |
| 4:P:96:ILE:CD1 | 4:P:100:LEU:HD22 | 1.60 | 1.19 |
| 1:F:351:TYR:CE1 | 2:M:29:TYR:OH | 1.94 | 1.19 |
| 1:L:381:THR:C | 1:L:382:SER:N | 1.96 | 1.19 |
| 3:N:80:ILE:HD13 | 3:N:116:PHE:CB | 1.71 | 1.19 |
| 3:N:68:ALA:H | 3:N:87:GLN:NE2 | 1.33 | 1.19 |
| 3:N:64:GLU:CB | 3:N:93:LEU:CB | 2.17 | 1.19 |
| 1:D:187:GLN:NE2 | 2:M:9:TYR:CD1 | 2.09 | 1.19 |
| 1:F:185:VAL:HA | 2:M:38:ILE:O | 1.35 | 1.19 |
| 1:J:384:THR:HG21 | 2:M:62:ALA:HB2 | 1.23 | 1.19 |
| 1:B:5:GLN:NE2 | 1:B:316:THR:HG23 | 1.40 | 1.19 |
| 1:L:64:ILE:HA | 1:L:181:VAL:O | 1.42 | 1.19 |
| 3:N:14:VAL:HG22 | 3:N:16:ASN:H | 1.04 | 1.19 |
| 4:P:96:ILE:HG21 | 4:P:100:LEU:CD1 | 1.73 | 1.19 |
| 1:E:182:LEU:HD21 | 1:E:184:ASN:ND2 | 0.87 | 1.18 |
| 1:F:239:GLN:CB | 2:M:45:MET:HE2 | 1.62 | 1.18 |
| 1:G:247:TYR:CZ | 2:M:2:LEU:HD23 | 1.77 | 1.18 |
| 1:I:281:LEU:CD1 | 1:I:385:GLU:HB3 | 1.74 | 1.18 |
| 1:K:282:TYR:HA | 1:K:381:THR:OG1 | 1.34 | 1.18 |
| 1:D:388:ASN:OD1 | 1:I:6:GLN:OE1 | 1.61 | 1.18 |
| 1:L:38:VAL:O | 1:L:236:TYR:N | 1.75 | 1.18 |
| 1:D:391:THR:OG1 | 1:I:356:GLY:O | 1.61 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:111:GLU:OE1 | 3:N:89:TYR:HB3 | 1.36 | 1.18 |
| 4:P:103:TYR:O | 4:P:107:LEU:HD13 | 1.01 | 1.18 |
| 2:M:24:MET:H | 2:M:25:PRO:CD | 1.57 | 1.17 |
| 1:L:312:ASN:CB | 2:M:73:PHE:CZ | 2.28 | 1.17 |
| 1:L:11:GLN:O | 1:L:15:LEU:HD13 | 1.01 | 1.17 |
| 1:H:281:LEU:CD1 | 1:H:385:GLU:OE1 | 1.92 | 1.17 |
| 1:L:312:ASN:HB2 | 2:M:73:PHE:CZ | 1.79 | 1.17 |
| 3:N:62:ASN:CB | 3:N:95:PRO:HG2 | 1.73 | 1.17 |
| 1:G:105:ASP:N | 2:M:7:PHE:CE2 | 2.13 | 1.17 |
| 1:J:9:PRO:HG3 | 1:K:34:GLN:HA | 1.19 | 1.17 |
| 1:D:187:GLN:NE2 | 2:M:9:TYR:CB | 2.08 | 1.17 |
| 3:N:61:ASP:CB | 3:N:75:GLU:HB2 | 1.73 | 1.17 |
| 1:L:182:LEU:CD1 | 1:L:184:ASN:ND2 | 2.08 | 1.17 |
| 1:L:104:PRO:CB | 1:L:188:SER:OG | 1.91 | 1.16 |
| 1:G:239:GLN:CD | 1:I:4:VAL:CA | 2.12 | 1.16 |
| 3:N:41:TYR:CB | 3:N:45:TYR:CG | 2.09 | 1.16 |
| 1:L:80:HIS:O | 1:L:156:ALA:CB | 1.92 | 1.16 |
| 1:L:312:ASN:HB2 | 2:M:73:PHE:HZ | 1.09 | 1.16 |
| 1:G:185:VAL:HG13 | 1:G:186:PRO:HD3 | 1.24 | 1.16 |
| 1:L:279:ALA:CA | 3:N:43:LEU:HD11 | 1.74 | 1.16 |
| 1:B:392:ILE:O | 1:B:393:SER:OG | 1.64 | 1.16 |
| 1:E:189:LYS:HZ2 | 1:K:61:ASN:CG | 1.49 | 1.16 |
| 3:N:39:VAL:CG1 | 3:N:90:PHE:HB3 | 1.76 | 1.15 |
| 1:K:102:TYR:O | 1:K:190:GLN:HA | 1.47 | 1.15 |
| 2:M:45:MET:HB2 | 2:M:48:LEU:CD1 | 1.77 | 1.15 |
| 2:M:45:MET:CB | 2:M:48:LEU:CD1 | 2.23 | 1.15 |
| 1:H:7:LEU:HD13 | 1:H:353:LEU:HD13 | 1.16 | 1.15 |
| 1:F:239:GLN:CG | 2:M:45:MET:HG2 | 1.75 | 1.15 |
| 1:B:7:LEU:CD2 | 1:B:353:LEU:HD22 | 1.77 | 1.15 |
| 1:H:265:GLN:NE2 | 1:H:393:SER:CB | 2.10 | 1.14 |
| 1:C:238:ASP:OD2 | 1:I:106:ASN:OD1 | 1.63 | 1.14 |
| 1:L:312:ASN:CB | 2:M:73:PHE:HZ | 1.60 | 1.14 |
| 1:B:272:VAL:HG11 | 1:I:264:ALA:CB | 1.77 | 1.14 |
| 1:F:383:ARG:HA | 2:M:31:VAL:HG21 | 1.26 | 1.14 |
| 3:N:25:GLN:HB2 | 3:N:107:SER:OG | 0.96 | 1.14 |
| 1:B:395:THR:OG1 | 1:D:394:THR:C | 1.87 | 1.14 |
| 1:E:187:GLN:HA | 1:K:185:VAL:HA | 1.14 | 1.14 |
| 1:L:7:LEU:HB3 | 1:L:11:GLN:CB | 1.55 | 1.14 |
| 1:E:8:THR:HB | 1:E:11:GLN:HB2 | 1.30 | 1.13 |
| 1:D:9:PRO:HG3 | 1:E:34:GLN:CD | 1.67 | 1.13 |
| 1:D:5:GLN:HE21 | 1:D:316:THR:HG21 | 1.11 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:384:THR:O | 2:M:33:GLY:HA3 | 1.42 | 1.13 |
| 1:I:17:ASN:CB | 1:I:20:ALA:CB | 2.15 | 1.13 |
| 2:M:24:MET:H | 2:M:25:PRO:HD3 | 1.06 | 1.13 |
| 4:P:19:ILE:CG2 | 4:P:23:PHE:HE1 | 1.62 | 1.13 |
| 1:C:190:GLN:C | 1:C:191:ARG:HG3 | 1.69 | 1.13 |
| 1:G:245:ASN:O | 1:G:246:GLY:N | 1.81 | 1.13 |
| 1:H:9:PRO:HB3 | 1:I:34:GLN:HE22 | 1.00 | 1.13 |
| 4:P:15:VAL:HG13 | 4:P:16:LEU:HD12 | 1.30 | 1.13 |
| 1:D:389:ALA:HB1 | 1:I:354:GLN:OE1 | 1.47 | 1.13 |
| 1:E:189:LYS:NZ | 1:K:61:ASN:CA | 2.11 | 1.13 |
| 1:F:239:GLN:HB3 | 2:M:45:MET:CE | 1.60 | 1.13 |
| 1:J:387:VAL:O | 1:J:388:ASN:OD1 | 1.67 | 1.13 |
| 1:L:78:ASN:O | 1:L:156:ALA:CA | 1.96 | 1.13 |
| 1:B:5:GLN:CG | 1:B:310:THR:HG21 | 1.79 | 1.13 |
| 1:D:387:VAL:CG2 | 1:I:6:GLN:NE2 | 2.10 | 1.12 |
| 1:L:353:LEU:HA | 2:M:76:PRO:CD | 1.79 | 1.12 |
| 4:P:42:THR:O | 4:P:45:GLN:HG3 | 1.49 | 1.12 |
| 1:D:257:LEU:HG | 1:D:383:ARG:HG2 | 1.13 | 1.12 |
| 3:N:62:ASN:HB2 | 3:N:95:PRO:O | 1.47 | 1.12 |
| 1:B:44:THR:N | 1:K:191:ARG:NH2 | 1.96 | 1.12 |
| 1:L:353:LEU:HA | 2:M:76:PRO:HG3 | 1.14 | 1.12 |
| 1:G:185:VAL:HG21 | 2:M:4:ASN:O | 1.46 | 1.12 |
| 1:A:245:ASN:O | 1:A:246:GLY:N | 1.81 | 1.12 |
| 1:L:108:ARG:HH11 | 3:N:89:TYR:HB3 | 1.01 | 1.12 |
| 1:K:7:LEU:HA | 1:K:12:GLN:NE2 | 1.64 | 1.12 |
| 1:K:182:LEU:HD13 | 1:K:254:LEU:HD13 | 1.24 | 1.11 |
| 1:B:269:THR:HG21 | 1:I:372:ARG:HD3 | 1.17 | 1.11 |
| 1:D:7:LEU:HD22 | 1:D:353:LEU:CD2 | 1.80 | 1.11 |
| 1:E:8:THR:HG22 | 1:E:11:GLN:H | 0.98 | 1.11 |
| 1:E:381:THR:CA | 1:E:382:SER:N | 2.12 | 1.11 |
| 1:G:239:GLN:CG | 1:I:4:VAL:N | 2.12 | 1.11 |
| 1:J:8:THR:HG23 | 1:J:9:PRO:HD2 | 1.12 | 1.11 |
| 1:D:108:ARG:HH22 | 1:I:314:SER:CA | 1.46 | 1.11 |
| 1:G:34:GLN:NE2 | 1:I:9:PRO:CB | 1.89 | 1.11 |
| 1:H:7:LEU:CD2 | 1:H:353:LEU:CD2 | 2.25 | 1.11 |
| 1:J:16:ARG:NH1 | 1:J:21:MET:HE1 | 1.64 | 1.11 |
| 1:F:312:ASN:HA | 2:M:21:THR:OG1 | 1.49 | 1.11 |
| 1:F:311:ALA:HB1 | 2:M:23:THR:HB | 1.25 | 1.11 |
| 1:B:44:THR:N | 1:K:191:ARG:CZ | 2.13 | 1.11 |
| 3:N:45:TYR:C | 3:N:46:LEU:HD12 | 1.71 | 1.11 |
| 3:N:61:ASP:CB | 3:N:75:GLU:CB | 2.26 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:257:LEU:HD12 | 1:I:386:LEU:HD22 | 1.32 | 1.10 |
| 3:N:41:TYR:HB3 | 3:N:45:TYR:HB2 | 1.27 | 1.10 |
| 3:N:80:ILE:HG12 | 3:N:117:LEU:H | 1.07 | 1.10 |
| 1:E:106:ASN:ND2 | 1:K:62:VAL:HG11 | 1.66 | 1.10 |
| 4:P:96:ILE:CD1 | 4:P:100:LEU:HD21 | 1.81 | 1.10 |
| 2:M:68:GLN:O | 4:P:41:MET:SD | 2.06 | 1.10 |
| 1:I:281:LEU:HD11 | 1:I:385:GLU:HB3 | 1.24 | 1.10 |
| 1:A:255:SER:C | 1:A:383:ARG:CD | 2.17 | 1.10 |
| 1:B:281:LEU:HD11 | 1:B:385:GLU:HB2 | 1.20 | 1.10 |
| 1:G:382:SER:CA | 1:G:383:ARG:N | 2.13 | 1.10 |
| 2:M:21:THR:HG22 | 2:M:23:THR:H | 1.16 | 1.10 |
| 1:F:353:LEU:HA | 2:M:26:LEU:HA | 1.13 | 1.10 |
| 4:P:18:LEU:O | 4:P:22:TRP:HD1 | 1.35 | 1.10 |
| 1:B:5:GLN:NE2 | 1:B:316:THR:HG21 | 1.34 | 1.10 |
| 1:B:389:ALA:HB2 | 1:D:354:GLN:HE22 | 1.17 | 1.10 |
| 1:L:104:PRO:HB3 | 1:L:188:SER:C | 1.72 | 1.10 |
| 3:N:62:ASN:HB3 | 3:N:95:PRO:HG2 | 1.26 | 1.09 |
| 1:D:11:GLN:OE1 | 1:D:351:TYR:CD2 | 2.04 | 1.09 |
| 1:J:313:PHE:HZ | 1:K:239:GLN:HG3 | 1.14 | 1.09 |
| 3:N:68:ALA:HB3 | 3:N:87:GLN:HG2 | 1.34 | 1.09 |
| 1:B:313:PHE:CE1 | 1:I:387:VAL:HG23 | 1.88 | 1.09 |
| 1:B:272:VAL:CG1 | 1:I:264:ALA:HB3 | 1.81 | 1.09 |
| 3:N:60:ILE:HD11 | 3:N:97:ARG:HH11 | 1.07 | 1.09 |
| 1:L:56:ASP:OD2 | 3:N:11:VAL:HG12 | 1.49 | 1.09 |
| 3:N:60:ILE:HD13 | 3:N:97:ARG:NH1 | 1.64 | 1.09 |
| 1:B:356:GLY:O | 1:I:391:THR:OG1 | 1.70 | 1.09 |
| 1:D:5:GLN:NE2 | 1:D:316:THR:HG21 | 1.67 | 1.09 |
| 1:D:5:GLN:N | 1:E:239:GLN:HE22 | 1.19 | 1.09 |
| 1:E:381:THR:HG1 | 1:E:382:SER:N | 1.50 | 1.09 |
| 1:J:255:SER:HA | 1:J:383:ARG:HD2 | 1.22 | 1.09 |
| 2:M:45:MET:HB3 | 2:M:48:LEU:HD11 | 1.30 | 1.08 |
| 1:B:4:VAL:O | 1:B:313:PHE:CD1 | 2.05 | 1.08 |
| 1:L:11:GLN:C | 1:L:15:LEU:HD13 | 1.72 | 1.08 |
| 1:L:265:GLN:NE2 | 3:N:40:LYS:HE3 | 1.50 | 1.08 |
| 1:K:101:TYR:OH | 1:K:190:GLN:CD | 1.73 | 1.08 |
| 1:L:312:ASN:CG | 2:M:73:PHE:CZ | 2.17 | 1.08 |
| 1:L:108:ARG:CA | 3:N:89:TYR:OH | 2.00 | 1.08 |
| 1:D:187:GLN:NE2 | 2:M:9:TYR:HD1 | 1.45 | 1.08 |
| 2:M:6:GLN:O | 2:M:8:PRO:HD3 | 1.52 | 1.08 |
| 1:L:353:LEU:CD2 | 2:M:76:PRO:HG3 | 1.84 | 1.08 |
| 3:N:39:VAL:HG13 | 3:N:90:PHE:HB3 | 1.09 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:181:VAL:CG1 | 1:C:182:LEU:N | 2.16 | 1.08 |
| 1:G:185:VAL:HG22 | 2:M:7:PHE:O | 1.45 | 1.07 |
| 1:F:247:TYR:HE2 | 2:M:43:GLN:NE2 | 1.44 | 1.07 |
| 3:N:80:ILE:HG12 | 3:N:117:LEU:N | 1.69 | 1.07 |
| 1:B:281:LEU:HD13 | 1:B:385:GLU:HB3 | 1.33 | 1.07 |
| 1:D:372:ARG:NH1 | 1:I:272:VAL:HG21 | 1.55 | 1.07 |
| 1:F:311:ALA:CB | 2:M:23:THR:CB | 2.32 | 1.07 |
| 1:F:255:SER:HB3 | 2:M:35:ILE:HD11 | 1.32 | 1.07 |
| 1:B:272:VAL:HG11 | 1:I:264:ALA:HB3 | 1.11 | 1.07 |
| 1:L:7:LEU:HB3 | 1:L:11:GLN:HB3 | 1.36 | 1.07 |
| 4:P:96:ILE:HD13 | 4:P:100:LEU:HD21 | 1.37 | 1.07 |
| 3:N:28:ARG:HH11 | 3:N:37:GLU:CD | 1.56 | 1.07 |
| 1:F:185:VAL:CG1 | 2:M:38:ILE:N | 2.16 | 1.07 |
| 1:F:185:VAL:HG21 | 2:M:37:GLY:HA3 | 1.09 | 1.07 |
| 1:D:7:LEU:HD22 | 1:D:353:LEU:HD22 | 1.25 | 1.06 |
| 1:A:63:GLY:N | 1:A:184:ASN:CG | 2.07 | 1.06 |
| 1:G:63:GLY:N | 1:G:184:ASN:CG | 2.07 | 1.06 |
| 1:D:387:VAL:HG22 | 1:I:6:GLN:CD | 1.74 | 1.06 |
| 1:G:239:GLN:CD | 1:I:4:VAL:HA | 1.74 | 1.06 |
| 1:J:184:ASN:ND2 | 1:J:247:TYR:CE1 | 2.22 | 1.06 |
| 1:J:4:VAL:N | 1:K:239:GLN:HG3 | 1.71 | 1.06 |
| 1:F:239:GLN:CD | 2:M:45:MET:SD | 2.34 | 1.06 |
| 1:G:185:VAL:HG21 | 2:M:7:PHE:O | 1.54 | 1.06 |
| 1:B:11:GLN:OE1 | 1:B:351:TYR:CD2 | 2.08 | 1.06 |
| 1:B:11:GLN:OE1 | 1:B:351:TYR:HD2 | 1.37 | 1.06 |
| 1:D:281:LEU:HD21 | 1:D:385:GLU:CB | 1.85 | 1.06 |
| 1:K:103:ASP:HA | 1:K:190:GLN:HG2 | 1.37 | 1.06 |
| 3:N:57:CYS:SG | 3:N:101:VAL:HG23 | 1.93 | 1.06 |
| 1:D:11:GLN:O | 1:D:15:LEU:CD1 | 2.04 | 1.06 |
| 1:K:63:GLY:O | 1:K:183:ALA:HB3 | 1.54 | 1.06 |
| 1:L:6:GLN:O | 1:L:7:LEU:HD13 | 1.56 | 1.06 |
| 1:B:11:GLN:O | 1:B:15:LEU:CD1 | 2.04 | 1.05 |
| 1:E:187:GLN:HA | 1:K:184:ASN:O | 1.54 | 1.05 |
| 1:E:182:LEU:CD2 | 1:E:184:ASN:CG | 2.16 | 1.05 |
| 1:K:7:LEU:CA | 1:K:12:GLN:HE22 | 1.69 | 1.05 |
| 4:P:96:ILE:HG21 | 4:P:100:LEU:HD13 | 1.11 | 1.05 |
| 1:H:281:LEU:HD13 | 1:H:385:GLU:CB | 1.70 | 1.05 |
| 1:G:239:GLN:OE1 | 1:I:4:VAL:HA | 1.57 | 1.05 |
| 1:F:311:ALA:HB1 | 2:M:21:THR:HG21 | 1.34 | 1.05 |
| 1:D:5:GLN:NE2 | 1:E:36:TYR:CD2 | 2.23 | 1.05 |
| 1:D:282:TYR:HE2 | 1:D:386:LEU:CG | 1.69 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:7:LEU:HD22 | 1:B:353:LEU:HD22 | 1.07 | 1.05 |
| 1:F:239:GLN:CG | 2:M:45:MET:CG | 2.30 | 1.05 |
| 1:I:11:GLN:O | 1:I:15:LEU:CD1 | 2.04 | 1.05 |
| 1:J:311:ALA:O | 1:J:312:ASN:OD1 | 1.72 | 1.05 |
| 1:D:387:VAL:CG2 | 1:I:6:GLN:CD | 2.24 | 1.04 |
| 1:B:5:GLN:CB | 1:B:310:THR:HG21 | 1.87 | 1.04 |
| 1:D:282:TYR:CE2 | 1:D:386:LEU:CG | 2.41 | 1.04 |
| 1:L:38:VAL:HG23 | 1:L:238:ASP:CB | 1.86 | 1.04 |
| 3:N:28:ARG:NH1 | 3:N:37:GLU:CD | 2.08 | 1.04 |
| 1:C:8:THR:HG23 | 1:C:9:PRO:HD2 | 1.08 | 1.04 |
| 1:F:383:ARG:HA | 2:M:31:VAL:CG2 | 1.86 | 1.04 |
| 1:G:34:GLN:HE22 | 1:I:9:PRO:HB2 | 0.90 | 1.04 |
| 1:L:111:GLU:OE1 | 3:N:89:TYR:CG | 2.10 | 1.04 |
| 1:F:239:GLN:HG2 | 2:M:45:MET:SD | 1.95 | 1.04 |
| 1:L:80:HIS:O | 1:L:156:ALA:HB2 | 1.54 | 1.04 |
| 4:P:106:SER:O | 4:P:110:TYR:CD2 | 2.11 | 1.04 |
| 3:N:37:GLU:HB2 | 3:N:92:LEU:HB3 | 1.38 | 1.03 |
| 1:D:9:PRO:CG | 1:E:34:GLN:OE1 | 2.05 | 1.03 |
| 3:N:66:ASP:O | 3:N:87:GLN:NE2 | 1.91 | 1.03 |
| 4:P:106:SER:O | 4:P:110:TYR:HD2 | 1.41 | 1.03 |
| 1:B:281:LEU:HD21 | 1:B:385:GLU:C | 1.78 | 1.03 |
| 1:C:14:ALA:HA | 1:C:17:ASN:ND2 | 1.73 | 1.03 |
| 1:D:108:ARG:HH22 | 1:I:314:SER:HA | 0.91 | 1.03 |
| 1:D:7:LEU:CD2 | 1:D:353:LEU:HD22 | 1.87 | 1.03 |
| 1:K:102:TYR:O | 1:K:190:GLN:CA | 2.06 | 1.03 |
| 1:I:5:GLN:CG | 1:I:310:THR:HG21 | 1.89 | 1.03 |
| 1:J:382:SER:O | 2:M:60:TYR:HE1 | 1.39 | 1.03 |
| 1:D:387:VAL:HG21 | 1:I:6:GLN:NE2 | 1.72 | 1.03 |
| 1:K:282:TYR:C | 1:K:381:THR:OG1 | 1.95 | 1.03 |
| 1:L:353:LEU:CA | 2:M:76:PRO:HG3 | 1.88 | 1.03 |
| 1:B:5:GLN:CD | 1:B:310:THR:CG2 | 2.27 | 1.03 |
| 3:N:37:GLU:O | 3:N:92:LEU:HB2 | 1.59 | 1.03 |
| 3:N:68:ALA:HB3 | 3:N:87:GLN:CG | 1.89 | 1.03 |
| 3:N:50:GLN:HE21 | 3:N:86:LYS:HE2 | 1.24 | 1.03 |
| 3:N:67:GLY:CA | 3:N:87:GLN:HE22 | 1.70 | 1.03 |
| 1:F:185:VAL:HG13 | 2:M:38:ILE:N | 1.74 | 1.02 |
| 1:F:35:SER:HB3 | 1:F:240:LEU:HD23 | 1.37 | 1.02 |
| 1:J:9:PRO:HG2 | 1:K:34:GLN:OE1 | 1.58 | 1.02 |
| 3:N:64:GLU:CD | 3:N:93:LEU:HB3 | 1.79 | 1.02 |
| 3:N:67:GLY:N | 3:N:87:GLN:NE2 | 1.96 | 1.02 |
| 1:L:108:ARG:CZ | 3:N:89:TYR:HA | 1.88 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:8:THR:HG23 | 1:J:9:PRO:CD | 1.80 | 1.02 |
| 1:L:38:VAL:CG2 | 1:L:238:ASP:HB2 | 1.88 | 1.02 |
| 1:F:356:GLY:HA3 | 2:M:23:THR:HG22 | 1.40 | 1.02 |
| 1:J:313:PHE:HE2 | 1:K:238:ASP:OD2 | 1.40 | 1.02 |
| 1:J:384:THR:HG22 | 2:M:62:ALA:HB2 | 1.04 | 1.02 |
| 3:N:89:TYR:O | 3:N:91:PRO:HD3 | 1.58 | 1.02 |
| 1:G:382:SER:HB2 | 1:G:383:ARG:N | 1.60 | 1.02 |
| 1:L:265:GLN:NE2 | 3:N:40:LYS:CD | 2.23 | 1.02 |
| 2:M:41:ALA:O | 2:M:42:ARG:CG | 2.06 | 1.02 |
| 1:L:108:ARG:HA | 3:N:89:TYR:OH | 1.58 | 1.02 |
| 1:A:63:GLY:N | 1:A:184:ASN:ND2 | 2.07 | 1.02 |
| 1:F:185:VAL:HG22 | 2:M:37:GLY:C | 1.75 | 1.02 |
| 2:M:72:THR:HG21 | 4:P:44:ASN:HB3 | 1.42 | 1.02 |
| 1:A:255:SER:CB | 1:A:383:ARG:HD2 | 1.89 | 1.01 |
| 1:B:5:GLN:CD | 1:B:310:THR:HG23 | 1.81 | 1.01 |
| 1:J:16:ARG:CZ | 1:J:21:MET:HE3 | 1.88 | 1.01 |
| 1:K:102:TYR:O | 1:K:190:GLN:CB | 2.07 | 1.01 |
| 1:L:6:GLN:O | 1:L:7:LEU:HB2 | 1.59 | 1.01 |
| 1:B:5:GLN:HB3 | 1:B:310:THR:HG21 | 1.40 | 1.01 |
| 1:H:281:LEU:HD11 | 1:H:385:GLU:HB2 | 1.02 | 1.01 |
| 1:B:5:GLN:OE1 | 1:B:310:THR:CG2 | 2.09 | 1.01 |
| 1:G:63:GLY:N | 1:G:184:ASN:ND2 | 2.07 | 1.01 |
| 1:F:185:VAL:CG2 | 2:M:37:GLY:CA | 2.35 | 1.01 |
| 3:N:81:LYS:CB | 3:N:113:PRO:CG | 2.27 | 1.01 |
| 4:P:52:THR:O | 4:P:53:LEU:HD12 | 1.58 | 1.01 |
| 1:D:281:LEU:HD21 | 1:D:386:LEU:N | 1.76 | 1.01 |
| 1:L:353:LEU:CA | 2:M:76:PRO:CD | 2.38 | 1.01 |
| 1:G:185:VAL:CG1 | 1:G:186:PRO:HD3 | 1.90 | 1.01 |
| 2:M:24:MET:N | 2:M:25:PRO:CD | 2.16 | 1.01 |
| 1:B:311:ALA:HB3 | 1:I:390:GLY:O | 1.60 | 1.01 |
| 4:P:96:ILE:HD12 | 4:P:100:LEU:HD23 | 1.41 | 1.01 |
| 1:C:104:PRO:CB | 1:C:188:SER:O | 2.07 | 1.01 |
| 1:F:353:LEU:HD12 | 2:M:29:TYR:CZ | 1.95 | 1.01 |
| 1:B:395:THR:CG2 | 1:I:395:THR:C | 2.21 | 1.01 |
| 1:L:104:PRO:HB2 | 1:L:188:SER:OG | 1.58 | 1.01 |
| 1:H:281:LEU:HD21 | 1:H:385:GLU:C | 1.81 | 1.01 |
| 1:G:185:VAL:CG2 | 2:M:4:ASN:HB2 | 1.90 | 1.01 |
| 3:N:5:ASN:CB | 3:N:6:PRO:HD3 | 1.72 | 1.00 |
| 3:N:65:ASN:ND2 | 3:N:85:GLY:O | 1.92 | 1.00 |
| 4:P:96:ILE:CB | 4:P:100:LEU:HD22 | 1.91 | 1.00 |
| 1:B:358:VAL:HG22 | 1:B:358:VAL:HA | 1.41 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:372:ARG:NH1 | 1:I:272:VAL:HG23 | 1.73 | 1.00 |
| 3:N:112:VAL:HG22 | 3:N:113:PRO:HD2 | 1.31 | 1.00 |
| 1:E:188:SER:OG | 1:E:189:LYS:O | 1.79 | 1.00 |
| 1:H:7:LEU:HD21 | 1:H:353:LEU:HD22 | 1.38 | 1.00 |
| 1:I:254:LEU:O | 1:I:383:ARG:NH1 | 1.95 | 1.00 |
| 3:N:64:GLU:HB3 | 3:N:93:LEU:HB2 | 1.39 | 1.00 |
| 1:J:382:SER:C | 2:M:60:TYR:CE1 | 2.34 | 1.00 |
| 3:N:47:ALA:O | 3:N:48:ASP:OD1 | 1.76 | 1.00 |
| 1:D:281:LEU:CD2 | 1:D:385:GLU:C | 2.29 | 1.00 |
| 1:D:389:ALA:HB1 | 1:I:354:GLN:CD | 1.82 | 1.00 |
| 1:F:185:VAL:CG2 | 2:M:38:ILE:N | 2.23 | 1.00 |
| 1:D:187:GLN:O | 1:G:187:GLN:HG2 | 1.62 | 1.00 |
| 1:L:282:TYR:CZ | 3:N:42:ASP:OD2 | 2.13 | 1.00 |
| 1:F:16:ARG:O | 1:F:17:ASN:N | 1.95 | 1.00 |
| 1:L:104:PRO:HB3 | 1:L:188:SER:O | 1.59 | 1.00 |
| 3:N:112:VAL:HG22 | 3:N:113:PRO:CD | 1.79 | 1.00 |
| 2:M:67:ILE:HG22 | 4:P:41:MET:HE1 | 1.44 | 1.00 |
| 1:B:108:ARG:CZ | 1:D:314:SER:HA | 1.84 | 0.99 |
| 1:J:16:ARG:NH1 | 1:J:21:MET:CE | 2.24 | 0.99 |
| 1:B:108:ARG:NE | 1:D:314:SER:HB2 | 1.76 | 0.99 |
| 2:M:2:LEU:O | 2:M:9:TYR:CE2 | 2.15 | 0.99 |
| 3:N:68:ALA:N | 3:N:87:GLN:CD | 2.00 | 0.99 |
| 1:F:239:GLN:CG | 2:M:45:MET:SD | 2.49 | 0.99 |
| 1:G:382:SER:HB2 | 1:G:383:ARG:H | 0.84 | 0.99 |
| 1:L:280:ASN:HB3 | 1:L:352:THR:OG1 | 1.62 | 0.99 |
| 1:D:281:LEU:HD21 | 1:D:385:GLU:C | 1.83 | 0.99 |
| 1:F:239:GLN:CA | 2:M:45:MET:HE2 | 1.92 | 0.99 |
| 1:D:11:GLN:O | 1:D:15:LEU:HD13 | 1.63 | 0.99 |
| 1:H:7:LEU:CD1 | 1:H:353:LEU:HD13 | 1.93 | 0.99 |
| 3:N:31:PHE:CZ | 3:N:100:PHE:CD2 | 2.36 | 0.99 |
| 2:M:78:ILE:O | 4:P:53:LEU:HD21 | 1.61 | 0.99 |
| 1:B:311:ALA:CB | 1:I:390:GLY:O | 2.11 | 0.99 |
| 1:D:277:GLN:HE21 | 1:D:394:THR:HG23 | 1.24 | 0.99 |
| 1:L:279:ALA:HA | 3:N:43:LEU:HD11 | 1.40 | 0.99 |
| 3:N:28:ARG:HH11 | 3:N:37:GLU:CG | 1.65 | 0.99 |
| 1:L:280:ASN:CG | 1:L:352:THR:HG21 | 1.82 | 0.99 |
| 1:F:35:SER:CB | 1:F:240:LEU:CD2 | 2.40 | 0.99 |
| 1:B:392:ILE:O | 1:B:393:SER:O | 1.80 | 0.99 |
| 1:D:187:GLN:CG | 2:M:9:TYR:CE1 | 2.43 | 0.99 |
| 1:H:281:LEU:HD21 | 1:H:386:LEU:N | 1.77 | 0.99 |
| 1:K:7:LEU:CA | 1:K:12:GLN:NE2 | 2.25 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:19:ILE:HG23 | 4:P:23:PHE:HE1 | 1.24 | 0.98 |
| 1:H:7:LEU:HD13 | 1:H:353:LEU:CD1 | 1.92 | 0.98 |
| 1:H:9:PRO:HG3 | 1:I:34:GLN:OE1 | 1.64 | 0.98 |
| 3:N:80:ILE:HG21 | 3:N:116:PHE:CG | 1.96 | 0.98 |
| 1:B:358:VAL:HB | 1:B:358:VAL:CA | 1.47 | 0.98 |
| 1:E:189:LYS:HZ2 | 1:K:61:ASN:HB2 | 0.83 | 0.98 |
| 1:J:386:LEU:CD1 | 2:M:62:ALA:HB1 | 1.93 | 0.98 |
| 1:L:104:PRO:HA | 1:L:189:LYS:O | 1.64 | 0.98 |
| 1:F:357:ASN:H | 2:M:23:THR:CG2 | 1.75 | 0.98 |
| 3:N:80:ILE:HG23 | 3:N:116:PHE:CA | 1.63 | 0.98 |
| 3:N:13:PRO:HD2 | 3:N:68:ALA:HB1 | 1.43 | 0.98 |
| 1:L:279:ALA:C | 3:N:43:LEU:HD11 | 1.83 | 0.98 |
| 1:L:38:VAL:HG23 | 1:L:238:ASP:HB2 | 1.00 | 0.98 |
| 1:G:309:ARG:CD | 1:G:314:SER:HA | 1.94 | 0.97 |
| 1:D:7:LEU:HD13 | 1:D:353:LEU:HD13 | 1.44 | 0.97 |
| 1:G:255:SER:OG | 1:G:386:LEU:HD21 | 1.64 | 0.97 |
| 1:H:9:PRO:CB | 1:I:34:GLN:HE22 | 1.77 | 0.97 |
| 3:N:91:PRO:O | 3:N:92:LEU:HD12 | 1.62 | 0.97 |
| 1:D:187:GLN:HG3 | 2:M:9:TYR:CD1 | 1.96 | 0.97 |
| 1:E:257:LEU:CG | 1:E:383:ARG:HE | 1.76 | 0.97 |
| 1:J:184:ASN:HD21 | 1:J:240:LEU:HD12 | 1.26 | 0.97 |
| 1:F:239:GLN:OE1 | 2:M:45:MET:SD | 2.22 | 0.97 |
| 3:N:82:CYS:SG | 3:N:116:PHE:HE2 | 1.72 | 0.97 |
| 1:D:281:LEU:CG | 1:D:385:GLU:HB3 | 1.78 | 0.97 |
| 4:P:96:ILE:HG22 | 4:P:100:LEU:HD13 | 1.46 | 0.97 |
| 1:B:384:THR:O | 1:B:387:VAL:CG1 | 2.13 | 0.97 |
| 1:D:281:LEU:HD22 | 1:D:385:GLU:CB | 1.79 | 0.97 |
| 1:D:281:LEU:HD22 | 1:D:385:GLU:HB3 | 1.01 | 0.97 |
| 1:D:108:ARG:CZ | 1:I:314:SER:N | 2.22 | 0.97 |
| 1:I:384:THR:O | 1:I:387:VAL:CG1 | 2.13 | 0.97 |
| 1:L:311:ALA:O | 1:L:312:ASN:OD1 | 1.81 | 0.97 |
| 1:L:354:GLN:HA | 2:M:75:GLN:HG2 | 1.43 | 0.97 |
| 3:N:39:VAL:HG13 | 3:N:90:PHE:CB | 1.94 | 0.97 |
| 1:D:389:ALA:HB2 | 1:I:354:GLN:HE22 | 0.96 | 0.97 |
| 1:E:8:THR:CG2 | 1:E:11:GLN:H | 1.78 | 0.97 |
| 1:F:185:VAL:CA | 2:M:38:ILE:O | 2.13 | 0.97 |
| 1:F:356:GLY:CA | 2:M:23:THR:HG22 | 1.94 | 0.97 |
| 3:N:80:ILE:HG12 | 3:N:117:LEU:O | 1.63 | 0.97 |
| 1:E:188:SER:OG | 1:E:189:LYS:N | 1.95 | 0.97 |
| 1:G:34:GLN:NE2 | 1:I:9:PRO:HB3 | 1.79 | 0.97 |
| 1:K:104:PRO:O | 1:K:188:SER:OG | 1.82 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:353:LEU:CA | 2:M:76:PRO:CG | 2.42 | 0.97 |
| 1:C:104:PRO:HB3 | 1:C:188:SER:HB3 | 1.44 | 0.97 |
| 1:F:353:LEU:HD13 | 2:M:27:LEU:O | 1.65 | 0.97 |
| 3:N:49:THR:CG2 | 3:N:112:VAL:CG1 | 2.37 | 0.97 |
| 1:F:384:THR:O | 2:M:33:GLY:N | 1.98 | 0.96 |
| 1:I:11:GLN:O | 1:I:15:LEU:HD13 | 1.63 | 0.96 |
| 3:N:5:ASN:HB3 | 3:N:6:PRO:HD3 | 1.44 | 0.96 |
| 1:B:11:GLN:O | 1:B:15:LEU:HD13 | 1.63 | 0.96 |
| 1:B:7:LEU:HD13 | 1:B:353:LEU:HD13 | 1.47 | 0.96 |
| 4:P:96:ILE:HD13 | 4:P:100:LEU:CD2 | 1.87 | 0.96 |
| 1:D:384:THR:O | 1:D:387:VAL:CG1 | 2.13 | 0.96 |
| 1:F:311:ALA:HB1 | 2:M:23:THR:CB | 1.92 | 0.96 |
| 4:P:50:SER:O | 4:P:51:VAL:HG12 | 1.65 | 0.96 |
| 1:B:108:ARG:HH21 | 1:D:314:SER:N | 1.54 | 0.96 |
| 1:C:184:ASN:HB2 | 1:C:247:TYR:CE1 | 2.00 | 0.96 |
| 1:F:16:ARG:C | 1:F:17:ASN:N | 2.18 | 0.96 |
| 1:G:247:TYR:OH | 2:M:2:LEU:CD2 | 2.14 | 0.96 |
| 1:B:6:GLN:HB2 | 1:I:388:ASN:HA | 1.45 | 0.96 |
| 1:F:35:SER:CB | 1:F:240:LEU:HD23 | 1.94 | 0.96 |
| 1:H:384:THR:O | 1:H:387:VAL:CG1 | 2.13 | 0.96 |
| 1:L:263:SER:CB | 3:N:40:LYS:CE | 2.37 | 0.96 |
| 1:B:17:ASN:C | 1:B:20:ALA:H | 1.65 | 0.96 |
| 1:E:187:GLN:HA | 1:K:185:VAL:CA | 1.96 | 0.96 |
| 4:P:38:PRO:N | 4:P:39:PRO:CD | 2.29 | 0.96 |
| 1:D:187:GLN:HA | 1:G:187:GLN:HE21 | 1.30 | 0.96 |
| 1:B:44:THR:H | 1:K:191:ARG:NH2 | 1.58 | 0.95 |
| 1:C:190:GLN:OE1 | 1:C:191:ARG:N | 1.99 | 0.95 |
| 1:G:239:GLN:NE2 | 1:I:313:PHE:HZ | 1.64 | 0.95 |
| 1:F:185:VAL:HG13 | 2:M:38:ILE:H | 1.26 | 0.95 |
| 1:D:21:MET:HA | 1:D:252:ILE:HD12 | 1.47 | 0.95 |
| 1:L:193:LYS:NZ | 3:N:67:GLY:O | 2.00 | 0.95 |
| 3:N:31:PHE:CZ | 3:N:100:PHE:HD2 | 1.80 | 0.95 |
| 1:B:358:VAL:CG1 | 1:B:358:VAL:HA | 1.80 | 0.95 |
| 1:F:185:VAL:HG11 | 2:M:38:ILE:H | 1.31 | 0.95 |
| 2:M:15:ILE:N | 2:M:16:PRO:CD | 2.30 | 0.95 |
| 1:B:277:GLN:HB2 | 1:B:394:THR:OG1 | 0.78 | 0.95 |
| 1:B:257:LEU:HG | 1:B:383:ARG:HG2 | 1.45 | 0.95 |
| 1:D:108:ARG:NH2 | 1:I:314:SER:HA | 1.46 | 0.95 |
| 1:E:182:LEU:CD2 | 1:E:184:ASN:HD21 | 1.53 | 0.95 |
| 3:N:62:ASN:HB3 | 3:N:95:PRO:CG | 1.95 | 0.95 |
| 1:J:384:THR:HG21 | 2:M:62:ALA:CB | 1.88 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:15:TYR:CE2 | 3:N:88:GLY:HA2 | 2.01 | 0.95 |
| 1:E:311:ALA:HB3 | 2:M:47:PHE:CE1 | 2.01 | 0.95 |
| 1:I:281:LEU:CD1 | 1:I:385:GLU:CB | 2.40 | 0.95 |
| 1:L:63:GLY:O | 1:L:183:ALA:N | 2.00 | 0.95 |
| 1:F:185:VAL:HG13 | 2:M:38:ILE:CB | 1.97 | 0.95 |
| 3:N:41:TYR:HB3 | 3:N:45:TYR:CD2 | 1.90 | 0.95 |
| 4:P:42:THR:O | 4:P:45:GLN:CG | 2.14 | 0.95 |
| 1:B:384:THR:O | 1:B:387:VAL:HG13 | 1.67 | 0.94 |
| 1:B:392:ILE:HG22 | 1:B:393:SER:H | 1.29 | 0.94 |
| 1:F:353:LEU:HA | 2:M:26:LEU:CA | 1.97 | 0.94 |
| 1:J:308:GLN:HE22 | 1:J:345:ASN:HD21 | 1.03 | 0.94 |
| 3:N:14:VAL:HG22 | 3:N:16:ASN:N | 1.80 | 0.94 |
| 1:A:312:ASN:ND2 | 1:K:281:LEU:HB3 | 1.82 | 0.94 |
| 1:B:281:LEU:CD2 | 1:B:385:GLU:HB3 | 1.96 | 0.94 |
| 1:F:185:VAL:HG13 | 2:M:38:ILE:HB | 1.48 | 0.94 |
| 1:D:11:GLN:CD | 1:D:351:TYR:HD2 | 1.71 | 0.94 |
| 1:D:372:ARG:HH12 | 1:I:272:VAL:CG2 | 1.75 | 0.94 |
| 1:F:386:LEU:HD13 | 2:M:33:GLY:O | 1.67 | 0.94 |
| 1:E:187:GLN:CA | 1:K:185:VAL:HA | 1.96 | 0.94 |
| 1:H:254:LEU:O | 1:H:383:ARG:CZ | 2.15 | 0.94 |
| 1:I:392:ILE:C | 1:I:393:SER:CA | 2.32 | 0.94 |
| 1:K:34:GLN:C | 1:K:35:SER:N | 2.20 | 0.94 |
| 1:F:15:LEU:C | 1:F:17:ASN:OD1 | 2.05 | 0.94 |
| 3:N:28:ARG:HH12 | 3:N:37:GLU:CG | 1.79 | 0.94 |
| 1:D:187:GLN:NE2 | 2:M:9:TYR:CG | 2.36 | 0.94 |
| 1:G:15:LEU:CD2 | 1:G:18:GLN:NE2 | 1.93 | 0.94 |
| 1:J:313:PHE:CE2 | 1:K:238:ASP:OD2 | 2.21 | 0.94 |
| 1:F:10:ALA:HB2 | 2:M:26:LEU:CD2 | 1.98 | 0.94 |
| 3:N:18:CYS:O | 3:N:19:ASP:OD1 | 1.85 | 0.94 |
| 1:B:281:LEU:CG | 1:B:385:GLU:HB3 | 1.98 | 0.93 |
| 1:F:383:ARG:CA | 2:M:31:VAL:HG21 | 1.98 | 0.93 |
| 3:N:92:LEU:C | 3:N:93:LEU:HD12 | 1.89 | 0.93 |
| 4:P:50:SER:O | 4:P:51:VAL:CG1 | 2.15 | 0.93 |
| 3:N:49:THR:CG2 | 3:N:82:CYS:C | 2.36 | 0.93 |
| 1:G:251:LEU:HD13 | 1:G:388:ASN:OD1 | 1.67 | 0.93 |
| 1:L:104:PRO:C | 1:L:188:SER:OG | 2.06 | 0.93 |
| 1:B:17:ASN:HB3 | 1:B:20:ALA:HB2 | 1.47 | 0.93 |
| 1:C:104:PRO:CB | 1:C:188:SER:HB3 | 1.97 | 0.93 |
| 1:D:281:LEU:HD11 | 1:D:382:SER:OG | 1.68 | 0.93 |
| 1:G:309:ARG:NE | 1:G:314:SER:HA | 1.82 | 0.93 |
| 1:I:384:THR:O | 1:I:387:VAL:HG13 | 1.67 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:16:ARG:CZ | 1:J:21:MET:CE | 2.47 | 0.93 |
| 1:B:395:THR:OG1 | 1:D:395:THR:N | 1.96 | 0.93 |
| 1:H:384:THR:O | 1:H:387:VAL:HG13 | 1.67 | 0.93 |
| 3:N:13:PRO:N | 3:N:69:PHE:CZ | 2.37 | 0.93 |
| 1:E:311:ALA:O | 2:M:47:PHE:CE1 | 2.21 | 0.93 |
| 1:C:181:VAL:C | 1:C:182:LEU:N | 2.23 | 0.93 |
| 1:F:185:VAL:HG22 | 2:M:38:ILE:O | 1.69 | 0.93 |
| 4:P:19:ILE:CG2 | 4:P:23:PHE:CE1 | 2.51 | 0.93 |
| 1:F:281:LEU:HG | 2:M:29:TYR:CE1 | 2.04 | 0.93 |
| 3:N:80:ILE:CG1 | 3:N:117:LEU:H | 1.82 | 0.93 |
| 1:B:5:GLN:CG | 1:B:310:THR:CG2 | 2.46 | 0.93 |
| 1:D:17:ASN:C | 1:D:21:MET:H | 1.73 | 0.93 |
| 2:M:45:MET:HB2 | 2:M:48:LEU:HD13 | 1.50 | 0.93 |
| 1:J:383:ARG:C | 2:M:60:TYR:CE1 | 2.41 | 0.93 |
| 1:D:387:VAL:HG21 | 1:I:6:GLN:HE22 | 1.32 | 0.92 |
| 1:D:372:ARG:HH11 | 1:I:272:VAL:HG21 | 0.77 | 0.92 |
| 3:N:37:GLU:HB2 | 3:N:92:LEU:CB | 1.99 | 0.92 |
| 1:H:7:LEU:HD22 | 1:H:353:LEU:HD21 | 1.45 | 0.92 |
| 1:H:281:LEU:HD13 | 1:H:385:GLU:HB3 | 0.94 | 0.92 |
| 1:L:80:HIS:O | 1:L:156:ALA:HB1 | 1.66 | 0.92 |
| 1:A:255:SER:HA | 1:A:383:ARG:NE | 1.83 | 0.92 |
| 1:D:384:THR:O | 1:D:387:VAL:HG13 | 1.67 | 0.92 |
| 1:J:182:LEU:CD2 | 1:J:249:LEU:HD13 | 1.98 | 0.92 |
| 1:E:189:LYS:NZ | 1:K:61:ASN:CG | 2.13 | 0.92 |
| 1:L:6:GLN:O | 1:L:7:LEU:CD1 | 2.16 | 0.92 |
| 1:J:385:GLU:C | 1:J:386:LEU:HD12 | 1.90 | 0.92 |
| 1:B:279:ALA:HB2 | 1:B:391:THR:O | 1.70 | 0.92 |
| 1:D:5:GLN:H | 1:E:239:GLN:NE2 | 1.61 | 0.92 |
| 3:N:41:TYR:CA | 3:N:45:TYR:HD2 | 1.66 | 0.92 |
| 4:P:96:ILE:CG1 | 4:P:100:LEU:HD22 | 2.00 | 0.92 |
| 4:P:37:GLY:C | 4:P:39:PRO:CD | 2.37 | 0.92 |
| 1:D:5:GLN:HE22 | 1:E:36:TYR:HE2 | 1.10 | 0.92 |
| 1:D:389:ALA:CB | 1:I:354:GLN:CD | 2.37 | 0.92 |
| 1:J:7:LEU:HD13 | 1:J:351:TYR:O | 1.70 | 0.92 |
| 1:F:354:GLN:HA | 2:M:26:LEU:HD21 | 1.52 | 0.92 |
| 1:B:392:ILE:HG22 | 1:B:393:SER:N | 1.83 | 0.92 |
| 1:K:7:LEU:HA | 1:K:12:GLN:HE22 | 1.25 | 0.92 |
| 1:I:185:VAL:HG13 | 1:I:186:PRO:HD3 | 1.51 | 0.92 |
| 1:A:312:ASN:HD21 | 1:K:281:LEU:HB3 | 1.32 | 0.91 |
| 1:F:185:VAL:HG22 | 2:M:38:ILE:N | 1.82 | 0.91 |
| 1:I:277:GLN:HB2 | 1:I:394:THR:OG1 | 1.70 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:17:ASN:O | 1:K:20:ALA:N | 2.03 | 0.91 |
| 1:L:280:ASN:CB | 1:L:352:THR:OG1 | 2.17 | 0.91 |
| 1:F:185:VAL:HG22 | 2:M:38:ILE:C | 1.90 | 0.91 |
| 1:B:282:TYR:CE2 | 1:B:386:LEU:HG | 2.05 | 0.91 |
| 2:M:75:GLN:CB | 4:P:51:VAL:H | 1.83 | 0.91 |
| 3:N:81:LYS:HD2 | 3:N:113:PRO:CB | 1.99 | 0.91 |
| 1:B:269:THR:HG21 | 1:I:372:ARG:CD | 2.00 | 0.91 |
| 1:E:8:THR:HG22 | 1:E:11:GLN:N | 1.84 | 0.91 |
| 3:N:45:TYR:O | 3:N:46:LEU:HD12 | 1.69 | 0.91 |
| 1:E:280:ASN:OD1 | 1:E:352:THR:HG21 | 1.71 | 0.91 |
| 1:E:187:GLN:O | 1:K:185:VAL:O | 1.88 | 0.91 |
| 1:J:382:SER:C | 2:M:60:TYR:HE1 | 1.71 | 0.91 |
| 1:D:11:GLN:CD | 1:D:351:TYR:CD2 | 2.44 | 0.91 |
| 1:I:257:LEU:CD2 | 1:I:383:ARG:HG2 | 2.01 | 0.91 |
| 1:J:313:PHE:CZ | 1:K:239:GLN:HG3 | 2.05 | 0.91 |
| 1:L:38:VAL:HG21 | 1:L:238:ASP:OD2 | 1.69 | 0.91 |
| 1:L:182:LEU:HD11 | 1:L:184:ASN:HD22 | 1.17 | 0.91 |
| 1:J:255:SER:HA | 1:J:383:ARG:CD | 2.01 | 0.91 |
| 1:K:245:ASN:O | 1:K:245:ASN:C | 0.71 | 0.91 |
| 1:B:185:VAL:HG13 | 1:B:186:PRO:HD3 | 1.51 | 0.91 |
| 1:D:386:LEU:C | 1:I:312:ASN:OD1 | 2.09 | 0.91 |
| 1:G:385:GLU:C | 1:G:386:LEU:HD12 | 1.92 | 0.91 |
| 1:F:311:ALA:HB3 | 2:M:23:THR:HB | 1.52 | 0.91 |
| 1:A:255:SER:O | 1:A:383:ARG:CB | 2.19 | 0.90 |
| 1:B:395:THR:HG22 | 1:I:395:THR:C | 1.67 | 0.90 |
| 1:K:7:LEU:CB | 1:K:12:GLN:HE22 | 1.84 | 0.90 |
| 1:A:313:PHE:HE1 | 1:K:383:ARG:HA | 1.29 | 0.90 |
| 1:L:265:GLN:HG2 | 3:N:40:LYS:HZ1 | 1.36 | 0.90 |
| 1:L:6:GLN:O | 1:L:7:LEU:CB | 2.19 | 0.90 |
| 1:F:311:ALA:HB2 | 2:M:23:THR:HG21 | 1.50 | 0.90 |
| 1:L:265:GLN:HE22 | 3:N:40:LYS:CE | 1.83 | 0.90 |
| 1:F:357:ASN:H | 2:M:23:THR:HG21 | 1.35 | 0.90 |
| 3:N:25:GLN:CB | 3:N:107:SER:HG | 1.77 | 0.90 |
| 1:A:63:GLY:N | 1:A:184:ASN:OD1 | 2.05 | 0.90 |
| 1:H:9:PRO:HB3 | 1:I:34:GLN:NE2 | 1.85 | 0.90 |
| 1:L:7:LEU:CB | 1:L:11:GLN:CB | 2.45 | 0.90 |
| 2:M:15:ILE:N | 2:M:16:PRO:HD2 | 1.74 | 0.90 |
| 4:P:42:THR:O | 4:P:45:GLN:NE2 | 2.00 | 0.90 |
| 1:H:265:GLN:HE22 | 1:H:393:SER:HB2 | 1.09 | 0.90 |
| 1:L:353:LEU:C | 2:M:76:PRO:CD | 2.40 | 0.90 |
| 3:N:60:ILE:HD12 | 3:N:97:ARG:HD3 | 1.48 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:245:ASN:C | 1:C:245:ASN:O | 0.70 | 0.90 |
| 1:F:353:LEU:CA | 2:M:26:LEU:HA | 2.00 | 0.90 |
| 1:D:187:GLN:HE22 | 2:M:9:TYR:CA | 1.84 | 0.90 |
| 1:J:11:GLN:OE1 | 1:J:353:LEU:HD21 | 1.71 | 0.90 |
| 1:J:184:ASN:ND2 | 1:J:240:LEU:HD12 | 1.85 | 0.90 |
| 1:E:187:GLN:C | 1:K:185:VAL:O | 2.11 | 0.90 |
| 1:L:265:GLN:NE2 | 3:N:40:LYS:HZ2 | 1.69 | 0.90 |
| 1:J:386:LEU:HD11 | 2:M:62:ALA:CB | 2.02 | 0.90 |
| 4:P:37:GLY:O | 4:P:39:PRO:HD2 | 1.70 | 0.90 |
| 1:C:14:ALA:HA | 1:C:17:ASN:HD22 | 1.34 | 0.90 |
| 1:D:281:LEU:CD2 | 1:D:385:GLU:HB2 | 1.98 | 0.90 |
| 1:D:257:LEU:CG | 1:D:383:ARG:HG2 | 2.01 | 0.90 |
| 3:N:65:ASN:HD21 | 3:N:71:ILE:HD12 | 1.17 | 0.90 |
| 1:A:245:ASN:C | 1:A:245:ASN:O | 0.69 | 0.89 |
| 1:H:255:SER:O | 1:H:383:ARG:HG3 | 1.71 | 0.89 |
| 1:L:353:LEU:O | 2:M:76:PRO:CD | 2.18 | 0.89 |
| 1:L:311:ALA:O | 1:L:312:ASN:CG | 2.10 | 0.89 |
| 1:L:6:GLN:C | 1:L:7:LEU:CD1 | 2.40 | 0.89 |
| 3:N:80:ILE:HG22 | 3:N:116:PHE:HA | 1.50 | 0.89 |
| 3:N:62:ASN:CB | 3:N:95:PRO:O | 2.21 | 0.89 |
| 1:D:185:VAL:HG13 | 1:D:186:PRO:HD3 | 1.50 | 0.89 |
| 1:D:281:LEU:HD21 | 1:D:386:LEU:HD12 | 1.52 | 0.89 |
| 1:G:245:ASN:C | 1:G:245:ASN:O | 0.69 | 0.89 |
| 1:H:185:VAL:HG13 | 1:H:186:PRO:HD3 | 1.50 | 0.89 |
| 1:I:17:ASN:CA | 1:I:20:ALA:H | 1.79 | 0.89 |
| 1:E:187:GLN:C | 1:K:185:VAL:C | 2.31 | 0.89 |
| 1:L:76:ILE:HB | 1:L:154:ILE:CD1 | 2.03 | 0.89 |
| 1:L:186:PRO:O | 1:L:187:GLN:HB2 | 1.71 | 0.89 |
| 3:N:66:ASP:C | 3:N:87:GLN:HE22 | 1.56 | 0.89 |
| 1:E:182:LEU:HD21 | 1:E:184:ASN:HD22 | 1.36 | 0.89 |
| 1:F:239:GLN:HG2 | 2:M:45:MET:HE2 | 1.04 | 0.89 |
| 1:F:280:ASN:OD1 | 1:F:352:THR:HG21 | 1.71 | 0.89 |
| 1:G:63:GLY:N | 1:G:184:ASN:OD1 | 2.05 | 0.89 |
| 1:F:185:VAL:CG2 | 2:M:37:GLY:HA3 | 2.00 | 0.89 |
| 3:N:61:ASP:HB2 | 3:N:75:GLU:HB2 | 0.90 | 0.89 |
| 1:B:355:TYR:OH | 1:B:393:SER:O | 1.88 | 0.89 |
| 1:I:254:LEU:O | 1:I:383:ARG:CZ | 2.21 | 0.89 |
| 1:C:104:PRO:HB3 | 1:C:188:SER:CB | 2.04 | 0.88 |
| 1:D:389:ALA:HB1 | 1:I:354:GLN:NE2 | 1.85 | 0.88 |
| 1:J:308:GLN:HE22 | 1:J:345:ASN:ND2 | 1.69 | 0.88 |
| 1:F:383:ARG:HG2 | 2:M:31:VAL:CG2 | 2.03 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:64:GLU:OE1 | 3:N:93:LEU:CB | 2.21 | 0.88 |
| 1:E:189:LYS:HZ1 | 1:K:61:ASN:N | 1.67 | 0.88 |
| 1:L:77:THR:HA | 1:L:158:ALA:O | 1.73 | 0.88 |
| 1:B:389:ALA:HB2 | 1:D:354:GLN:NE2 | 1.88 | 0.88 |
| 4:P:38:PRO:N | 4:P:39:PRO:HD2 | 1.84 | 0.88 |
| 1:L:151:PRO:HD2 | 1:L:162:LEU:HD22 | 1.56 | 0.88 |
| 3:N:37:GLU:CB | 3:N:92:LEU:HB3 | 2.03 | 0.88 |
| 3:N:49:THR:HG21 | 3:N:112:VAL:CG1 | 2.01 | 0.88 |
| 4:P:35:TRP:CD2 | 4:P:110:TYR:HD1 | 1.74 | 0.88 |
| 1:D:282:TYR:HE2 | 1:D:386:LEU:HG | 0.80 | 0.88 |
| 1:H:254:LEU:O | 1:H:383:ARG:NH2 | 2.06 | 0.88 |
| 1:L:64:ILE:CA | 1:L:181:VAL:O | 2.21 | 0.88 |
| 1:L:263:SER:OG | 3:N:40:LYS:HE2 | 0.70 | 0.88 |
| 1:B:106:ASN:OD1 | 1:E:238:ASP:OD2 | 1.92 | 0.88 |
| 1:D:187:GLN:O | 1:G:187:GLN:CG | 2.22 | 0.88 |
| 1:L:353:LEU:C | 2:M:76:PRO:HD2 | 1.94 | 0.88 |
| 1:L:353:LEU:HD23 | 2:M:76:PRO:HG3 | 1.53 | 0.88 |
| 1:C:8:THR:HG22 | 1:C:9:PRO:HD2 | 0.88 | 0.87 |
| 1:B:395:THR:HG1 | 1:D:394:THR:C | 1.73 | 0.87 |
| 1:F:16:ARG:C | 1:F:17:ASN:CG | 2.25 | 0.87 |
| 1:H:281:LEU:CD1 | 1:H:385:GLU:CG | 2.52 | 0.87 |
| 1:I:355:TYR:HE2 | 1:I:394:THR:HG1 | 0.89 | 0.87 |
| 1:B:5:GLN:HE22 | 1:B:316:THR:CG2 | 1.87 | 0.87 |
| 1:G:185:VAL:HG13 | 2:M:7:PHE:HB2 | 1.55 | 0.87 |
| 3:N:64:GLU:OE1 | 3:N:93:LEU:HD23 | 1.75 | 0.87 |
| 1:L:183:ALA:C | 1:L:184:ASN:N | 2.27 | 0.87 |
| 1:F:312:ASN:HB3 | 2:M:20:PRO:HG2 | 1.56 | 0.87 |
| 1:K:182:LEU:HD13 | 1:K:254:LEU:CD1 | 2.04 | 0.87 |
| 1:G:257:LEU:HD21 | 1:G:383:ARG:HH21 | 1.38 | 0.87 |
| 1:F:255:SER:CB | 2:M:35:ILE:HD11 | 2.05 | 0.87 |
| 3:N:49:THR:CB | 3:N:112:VAL:HG12 | 2.02 | 0.87 |
| 3:N:60:ILE:CG1 | 3:N:97:ARG:HD2 | 2.04 | 0.87 |
| 1:D:187:GLN:HE22 | 2:M:9:TYR:CB | 1.80 | 0.87 |
| 1:I:7:LEU:HD22 | 1:I:353:LEU:CD2 | 2.05 | 0.87 |
| 1:J:254:LEU:O | 1:J:383:ARG:NE | 2.08 | 0.87 |
| 1:E:311:ALA:CB | 2:M:47:PHE:HE1 | 1.87 | 0.87 |
| 1:E:8:THR:O | 1:E:12:GLN:HG3 | 1.75 | 0.87 |
| 4:P:19:ILE:O | 4:P:23:PHE:HD1 | 1.58 | 0.86 |
| 1:I:382:SER:O | 1:I:386:LEU:HD13 | 1.75 | 0.86 |
| 1:L:265:GLN:HE22 | 3:N:40:LYS:CD | 1.84 | 0.86 |
| 1:B:382:SER:O | 1:B:386:LEU:HD13 | 1.75 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:281:LEU:CD2 | 1:H:385:GLU:C | 2.44 | 0.86 |
| 1:H:5:GLN:OE1 | 1:I:36:TYR:CE1 | 2.28 | 0.86 |
| 1:B:354:GLN:OE1 | 1:I:389:ALA:HB1 | 1.75 | 0.86 |
| 1:D:9:PRO:HG3 | 1:E:34:GLN:NE2 | 1.90 | 0.86 |
| 1:E:187:GLN:O | 1:K:186:PRO:HD3 | 1.75 | 0.86 |
| 1:G:239:GLN:CD | 1:I:313:PHE:HZ | 1.79 | 0.86 |
| 1:L:108:ARG:NH1 | 3:N:89:TYR:HB3 | 1.68 | 0.86 |
| 3:N:27:VAL:CB | 3:N:27:VAL:N | 2.37 | 0.86 |
| 1:L:280:ASN:OD1 | 1:L:352:THR:CG2 | 2.21 | 0.86 |
| 3:N:13:PRO:N | 3:N:69:PHE:CE1 | 2.43 | 0.86 |
| 4:P:16:LEU:O | 4:P:20:TRP:HD1 | 1.58 | 0.86 |
| 1:H:382:SER:OG | 1:H:385:GLU:HG3 | 1.76 | 0.86 |
| 1:L:353:LEU:HA | 2:M:76:PRO:HD3 | 1.57 | 0.86 |
| 3:N:112:VAL:O | 3:N:114:LEU:HD12 | 1.76 | 0.86 |
| 3:N:64:GLU:HB2 | 3:N:93:LEU:HB2 | 0.86 | 0.86 |
| 1:D:382:SER:OG | 1:D:385:GLU:HG3 | 1.76 | 0.85 |
| 1:K:104:PRO:HB2 | 1:K:187:GLN:OE1 | 1.75 | 0.85 |
| 3:N:49:THR:CG2 | 3:N:83:PRO:CA | 2.27 | 0.85 |
| 4:P:24:ARG:O | 4:P:28:ALA:HB2 | 1.76 | 0.85 |
| 1:F:239:GLN:HA | 2:M:45:MET:HE2 | 1.58 | 0.85 |
| 1:H:185:VAL:CG1 | 1:H:186:PRO:HD3 | 2.06 | 0.85 |
| 1:H:265:GLN:HE22 | 1:H:393:SER:CB | 1.83 | 0.85 |
| 1:B:313:PHE:CZ | 1:I:387:VAL:HG23 | 2.10 | 0.85 |
| 4:P:18:LEU:O | 4:P:22:TRP:CD1 | 2.27 | 0.85 |
| 1:B:277:GLN:HB2 | 1:B:394:THR:CB | 2.06 | 0.85 |
| 1:D:387:VAL:HG22 | 1:I:6:GLN:OE1 | 1.74 | 0.85 |
| 1:G:353:LEU:HD12 | 1:G:353:LEU:H | 1.41 | 0.85 |
| 1:I:257:LEU:HG | 1:I:383:ARG:HG2 | 1.59 | 0.85 |
| 1:D:108:ARG:CZ | 1:I:313:PHE:O | 2.23 | 0.85 |
| 3:N:55:VAL:HG22 | 3:N:56:GLN:N | 1.91 | 0.85 |
| 3:N:61:ASP:HB2 | 3:N:75:GLU:HB3 | 1.54 | 0.85 |
| 3:N:62:ASN:CB | 3:N:95:PRO:CG | 2.52 | 0.85 |
| 1:G:309:ARG:HG3 | 1:G:313:PHE:O | 1.76 | 0.85 |
| 1:H:355:TYR:CZ | 1:H:394:THR:OG1 | 2.28 | 0.85 |
| 2:M:6:GLN:O | 2:M:8:PRO:CD | 2.25 | 0.85 |
| 1:I:382:SER:OG | 1:I:385:GLU:HG3 | 1.76 | 0.85 |
| 1:F:383:ARG:HG2 | 2:M:31:VAL:HG21 | 1.59 | 0.85 |
| 1:E:187:GLN:CA | 1:K:184:ASN:O | 2.24 | 0.85 |
| 1:H:382:SER:O | 1:H:386:LEU:HD13 | 1.75 | 0.85 |
| 1:I:185:VAL:CG1 | 1:I:186:PRO:HD3 | 2.06 | 0.85 |
| 3:N:80:ILE:HD13 | 3:N:116:PHE:HB3 | 0.87 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:80:ILE:HG23 | 3:N:116:PHE:HA | 0.86 | 0.85 |
| 1:B:382:SER:OG | 1:B:385:GLU:HG3 | 1.76 | 0.85 |
| 1:C:181:VAL:C | 1:C:182:LEU:CA | 2.45 | 0.85 |
| 1:K:102:TYR:O | 1:K:190:GLN:HB3 | 1.76 | 0.85 |
| 1:J:386:LEU:HD11 | 2:M:62:ALA:HB1 | 1.59 | 0.84 |
| 1:B:358:VAL:CB | 1:B:358:VAL:CA | 0.85 | 0.84 |
| 1:E:187:GLN:O | 1:K:185:VAL:C | 2.14 | 0.84 |
| 1:G:62:VAL:C | 1:G:184:ASN:OD1 | 2.15 | 0.84 |
| 2:M:2:LEU:O | 2:M:9:TYR:HE2 | 1.57 | 0.84 |
| 1:J:382:SER:O | 2:M:60:TYR:CE1 | 2.28 | 0.84 |
| 4:P:103:TYR:C | 4:P:107:LEU:HD13 | 1.97 | 0.84 |
| 1:A:384:THR:O | 1:A:385:GLU:HB2 | 1.75 | 0.84 |
| 1:D:382:SER:O | 1:D:386:LEU:HD13 | 1.75 | 0.84 |
| 3:N:68:ALA:CB | 3:N:87:GLN:HG2 | 2.07 | 0.84 |
| 1:H:355:TYR:CE2 | 1:H:394:THR:OG1 | 2.31 | 0.84 |
| 1:B:382:SER:OG | 1:B:385:GLU:CG | 2.26 | 0.84 |
| 1:J:8:THR:HG22 | 1:J:9:PRO:HD2 | 0.85 | 0.84 |
| 1:L:151:PRO:O | 1:L:215:TYR:OH | 1.94 | 0.84 |
| 4:P:35:TRP:O | 4:P:36:GLU:HB2 | 1.77 | 0.84 |
| 1:C:8:THR:HG23 | 1:C:9:PRO:CD | 1.89 | 0.84 |
| 1:E:187:GLN:HA | 1:K:184:ASN:C | 1.97 | 0.84 |
| 1:F:247:TYR:CZ | 2:M:43:GLN:NE2 | 2.45 | 0.84 |
| 2:M:67:ILE:CG2 | 4:P:41:MET:HE1 | 2.07 | 0.84 |
| 3:N:28:ARG:O | 3:N:103:ARG:HB2 | 1.78 | 0.84 |
| 3:N:65:ASN:ND2 | 3:N:71:ILE:CD1 | 2.39 | 0.84 |
| 1:D:17:ASN:CA | 1:D:20:ALA:H | 1.79 | 0.83 |
| 1:D:382:SER:OG | 1:D:385:GLU:CG | 2.26 | 0.83 |
| 1:E:189:LYS:HZ3 | 1:K:61:ASN:CA | 1.79 | 0.83 |
| 1:E:191:ARG:HE | 1:K:62:VAL:HG23 | 1.42 | 0.83 |
| 1:K:104:PRO:HB3 | 1:K:187:GLN:HB2 | 1.58 | 0.83 |
| 1:G:247:TYR:CZ | 2:M:2:LEU:CD2 | 2.60 | 0.83 |
| 1:B:185:VAL:CG1 | 1:B:186:PRO:HD3 | 2.06 | 0.83 |
| 1:H:382:SER:OG | 1:H:385:GLU:CG | 2.26 | 0.83 |
| 1:J:21:MET:HA | 1:J:252:ILE:HD12 | 1.60 | 0.83 |
| 1:L:265:GLN:NE2 | 3:N:40:LYS:HD2 | 1.93 | 0.83 |
| 3:N:81:LYS:CG | 3:N:113:PRO:CG | 2.56 | 0.83 |
| 1:D:11:GLN:NE2 | 1:D:351:TYR:HD2 | 1.76 | 0.83 |
| 1:H:12:GLN:HA | 1:H:15:LEU:HD13 | 1.58 | 0.83 |
| 1:I:382:SER:OG | 1:I:385:GLU:CG | 2.26 | 0.83 |
| 3:N:60:ILE:HD12 | 3:N:97:ARG:NE | 1.93 | 0.83 |
| 4:P:19:ILE:HG23 | 4:P:23:PHE:CE1 | 2.13 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:309:ARG:HG3 | 1:G:314:SER:C | 1.99 | 0.83 |
| 1:F:239:GLN:CA | 2:M:45:MET:CE | 2.53 | 0.83 |
| 1:L:312:ASN:CG | 2:M:73:PHE:HE2 | 1.78 | 0.83 |
| 1:B:264:ALA:HB3 | 1:D:272:VAL:HG11 | 1.60 | 0.83 |
| 1:B:279:ALA:CB | 1:B:391:THR:O | 2.27 | 0.83 |
| 1:D:187:GLN:HE21 | 2:M:9:TYR:HB3 | 1.41 | 0.83 |
| 3:N:81:LYS:HB2 | 3:N:113:PRO:HB2 | 1.61 | 0.83 |
| 1:K:282:TYR:HA | 1:K:381:THR:HB | 1.61 | 0.83 |
| 1:J:5:GLN:HE22 | 1:K:38:VAL:CG2 | 1.92 | 0.83 |
| 1:B:282:TYR:HE2 | 1:B:386:LEU:HG | 1.43 | 0.83 |
| 1:G:15:LEU:HD22 | 1:G:18:GLN:HE22 | 1.42 | 0.83 |
| 1:H:281:LEU:CD1 | 1:H:385:GLU:CD | 2.47 | 0.83 |
| 1:F:185:VAL:HG13 | 2:M:38:ILE:CA | 2.08 | 0.82 |
| 1:F:312:ASN:HB3 | 2:M:20:PRO:CG | 2.08 | 0.82 |
| 1:F:382:SER:HB3 | 1:F:383:ARG:CA | 2.09 | 0.82 |
| 1:F:251:LEU:HB3 | 1:F:385:GLU:OE1 | 1.78 | 0.82 |
| 1:H:355:TYR:OH | 1:H:392:ILE:O | 1.95 | 0.82 |
| 1:I:16:ARG:O | 1:I:18:GLN:N | 2.12 | 0.82 |
| 1:L:111:GLU:OE1 | 3:N:89:TYR:HB2 | 1.77 | 0.82 |
| 3:N:67:GLY:C | 3:N:87:GLN:NE2 | 2.31 | 0.82 |
| 1:A:62:VAL:C | 1:A:184:ASN:OD1 | 2.16 | 0.82 |
| 1:E:189:LYS:HD3 | 1:K:61:ASN:HD22 | 1.42 | 0.82 |
| 1:H:5:GLN:OE1 | 1:I:36:TYR:CD1 | 2.31 | 0.82 |
| 1:K:283:ARG:H | 1:K:381:THR:HG1 | 1.24 | 0.82 |
| 1:A:255:SER:C | 1:A:383:ARG:CG | 2.41 | 0.82 |
| 1:F:251:LEU:O | 1:F:385:GLU:OE2 | 1.98 | 0.82 |
| 1:H:381:THR:CA | 1:H:382:SER:N | 2.42 | 0.82 |
| 1:L:65:VAL:HG21 | 1:L:190:GLN:OE1 | 1.78 | 0.82 |
| 3:N:14:VAL:CG2 | 3:N:16:ASN:H | 1.88 | 0.82 |
| 1:H:282:TYR:CE2 | 1:H:386:LEU:HG | 2.13 | 0.82 |
| 1:F:383:ARG:CB | 2:M:31:VAL:CG2 | 2.58 | 0.82 |
| 4:P:19:ILE:HG22 | 4:P:23:PHE:CE1 | 2.14 | 0.82 |
| 1:B:354:GLN:HE22 | 1:I:389:ALA:HB2 | 1.45 | 0.82 |
| 3:N:49:THR:OG1 | 3:N:112:VAL:CG1 | 2.28 | 0.82 |
| 1:B:17:ASN:C | 1:B:20:ALA:N | 2.28 | 0.82 |
| 1:E:311:ALA:CB | 2:M:47:PHE:CE1 | 2.60 | 0.82 |
| 3:N:41:TYR:CB | 3:N:45:TYR:CB | 2.46 | 0.82 |
| 1:B:382:SER:HG | 1:B:385:GLU:HG3 | 1.45 | 0.81 |
| 1:J:383:ARG:HB2 | 1:J:384:THR:N | 1.95 | 0.81 |
| 1:F:384:THR:O | 2:M:33:GLY:C | 2.17 | 0.81 |
| 1:H:7:LEU:HD22 | 1:H:353:LEU:HD22 | 1.30 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:101:TYR:O | 3:N:89:TYR:OH | 1.98 | 0.81 |
| 1:A:353:LEU:H | 1:A:353:LEU:HD12 | 1.41 | 0.81 |
| 1:D:384:THR:HA | 1:D:387:VAL:CG1 | 2.11 | 0.81 |
| 1:E:28:ARG:HD3 | 1:E:175:THR:O | 1.80 | 0.81 |
| 1:L:170:LEU:HD13 | 1:L:181:VAL:HG21 | 1.60 | 0.81 |
| 1:F:239:GLN:HB3 | 2:M:45:MET:HE1 | 0.83 | 0.81 |
| 3:N:81:LYS:CG | 3:N:113:PRO:HG3 | 2.10 | 0.81 |
| 1:L:282:TYR:HE1 | 3:N:42:ASP:OD2 | 1.63 | 0.81 |
| 3:N:81:LYS:CD | 3:N:113:PRO:CB | 2.57 | 0.81 |
| 1:A:309:ARG:HG2 | 1:A:310:THR:C | 2.00 | 0.81 |
| 1:B:354:GLN:NE2 | 1:I:389:ALA:HB2 | 1.94 | 0.81 |
| 3:N:49:THR:HG23 | 3:N:83:PRO:HA | 0.82 | 0.81 |
| 1:B:17:ASN:CB | 1:B:20:ALA:HB2 | 2.10 | 0.81 |
| 1:D:257:LEU:HG | 1:D:383:ARG:CG | 2.05 | 0.81 |
| 1:D:281:LEU:HD21 | 1:D:385:GLU:HB2 | 1.56 | 0.81 |
| 1:E:7:LEU:O | 1:E:8:THR:OG1 | 1.98 | 0.81 |
| 1:F:255:SER:HB3 | 2:M:35:ILE:CD1 | 2.10 | 0.81 |
| 1:G:257:LEU:HD21 | 1:G:383:ARG:NH2 | 1.95 | 0.81 |
| 1:J:384:THR:CG2 | 2:M:62:ALA:CA | 2.58 | 0.81 |
| 3:N:103:ARG:HB3 | 3:N:105:LEU:HD11 | 1.61 | 0.81 |
| 1:F:311:ALA:CB | 2:M:23:THR:CG2 | 2.57 | 0.81 |
| 1:I:8:THR:C | 1:I:9:PRO:CA | 2.49 | 0.81 |
| 1:J:384:THR:OG1 | 2:M:60:TYR:HB3 | 1.79 | 0.81 |
| 1:F:386:LEU:CD1 | 2:M:33:GLY:O | 2.28 | 0.81 |
| 1:I:277:GLN:CG | 1:I:394:THR:HB | 2.08 | 0.81 |
| 3:N:80:ILE:CG1 | 3:N:117:LEU:O | 2.28 | 0.81 |
| 4:P:15:VAL:HG13 | 4:P:16:LEU:CD1 | 2.09 | 0.81 |
| 1:A:255:SER:C | 1:A:383:ARG:HG3 | 2.00 | 0.81 |
| 1:B:384:THR:HA | 1:B:387:VAL:CG1 | 2.11 | 0.81 |
| 1:F:11:GLN:C | 1:F:15:LEU:HD13 | 2.01 | 0.81 |
| 1:I:384:THR:HA | 1:I:387:VAL:CG1 | 2.11 | 0.81 |
| 1:L:265:GLN:HE22 | 3:N:40:LYS:HD2 | 1.43 | 0.81 |
| 1:H:384:THR:HA | 1:H:387:VAL:CG1 | 2.11 | 0.81 |
| 4:P:24:ARG:O | 4:P:28:ALA:N | 2.14 | 0.81 |
| 1:D:16:ARG:C | 1:D:18:GLN:N | 2.34 | 0.81 |
| 1:F:312:ASN:OD1 | 2:M:21:THR:CB | 2.20 | 0.81 |
| 1:A:309:ARG:HG3 | 1:A:313:PHE:O | 1.79 | 0.80 |
| 1:F:383:ARG:CA | 2:M:31:VAL:CG2 | 2.57 | 0.80 |
| 1:G:23:ALA:O | 1:G:24:ASN:N | 2.14 | 0.80 |
| 4:P:24:ARG:O | 4:P:28:ALA:CB | 2.29 | 0.80 |
| 1:B:384:THR:C | 1:B:387:VAL:HG12 | 2.02 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:44:THR:H | 1:K:191:ARG:NE | 1.79 | 0.80 |
| 3:N:50:GLN:HE21 | 3:N:86:LYS:CE | 1.93 | 0.80 |
| 1:B:8:THR:C | 1:B:9:PRO:CA | 2.49 | 0.80 |
| 1:I:7:LEU:HD13 | 1:I:353:LEU:HD22 | 1.61 | 0.80 |
| 1:E:182:LEU:HD21 | 1:E:184:ASN:HD21 | 1.09 | 0.80 |
| 1:G:251:LEU:HD11 | 1:G:388:ASN:CG | 2.01 | 0.80 |
| 1:B:358:VAL:CB | 1:B:358:VAL:C | 2.50 | 0.80 |
| 1:E:108:ARG:HD3 | 1:J:314:SER:HB2 | 1.60 | 0.80 |
| 1:K:104:PRO:CB | 1:K:187:GLN:HB2 | 2.12 | 0.80 |
| 4:P:7:LEU:HD12 | 4:P:7:LEU:H | 1.46 | 0.80 |
| 1:G:23:ALA:CA | 1:G:24:ASN:N | 2.44 | 0.80 |
| 1:H:384:THR:C | 1:H:387:VAL:HG12 | 2.02 | 0.80 |
| 1:J:308:GLN:NE2 | 1:J:345:ASN:HD21 | 1.78 | 0.80 |
| 1:G:247:TYR:OH | 2:M:2:LEU:HD23 | 1.76 | 0.80 |
| 1:F:239:GLN:CD | 2:M:45:MET:HG2 | 2.00 | 0.80 |
| 4:P:96:ILE:HB | 4:P:100:LEU:HD22 | 1.64 | 0.80 |
| 1:H:5:GLN:NE2 | 1:I:36:TYR:CG | 2.49 | 0.80 |
| 1:I:7:LEU:HD13 | 1:I:353:LEU:HD13 | 1.61 | 0.80 |
| 3:N:49:THR:OG1 | 3:N:112:VAL:HG12 | 1.81 | 0.80 |
| 1:G:239:GLN:NE2 | 1:I:313:PHE:CZ | 2.50 | 0.80 |
| 1:K:63:GLY:O | 1:K:183:ALA:CB | 2.30 | 0.80 |
| 1:F:10:ALA:HB2 | 2:M:26:LEU:HD23 | 1.61 | 0.80 |
| 3:N:37:GLU:CB | 3:N:92:LEU:CB | 2.59 | 0.80 |
| 1:H:265:GLN:HE21 | 1:H:393:SER:HB2 | 1.41 | 0.80 |
| 1:B:395:THR:HG21 | 1:I:395:THR:C | 2.00 | 0.80 |
| 1:L:78:ASN:CB | 1:L:154:ILE:O | 2.30 | 0.80 |
| 3:N:55:VAL:HG22 | 3:N:56:GLN:H | 1.45 | 0.80 |
| 1:C:186:PRO:O | 1:C:187:GLN:HG3 | 1.82 | 0.79 |
| 1:C:104:PRO:O | 1:C:188:SER:OG | 1.99 | 0.79 |
| 1:J:384:THR:HG21 | 2:M:61:HIS:C | 2.00 | 0.79 |
| 1:J:5:GLN:N | 1:J:313:PHE:CZ | 2.50 | 0.79 |
| 1:F:239:GLN:CD | 2:M:45:MET:CG | 2.50 | 0.79 |
| 1:L:353:LEU:CD2 | 2:M:76:PRO:CG | 2.60 | 0.79 |
| 1:B:9:PRO:CG | 1:C:34:GLN:OE1 | 2.23 | 0.79 |
| 1:J:28:ARG:HG3 | 1:J:177:LEU:HD12 | 1.65 | 0.79 |
| 3:N:27:VAL:CB | 3:N:27:VAL:C | 2.48 | 0.79 |
| 1:B:281:LEU:CD2 | 1:B:385:GLU:C | 2.51 | 0.79 |
| 2:M:14:PRO:O | 2:M:16:PRO:HD2 | 1.82 | 0.79 |
| 1:I:355:TYR:HE2 | 1:I:394:THR:OG1 | 1.66 | 0.79 |
| 1:A:313:PHE:HE1 | 1:K:383:ARG:CA | 1.81 | 0.79 |
| 1:L:353:LEU:HD22 | 2:M:76:PRO:CG | 2.12 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:77:THR:HG23 | 1:L:158:ALA:O | 1.81 | 0.79 |
| 3:N:49:THR:HG21 | 3:N:82:CYS:O | 1.80 | 0.79 |
| 1:F:351:TYR:HH | 2:M:29:TYR:HE2 | 1.20 | 0.79 |
| 1:B:313:PHE:HE1 | 1:I:387:VAL:HG23 | 1.41 | 0.79 |
| 1:L:7:LEU:O | 1:L:11:GLN:HG3 | 1.82 | 0.79 |
| 1:D:384:THR:C | 1:D:387:VAL:HG12 | 2.02 | 0.79 |
| 1:G:185:VAL:HB | 2:M:4:ASN:HB2 | 0.81 | 0.79 |
| 1:I:80:HIS:CD2 | 1:I:83:GLU:H | 2.01 | 0.79 |
| 3:N:60:ILE:CD1 | 3:N:97:ARG:CD | 2.19 | 0.79 |
| 1:B:357:ASN:C | 1:B:358:VAL:CA | 2.50 | 0.79 |
| 1:H:282:TYR:HE2 | 1:H:386:LEU:HG | 1.44 | 0.79 |
| 1:J:16:ARG:HD3 | 1:J:21:MET:CE | 2.12 | 0.79 |
| 1:A:80:HIS:CD2 | 1:A:83:GLU:H | 2.01 | 0.78 |
| 1:C:104:PRO:HB3 | 1:C:188:SER:C | 2.02 | 0.78 |
| 3:N:60:ILE:CD1 | 3:N:97:ARG:CZ | 2.60 | 0.78 |
| 3:N:28:ARG:CZ | 3:N:37:GLU:HG2 | 2.12 | 0.78 |
| 1:D:17:ASN:HA | 1:D:20:ALA:H | 1.48 | 0.78 |
| 1:D:21:MET:HA | 1:D:252:ILE:CD1 | 2.12 | 0.78 |
| 1:I:277:GLN:CB | 1:I:394:THR:OG1 | 2.31 | 0.78 |
| 1:I:384:THR:C | 1:I:387:VAL:HG12 | 2.02 | 0.78 |
| 3:N:27:VAL:CG1 | 3:N:27:VAL:CA | 2.61 | 0.78 |
| 1:G:80:HIS:CD2 | 1:G:83:GLU:H | 2.01 | 0.78 |
| 1:C:102:TYR:O | 1:C:190:GLN:HG2 | 1.84 | 0.78 |
| 1:C:184:ASN:HB2 | 1:C:247:TYR:HE1 | 1.47 | 0.78 |
| 1:I:17:ASN:C | 1:I:21:MET:H | 1.86 | 0.78 |
| 1:J:80:HIS:CD2 | 1:J:83:GLU:H | 2.01 | 0.78 |
| 1:G:182:LEU:CD2 | 2:M:4:ASN:HB3 | 2.13 | 0.78 |
| 3:N:67:GLY:C | 3:N:87:GLN:HE22 | 1.87 | 0.78 |
| 1:B:80:HIS:CD2 | 1:B:83:GLU:H | 2.01 | 0.78 |
| 1:D:187:GLN:HE22 | 2:M:9:TYR:HA | 1.48 | 0.78 |
| 1:I:7:LEU:HD22 | 1:I:353:LEU:HD22 | 1.63 | 0.78 |
| 1:J:31:VAL:O | 1:J:35:SER:N | 2.17 | 0.78 |
| 1:L:6:GLN:C | 1:L:7:LEU:HD12 | 2.04 | 0.78 |
| 3:N:49:THR:HB | 3:N:112:VAL:HG11 | 0.78 | 0.78 |
| 1:B:389:ALA:CB | 1:D:354:GLN:OE1 | 2.32 | 0.78 |
| 1:L:180:ALA:HB3 | 1:L:254:LEU:HD23 | 1.65 | 0.78 |
| 3:N:80:ILE:HG23 | 3:N:116:PHE:C | 2.03 | 0.78 |
| 1:F:247:TYR:HE2 | 2:M:43:GLN:HE21 | 1.23 | 0.78 |
| 3:N:94:VAL:CG2 | 3:N:103:ARG:NH1 | 2.42 | 0.78 |
| 3:N:41:TYR:C | 3:N:45:TYR:HD2 | 1.85 | 0.78 |
| 1:B:4:VAL:N | 1:B:4:VAL:CB | 2.46 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:80:HIS:CD2 | 1:D:83:GLU:H | 2.01 | 0.77 |
| 1:L:283:ARG:NH1 | 1:L:382:SER:HB3 | 1.99 | 0.77 |
| 3:N:112:VAL:O | 3:N:114:LEU:CD1 | 2.32 | 0.77 |
| 1:B:108:ARG:NH2 | 1:D:313:PHE:O | 2.17 | 0.77 |
| 1:E:182:LEU:HD23 | 1:E:184:ASN:OD1 | 1.83 | 0.77 |
| 1:E:189:LYS:HD3 | 1:K:61:ASN:ND2 | 1.98 | 0.77 |
| 1:I:257:LEU:CG | 1:I:383:ARG:HG2 | 2.13 | 0.77 |
| 1:J:239:GLN:O | 1:J:241:PRO:HD3 | 1.84 | 0.77 |
| 3:N:91:PRO:C | 3:N:92:LEU:CD1 | 2.46 | 0.77 |
| 1:I:17:ASN:CB | 1:I:20:ALA:HB3 | 2.05 | 0.77 |
| 4:P:35:TRP:CD2 | 4:P:110:TYR:CD1 | 2.38 | 0.77 |
| 4:P:52:THR:C | 4:P:53:LEU:CD1 | 2.45 | 0.77 |
| 1:D:108:ARG:NH2 | 1:I:313:PHE:O | 2.17 | 0.77 |
| 2:M:45:MET:HB3 | 2:M:48:LEU:CD1 | 2.01 | 0.77 |
| 1:G:185:VAL:HG23 | 2:M:4:ASN:H | 1.50 | 0.77 |
| 1:G:106:ASN:ND2 | 1:G:191:ARG:HH22 | 1.83 | 0.77 |
| 1:I:17:ASN:HA | 1:I:20:ALA:H | 1.48 | 0.77 |
| 1:I:382:SER:HG | 1:I:385:GLU:HG3 | 1.47 | 0.77 |
| 1:J:391:THR:OG1 | 2:M:67:ILE:HG23 | 1.84 | 0.77 |
| 1:L:11:GLN:O | 1:L:15:LEU:HD12 | 1.83 | 0.77 |
| 1:L:265:GLN:NE2 | 3:N:40:LYS:HZ1 | 1.79 | 0.77 |
| 1:L:7:LEU:HB3 | 1:L:11:GLN:HB2 | 1.63 | 0.77 |
| 1:D:4:VAL:O | 1:D:313:PHE:CE1 | 2.37 | 0.77 |
| 1:H:80:HIS:CD2 | 1:H:83:GLU:H | 2.01 | 0.77 |
| 1:I:7:LEU:CD2 | 1:I:353:LEU:HD22 | 2.14 | 0.77 |
| 1:B:354:GLN:HE22 | 1:I:389:ALA:CB | 1.97 | 0.77 |
| 1:L:265:GLN:CG | 3:N:40:LYS:HZ1 | 1.97 | 0.77 |
| 1:D:372:ARG:HH12 | 1:I:272:VAL:HG23 | 1.39 | 0.77 |
| 1:L:353:LEU:CB | 2:M:76:PRO:HG3 | 2.15 | 0.77 |
| 3:N:116:PHE:C | 3:N:117:LEU:HD12 | 2.05 | 0.77 |
| 3:N:53:THR:O | 3:N:79:ARG:NE | 2.12 | 0.77 |
| 1:I:17:ASN:HB3 | 1:I:20:ALA:HB2 | 0.79 | 0.77 |
| 1:D:187:GLN:OE1 | 2:M:9:TYR:CD1 | 2.37 | 0.77 |
| 3:N:65:ASN:HD22 | 3:N:71:ILE:HD12 | 1.47 | 0.77 |
| 4:P:13:GLY:O | 4:P:17:ILE:HG13 | 1.85 | 0.77 |
| 1:B:106:ASN:ND2 | 1:B:191:ARG:HH22 | 1.83 | 0.77 |
| 1:B:257:LEU:CG | 1:B:383:ARG:HG2 | 2.14 | 0.77 |
| 1:I:7:LEU:CD1 | 1:I:353:LEU:HD22 | 2.14 | 0.77 |
| 1:I:4:VAL:CB | 1:I:4:VAL:N | 2.46 | 0.77 |
| 1:E:311:ALA:O | 2:M:47:PHE:HE1 | 1.65 | 0.77 |
| 1:F:11:GLN:O | 1:F:15:LEU:HD12 | 1.85 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:106:ASN:ND2 | 1:A:191:ARG:HH22 | 1.83 | 0.76 |
| 1:B:63:GLY:HA2 | 1:B:184:ASN:ND2 | 2.01 | 0.76 |
| 1:B:5:GLN:CD | 1:B:310:THR:HG21 | 1.99 | 0.76 |
| 1:D:106:ASN:ND2 | 1:D:191:ARG:HH22 | 1.83 | 0.76 |
| 2:M:75:GLN:HB3 | 4:P:51:VAL:H | 1.51 | 0.76 |
| 4:P:42:THR:O | 4:P:45:GLN:CD | 2.23 | 0.76 |
| 1:A:354:GLN:HB2 | 1:A:357:ASN:ND2 | 1.99 | 0.76 |
| 1:A:63:GLY:H | 1:A:184:ASN:HD21 | 1.32 | 0.76 |
| 1:E:106:ASN:ND2 | 1:K:62:VAL:CG1 | 2.46 | 0.76 |
| 1:H:106:ASN:ND2 | 1:H:191:ARG:HH22 | 1.83 | 0.76 |
| 1:H:63:GLY:HA2 | 1:H:184:ASN:ND2 | 2.01 | 0.76 |
| 1:B:272:VAL:CG1 | 1:I:264:ALA:CB | 2.51 | 0.76 |
| 1:G:354:GLN:HB2 | 1:G:357:ASN:ND2 | 1.99 | 0.76 |
| 1:G:63:GLY:H | 1:G:184:ASN:HD21 | 1.32 | 0.76 |
| 1:H:308:GLN:HE22 | 1:H:345:ASN:HD21 | 1.34 | 0.76 |
| 1:L:78:ASN:O | 1:L:157:GLY:N | 2.18 | 0.76 |
| 3:N:25:GLN:HB2 | 3:N:107:SER:HG | 0.95 | 0.76 |
| 4:P:5:LYS:C | 4:P:6:LEU:HD12 | 2.06 | 0.76 |
| 1:B:358:VAL:CB | 1:B:358:VAL:N | 2.48 | 0.76 |
| 1:I:308:GLN:HE22 | 1:I:345:ASN:HD21 | 1.34 | 0.76 |
| 4:P:6:LEU:HB3 | 4:P:7:LEU:HD12 | 1.68 | 0.76 |
| 1:B:257:LEU:HD12 | 1:B:386:LEU:HD22 | 1.67 | 0.76 |
| 1:C:280:ASN:OD1 | 1:C:352:THR:HG21 | 1.86 | 0.76 |
| 1:I:106:ASN:ND2 | 1:I:191:ARG:HH22 | 1.83 | 0.76 |
| 1:K:380:PHE:O | 1:K:381:THR:OG1 | 2.01 | 0.76 |
| 1:A:255:SER:HA | 1:A:383:ARG:CZ | 2.14 | 0.76 |
| 1:K:280:ASN:OD1 | 1:K:352:THR:HG21 | 1.86 | 0.76 |
| 1:F:185:VAL:CG2 | 2:M:38:ILE:O | 2.33 | 0.76 |
| 3:N:49:THR:HG21 | 3:N:112:VAL:HG13 | 1.67 | 0.76 |
| 1:D:7:LEU:HD13 | 1:D:353:LEU:HD22 | 1.68 | 0.76 |
| 1:B:4:VAL:C | 1:B:4:VAL:CB | 2.55 | 0.75 |
| 1:H:4:VAL:N | 1:I:239:GLN:OE1 | 2.19 | 0.75 |
| 1:I:257:LEU:N | 1:I:381:THR:O | 2.15 | 0.75 |
| 1:J:106:ASN:ND2 | 1:J:191:ARG:HH22 | 1.83 | 0.75 |
| 1:C:14:ALA:CA | 1:C:17:ASN:ND2 | 2.49 | 0.75 |
| 1:L:7:LEU:O | 1:L:11:GLN:CG | 2.35 | 0.75 |
| 1:F:281:LEU:HA | 2:M:29:TYR:CE1 | 2.21 | 0.75 |
| 1:K:101:TYR:OH | 1:K:190:GLN:CG | 2.34 | 0.75 |
| 2:M:4:ASN:O | 2:M:7:PHE:O | 2.03 | 0.75 |
| 1:B:280:ASN:O | 1:B:281:LEU:HB3 | 1.87 | 0.75 |
| 1:D:17:ASN:CB | 1:D:20:ALA:HB3 | 2.05 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:257:LEU:HG | 1:E:383:ARG:HE | 1.49 | 0.75 |
| 1:B:311:ALA:CB | 1:I:390:GLY:C | 2.54 | 0.75 |
| 1:J:21:MET:HA | 1:J:252:ILE:CD1 | 2.16 | 0.75 |
| 1:H:281:LEU:HD13 | 1:H:385:GLU:CG | 2.14 | 0.75 |
| 4:P:96:ILE:HD12 | 4:P:100:LEU:HD22 | 1.32 | 0.75 |
| 1:B:354:GLN:HB2 | 1:B:357:ASN:ND2 | 2.01 | 0.75 |
| 1:D:389:ALA:CB | 1:I:354:GLN:OE1 | 2.31 | 0.75 |
| 1:B:108:ARG:NH1 | 1:D:314:SER:CA | 2.37 | 0.75 |
| 1:D:354:GLN:HB2 | 1:D:357:ASN:ND2 | 2.02 | 0.75 |
| 1:E:8:THR:CB | 1:E:11:GLN:HB2 | 2.13 | 0.75 |
| 1:G:382:SER:C | 1:G:383:ARG:CA | 2.54 | 0.75 |
| 1:B:354:GLN:NE2 | 1:I:389:ALA:CB | 2.49 | 0.75 |
| 1:G:35:SER:C | 1:G:36:TYR:CA | 2.56 | 0.75 |
| 3:N:66:ASP:C | 3:N:87:GLN:HE21 | 1.74 | 0.75 |
| 1:A:255:SER:HA | 1:A:383:ARG:HD2 | 0.79 | 0.74 |
| 1:L:76:ILE:O | 1:L:154:ILE:HD13 | 1.86 | 0.74 |
| 3:N:62:ASN:ND2 | 3:N:95:PRO:HG2 | 2.02 | 0.74 |
| 1:A:308:GLN:HE22 | 1:A:345:ASN:HD21 | 1.34 | 0.74 |
| 1:F:351:TYR:OH | 2:M:29:TYR:HE2 | 1.60 | 0.74 |
| 1:F:383:ARG:CG | 2:M:31:VAL:HG21 | 2.17 | 0.74 |
| 1:L:257:LEU:CA | 1:L:258:TYR:N | 2.50 | 0.74 |
| 1:D:63:GLY:HA2 | 1:D:184:ASN:ND2 | 2.01 | 0.74 |
| 1:K:104:PRO:CB | 1:K:187:GLN:CB | 2.65 | 0.74 |
| 1:F:357:ASN:N | 2:M:23:THR:CG2 | 2.50 | 0.74 |
| 1:E:312:ASN:OD1 | 2:M:47:PHE:CE1 | 2.39 | 0.74 |
| 1:D:281:LEU:CD2 | 1:D:386:LEU:HD12 | 2.17 | 0.74 |
| 1:G:185:VAL:CG1 | 2:M:7:PHE:HB2 | 2.18 | 0.74 |
| 1:I:11:GLN:OE1 | 1:I:351:TYR:CD2 | 2.40 | 0.74 |
| 1:B:281:LEU:HD21 | 1:B:386:LEU:N | 2.01 | 0.74 |
| 1:J:354:GLN:HB2 | 1:J:357:ASN:ND2 | 2.02 | 0.74 |
| 1:L:182:LEU:HD11 | 1:L:184:ASN:HD21 | 1.43 | 0.74 |
| 1:L:280:ASN:CG | 1:L:352:THR:CG2 | 2.55 | 0.74 |
| 3:N:50:GLN:NE2 | 3:N:86:LYS:HE2 | 2.00 | 0.74 |
| 1:D:17:ASN:HB3 | 1:D:20:ALA:HB2 | 0.79 | 0.74 |
| 1:L:64:ILE:CG2 | 1:L:180:ALA:HB1 | 2.17 | 0.74 |
| 4:P:26:ARG:HB2 | 4:P:27:PRO:HD3 | 1.68 | 0.74 |
| 1:A:384:THR:O | 1:A:385:GLU:CB | 2.36 | 0.74 |
| 1:D:281:LEU:CD2 | 1:D:385:GLU:CA | 2.65 | 0.74 |
| 1:D:386:LEU:O | 1:I:312:ASN:OD1 | 2.06 | 0.74 |
| 1:B:41:GLN:HG2 | 1:K:106:ASN:ND2 | 2.03 | 0.74 |
| 1:C:14:ALA:O | 1:C:17:ASN:ND2 | 2.21 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:60:ILE:HD12 | 3:N:97:ARG:HD2 | 0.74 | 0.74 |
| 1:D:17:ASN:HB2 | 1:D:20:ALA:CB | 2.18 | 0.74 |
| 1:D:308:GLN:HE22 | 1:D:345:ASN:HD21 | 1.34 | 0.74 |
| 1:F:311:ALA:O | 1:F:312:ASN:OD1 | 2.05 | 0.74 |
| 1:K:17:ASN:O | 1:K:20:ALA:HB3 | 1.87 | 0.74 |
| 1:L:312:ASN:ND2 | 2:M:73:PHE:CE1 | 2.51 | 0.74 |
| 1:I:63:GLY:HA2 | 1:I:184:ASN:ND2 | 2.01 | 0.74 |
| 1:I:281:LEU:HD11 | 1:I:385:GLU:HB2 | 1.68 | 0.74 |
| 1:I:354:GLN:HB2 | 1:I:357:ASN:ND2 | 2.02 | 0.74 |
| 1:K:191:ARG:C | 1:K:192:LEU:CA | 2.56 | 0.74 |
| 1:L:353:LEU:CA | 2:M:76:PRO:HD3 | 2.11 | 0.74 |
| 1:H:355:TYR:CE1 | 1:H:391:THR:HB | 2.23 | 0.73 |
| 1:H:355:TYR:OH | 1:H:394:THR:OG1 | 1.83 | 0.73 |
| 1:J:280:ASN:HD22 | 1:J:355:TYR:N | 1.86 | 0.73 |
| 4:P:103:TYR:O | 4:P:107:LEU:HD12 | 1.87 | 0.73 |
| 1:L:104:PRO:CA | 1:L:188:SER:OG | 2.35 | 0.73 |
| 3:N:15:TYR:CD2 | 3:N:47:ALA:CB | 2.72 | 0.73 |
| 1:B:185:VAL:HG13 | 1:B:186:PRO:CD | 2.18 | 0.73 |
| 1:J:28:ARG:NH2 | 1:J:253:ASP:OD1 | 2.19 | 0.73 |
| 1:L:78:ASN:C | 1:L:156:ALA:HA | 2.08 | 0.73 |
| 3:N:103:ARG:HB3 | 3:N:105:LEU:CD1 | 2.17 | 0.73 |
| 3:N:28:ARG:HH12 | 3:N:37:GLU:CB | 2.00 | 0.73 |
| 1:C:190:GLN:C | 1:C:191:ARG:CG | 2.55 | 0.73 |
| 1:D:280:ASN:HD22 | 1:D:355:TYR:N | 1.86 | 0.73 |
| 1:H:354:GLN:HB2 | 1:H:357:ASN:ND2 | 2.02 | 0.73 |
| 1:B:43:GLU:C | 1:K:191:ARG:NH2 | 2.34 | 0.73 |
| 1:L:312:ASN:CB | 2:M:73:PHE:CE2 | 2.63 | 0.73 |
| 1:F:311:ALA:HB2 | 2:M:23:THR:CG2 | 2.18 | 0.73 |
| 1:H:392:ILE:CG2 | 1:H:393:SER:N | 2.11 | 0.73 |
| 1:L:263:SER:HB2 | 3:N:40:LYS:CE | 2.16 | 0.73 |
| 1:D:5:GLN:HE21 | 1:D:316:THR:CG2 | 1.97 | 0.73 |
| 1:F:382:SER:O | 1:F:383:ARG:HG3 | 1.88 | 0.73 |
| 1:H:384:THR:O | 1:H:387:VAL:HG12 | 1.89 | 0.73 |
| 1:J:384:THR:HG21 | 2:M:62:ALA:CA | 2.16 | 0.73 |
| 3:N:112:VAL:CB | 3:N:113:PRO:HD2 | 2.13 | 0.73 |
| 3:N:80:ILE:CG2 | 3:N:116:PHE:CB | 2.41 | 0.73 |
| 1:L:265:GLN:CD | 3:N:40:LYS:NZ | 2.41 | 0.73 |
| 1:B:308:GLN:HE22 | 1:B:345:ASN:HD21 | 1.34 | 0.73 |
| 1:D:277:GLN:N | 1:D:394:THR:OG1 | 2.19 | 0.73 |
| 1:E:311:ALA:O | 1:E:312:ASN:OD1 | 2.05 | 0.73 |
| 1:G:309:ARG:HG3 | 1:G:314:SER:O | 1.89 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:309:ARG:HG3 | 1:G:314:SER:CA | 2.19 | 0.73 |
| 1:H:12:GLN:CA | 1:H:15:LEU:HD13 | 2.17 | 0.73 |
| 1:J:182:LEU:HD22 | 1:J:249:LEU:HD13 | 1.71 | 0.73 |
| 1:B:254:LEU:O | 1:B:383:ARG:CZ | 2.37 | 0.73 |
| 1:I:185:VAL:HG13 | 1:I:186:PRO:CD | 2.18 | 0.73 |
| 3:N:15:TYR:CD2 | 3:N:47:ALA:HB3 | 2.23 | 0.73 |
| 1:F:351:TYR:CZ | 2:M:29:TYR:CZ | 2.75 | 0.73 |
| 1:G:247:TYR:CE1 | 2:M:2:LEU:HD23 | 2.24 | 0.73 |
| 1:I:280:ASN:HD22 | 1:I:355:TYR:N | 1.86 | 0.73 |
| 1:H:5:GLN:NE2 | 1:I:36:TYR:CE2 | 2.38 | 0.73 |
| 1:L:182:LEU:HD21 | 1:L:184:ASN:HD21 | 1.54 | 0.73 |
| 1:A:309:ARG:HG2 | 1:A:310:THR:O | 1.88 | 0.73 |
| 1:H:185:VAL:HG13 | 1:H:186:PRO:CD | 2.18 | 0.73 |
| 1:B:352:THR:HB | 1:B:357:ASN:HB2 | 1.71 | 0.72 |
| 1:I:384:THR:O | 1:I:387:VAL:HG12 | 1.89 | 0.72 |
| 1:F:383:ARG:CB | 2:M:31:VAL:HG21 | 2.18 | 0.72 |
| 1:I:17:ASN:N | 1:I:18:GLN:N | 2.38 | 0.72 |
| 3:N:59:TYR:HB3 | 3:N:98:ALA:N | 2.02 | 0.72 |
| 1:A:255:SER:HA | 1:A:383:ARG:NH1 | 1.97 | 0.72 |
| 1:G:280:ASN:HD22 | 1:G:355:TYR:N | 1.86 | 0.72 |
| 1:H:7:LEU:O | 1:H:8:THR:HB | 1.89 | 0.72 |
| 1:I:281:LEU:CD2 | 1:I:385:GLU:HB3 | 2.18 | 0.72 |
| 1:H:280:ASN:HD22 | 1:H:355:TYR:N | 1.86 | 0.72 |
| 1:H:254:LEU:O | 1:H:383:ARG:NH1 | 2.21 | 0.72 |
| 1:F:354:GLN:HA | 2:M:26:LEU:CD2 | 2.19 | 0.72 |
| 2:M:47:PHE:C | 2:M:48:LEU:HD12 | 2.08 | 0.72 |
| 1:E:381:THR:HA | 1:E:382:SER:N | 2.02 | 0.72 |
| 1:F:383:ARG:CG | 2:M:31:VAL:CG2 | 2.67 | 0.72 |
| 1:J:313:PHE:HZ | 1:K:239:GLN:CG | 1.99 | 0.72 |
| 1:B:358:VAL:CB | 1:B:358:VAL:HA | 0.99 | 0.72 |
| 1:E:182:LEU:HD23 | 1:E:184:ASN:CG | 2.10 | 0.72 |
| 1:J:182:LEU:HD21 | 1:J:249:LEU:CD1 | 2.20 | 0.72 |
| 1:J:9:PRO:HG2 | 1:K:34:GLN:CD | 2.09 | 0.72 |
| 3:N:64:GLU:CB | 3:N:93:LEU:HB3 | 2.19 | 0.72 |
| 1:A:280:ASN:HD22 | 1:A:355:TYR:N | 1.86 | 0.72 |
| 1:B:280:ASN:HD22 | 1:B:355:TYR:N | 1.86 | 0.72 |
| 1:G:310:THR:OG1 | 1:G:313:PHE:HB2 | 1.89 | 0.72 |
| 1:K:29:GLN:O | 1:K:33:GLN:HG3 | 1.90 | 0.72 |
| 1:K:348:LYS:CE | 1:L:35:SER:O | 2.38 | 0.72 |
| 3:N:112:VAL:HG22 | 3:N:113:PRO:N | 2.04 | 0.72 |
| 1:L:102:TYR:CE2 | 3:N:13:PRO:HG3 | 2.24 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:29:GLN:O | 1:C:33:GLN:HG3 | 1.90 | 0.72 |
| 1:G:308:GLN:HE22 | 1:G:345:ASN:HD21 | 1.34 | 0.72 |
| 1:F:281:LEU:HA | 2:M:29:TYR:HE1 | 1.55 | 0.72 |
| 3:N:80:ILE:HG21 | 3:N:116:PHE:HA | 0.88 | 0.72 |
| 1:B:384:THR:O | 1:B:387:VAL:HG12 | 1.89 | 0.72 |
| 1:B:394:THR:O | 1:B:395:THR:O | 2.08 | 0.72 |
| 1:E:108:ARG:NH1 | 1:J:314:SER:HA | 2.04 | 0.72 |
| 1:E:106:ASN:CG | 1:K:62:VAL:CG1 | 2.58 | 0.72 |
| 3:N:62:ASN:HD22 | 3:N:95:PRO:HG2 | 1.53 | 0.72 |
| 1:B:392:ILE:O | 1:B:393:SER:CB | 2.24 | 0.71 |
| 1:D:185:VAL:HG13 | 1:D:186:PRO:CD | 2.18 | 0.71 |
| 1:L:102:TYR:CE2 | 3:N:89:TYR:HE2 | 2.08 | 0.71 |
| 1:H:281:LEU:CG | 1:H:385:GLU:HB3 | 2.17 | 0.71 |
| 1:I:8:THR:CA | 1:I:9:PRO:N | 2.47 | 0.71 |
| 1:B:11:GLN:CD | 1:B:351:TYR:HD2 | 1.92 | 0.71 |
| 1:C:104:PRO:CB | 1:C:188:SER:CB | 2.65 | 0.71 |
| 1:C:311:ALA:O | 1:C:312:ASN:OD1 | 2.09 | 0.71 |
| 1:G:15:LEU:HD23 | 1:G:18:GLN:HE21 | 1.44 | 0.71 |
| 1:I:355:TYR:OH | 1:I:393:SER:C | 2.29 | 0.71 |
| 1:K:311:ALA:O | 1:K:312:ASN:OD1 | 2.09 | 0.71 |
| 1:H:384:THR:HA | 1:H:387:VAL:HG12 | 1.72 | 0.71 |
| 1:H:4:VAL:N | 1:I:239:GLN:CG | 2.53 | 0.71 |
| 1:I:384:THR:CA | 1:I:387:VAL:HG12 | 2.21 | 0.71 |
| 1:I:384:THR:HA | 1:I:387:VAL:HG12 | 1.72 | 0.71 |
| 1:J:186:PRO:HB3 | 2:M:66:GLY:HA2 | 1.72 | 0.71 |
| 1:K:282:TYR:HA | 1:K:381:THR:CG2 | 2.21 | 0.71 |
| 1:B:384:THR:CA | 1:B:387:VAL:HG12 | 2.21 | 0.71 |
| 1:D:254:LEU:O | 1:D:383:ARG:NH1 | 2.24 | 0.71 |
| 1:G:34:GLN:NE2 | 1:I:9:PRO:HB2 | 1.76 | 0.71 |
| 1:L:65:VAL:N | 1:L:181:VAL:O | 2.23 | 0.71 |
| 1:F:351:TYR:CZ | 2:M:29:TYR:CE2 | 2.77 | 0.71 |
| 1:F:239:GLN:CD | 2:M:45:MET:CE | 2.58 | 0.71 |
| 1:L:265:GLN:CG | 3:N:40:LYS:NZ | 2.53 | 0.71 |
| 1:D:7:LEU:CD1 | 1:D:353:LEU:HD22 | 2.19 | 0.71 |
| 1:D:384:THR:CA | 1:D:387:VAL:HG12 | 2.21 | 0.71 |
| 1:F:29:GLN:O | 1:F:33:GLN:HG3 | 1.90 | 0.71 |
| 1:F:357:ASN:N | 2:M:23:THR:HG21 | 2.05 | 0.71 |
| 1:H:265:GLN:HE21 | 1:H:393:SER:CB | 2.00 | 0.71 |
| 1:E:187:GLN:HG2 | 1:K:184:ASN:O | 1.89 | 0.71 |
| 1:L:38:VAL:CG2 | 1:L:238:ASP:CB | 2.59 | 0.71 |
| 1:B:5:GLN:HG2 | 1:B:310:THR:CG2 | 2.20 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:8:THR:CG2 | 1:E:11:GLN:CG | 2.42 | 0.71 |
| 1:E:29:GLN:O | 1:E:33:GLN:HG3 | 1.90 | 0.71 |
| 1:L:28:ARG:HD3 | 1:L:175:THR:O | 1.90 | 0.71 |
| 1:J:386:LEU:HD13 | 2:M:62:ALA:HB1 | 1.69 | 0.71 |
| 1:D:17:ASN:N | 1:D:18:GLN:N | 2.38 | 0.71 |
| 1:D:16:ARG:O | 1:D:17:ASN:OD1 | 2.09 | 0.71 |
| 1:D:7:LEU:HD13 | 1:D:353:LEU:CD1 | 2.19 | 0.71 |
| 1:F:311:ALA:CB | 2:M:21:THR:HG21 | 2.19 | 0.71 |
| 3:N:28:ARG:HH12 | 3:N:37:GLU:HB3 | 1.55 | 0.71 |
| 3:N:15:TYR:CG | 3:N:47:ALA:HB3 | 2.25 | 0.71 |
| 1:F:351:TYR:CZ | 2:M:29:TYR:OH | 2.23 | 0.71 |
| 1:F:393:SER:OG | 1:F:394:THR:N | 2.24 | 0.71 |
| 2:M:24:MET:N | 2:M:25:PRO:HD2 | 2.03 | 0.71 |
| 1:D:394:THR:O | 1:D:395:THR:O | 2.08 | 0.71 |
| 1:G:182:LEU:HD21 | 2:M:4:ASN:HB3 | 1.73 | 0.71 |
| 1:I:80:HIS:HD2 | 1:I:83:GLU:H | 1.39 | 0.71 |
| 1:G:35:SER:CA | 1:G:36:TYR:N | 2.53 | 0.70 |
| 1:L:64:ILE:HD11 | 1:L:249:LEU:HD22 | 1.73 | 0.70 |
| 1:L:108:ARG:HH12 | 3:N:89:TYR:CA | 1.99 | 0.70 |
| 1:B:108:ARG:CZ | 1:D:313:PHE:O | 2.37 | 0.70 |
| 1:G:280:ASN:O | 1:G:281:LEU:HB3 | 1.91 | 0.70 |
| 1:K:282:TYR:CA | 1:K:381:THR:CB | 2.51 | 0.70 |
| 1:F:311:ALA:CB | 2:M:23:THR:HG21 | 2.20 | 0.70 |
| 1:J:384:THR:HG21 | 2:M:62:ALA:N | 2.06 | 0.70 |
| 1:B:354:GLN:HB2 | 1:B:357:ASN:HD21 | 1.54 | 0.70 |
| 1:H:4:VAL:N | 1:I:239:GLN:NE2 | 2.39 | 0.70 |
| 1:L:279:ALA:HA | 3:N:43:LEU:CD1 | 2.19 | 0.70 |
| 3:N:65:ASN:HB2 | 3:N:69:PHE:O | 1.92 | 0.70 |
| 1:H:280:ASN:O | 1:H:281:LEU:HB3 | 1.91 | 0.70 |
| 1:H:384:THR:CA | 1:H:387:VAL:HG12 | 2.21 | 0.70 |
| 1:I:354:GLN:HB2 | 1:I:357:ASN:HD21 | 1.56 | 0.70 |
| 3:N:112:VAL:CG2 | 3:N:113:PRO:N | 2.54 | 0.70 |
| 3:N:15:TYR:HE2 | 3:N:88:GLY:HA2 | 1.51 | 0.70 |
| 1:L:109:HIS:N | 3:N:89:TYR:OH | 2.24 | 0.70 |
| 4:P:7:LEU:CD1 | 4:P:7:LEU:H | 2.03 | 0.70 |
| 1:L:104:PRO:HB3 | 1:L:188:SER:CB | 2.21 | 0.70 |
| 1:L:279:ALA:CA | 3:N:43:LEU:CD1 | 2.63 | 0.70 |
| 3:N:7:ASN:HB3 | 3:N:8:GLN:HA | 1.74 | 0.70 |
| 1:B:384:THR:HA | 1:B:387:VAL:HG12 | 1.72 | 0.70 |
| 1:E:98:ARG:NH2 | 1:E:111:GLU:OE2 | 2.25 | 0.70 |
| 1:H:16:ARG:O | 1:H:17:ASN:OD1 | 2.09 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:348:LYS:HE3 | 1:L:35:SER:O | 1.92 | 0.70 |
| 3:N:89:TYR:O | 3:N:91:PRO:CD | 2.36 | 0.70 |
| 1:F:354:GLN:CA | 2:M:26:LEU:HD21 | 2.21 | 0.70 |
| 1:F:382:SER:CA | 1:F:383:ARG:N | 2.53 | 0.70 |
| 1:F:392:ILE:HG22 | 1:F:394:THR:O | 1.90 | 0.70 |
| 1:J:34:GLN:C | 1:J:35:SER:N | 2.45 | 0.70 |
| 1:L:104:PRO:HB3 | 1:L:188:SER:OG | 1.88 | 0.70 |
| 1:E:106:ASN:CG | 1:K:62:VAL:HG11 | 2.10 | 0.70 |
| 1:H:392:ILE:HG22 | 1:H:393:SER:H | 0.57 | 0.70 |
| 4:P:12:GLY:O | 4:P:15:VAL:CG1 | 2.40 | 0.70 |
| 1:B:8:THR:CA | 1:B:9:PRO:N | 2.47 | 0.70 |
| 1:G:185:VAL:CG2 | 2:M:4:ASN:CB | 2.67 | 0.70 |
| 1:K:104:PRO:HB2 | 1:K:187:GLN:CB | 2.21 | 0.70 |
| 1:L:75:ALA:CA | 1:L:160:GLY:O | 2.31 | 0.70 |
| 1:L:182:LEU:CG | 1:L:184:ASN:ND2 | 2.55 | 0.70 |
| 1:L:98:ARG:NH2 | 1:L:111:GLU:OE2 | 2.25 | 0.70 |
| 1:A:280:ASN:O | 1:A:281:LEU:HB3 | 1.91 | 0.70 |
| 1:B:108:ARG:NH1 | 1:D:314:SER:HB2 | 1.75 | 0.70 |
| 1:J:80:HIS:HD2 | 1:J:83:GLU:H | 1.39 | 0.70 |
| 1:L:78:ASN:HB2 | 1:L:154:ILE:O | 1.92 | 0.70 |
| 1:D:5:GLN:CD | 1:E:36:TYR:CE2 | 2.65 | 0.69 |
| 1:F:353:LEU:HD22 | 2:M:26:LEU:C | 2.06 | 0.69 |
| 2:M:67:ILE:CG2 | 4:P:41:MET:CE | 2.70 | 0.69 |
| 1:H:7:LEU:CD1 | 1:H:353:LEU:HD22 | 2.22 | 0.69 |
| 3:N:15:TYR:HB2 | 3:N:47:ALA:HB3 | 1.73 | 0.69 |
| 3:N:41:TYR:CA | 3:N:45:TYR:CE2 | 2.49 | 0.69 |
| 1:B:5:GLN:OE1 | 1:B:310:THR:HG23 | 1.83 | 0.69 |
| 1:D:280:ASN:O | 1:D:281:LEU:HB3 | 1.91 | 0.69 |
| 1:H:310:THR:HG22 | 1:H:358:VAL:HG22 | 1.75 | 0.69 |
| 1:I:277:GLN:HB2 | 1:I:394:THR:CB | 2.21 | 0.69 |
| 3:N:60:ILE:HG22 | 3:N:62:ASN:OD1 | 1.91 | 0.69 |
| 3:N:80:ILE:CG1 | 3:N:117:LEU:N | 2.47 | 0.69 |
| 1:C:181:VAL:C | 1:C:182:LEU:HB2 | 2.13 | 0.69 |
| 1:E:381:THR:OG1 | 1:E:382:SER:N | 2.24 | 0.69 |
| 1:E:80:HIS:CD2 | 1:E:83:GLU:H | 2.11 | 0.69 |
| 1:G:239:GLN:CG | 1:I:4:VAL:HA | 1.99 | 0.69 |
| 1:L:29:GLN:O | 1:L:33:GLN:HG3 | 1.90 | 0.69 |
| 1:G:382:SER:OG | 1:G:383:ARG:N | 2.25 | 0.69 |
| 1:L:80:HIS:CD2 | 1:L:83:GLU:H | 2.11 | 0.69 |
| 4:P:19:ILE:O | 4:P:23:PHE:CD1 | 2.45 | 0.69 |
| 1:D:310:THR:HG22 | 1:D:358:VAL:HG22 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:80:HIS:CD2 | 1:K:83:GLU:H | 2.10 | 0.69 |
| 1:B:4:VAL:O | 1:B:313:PHE:CZ | 2.44 | 0.69 |
| 1:G:80:HIS:HD2 | 1:G:83:GLU:H | 1.39 | 0.69 |
| 1:H:354:GLN:HB2 | 1:H:357:ASN:HD21 | 1.56 | 0.69 |
| 1:I:394:THR:O | 1:I:395:THR:O | 2.08 | 0.69 |
| 1:L:52:ARG:NH1 | 3:N:8:GLN:HG2 | 2.08 | 0.69 |
| 4:P:107:LEU:C | 4:P:111:LEU:HD13 | 2.07 | 0.69 |
| 1:K:98:ARG:NH2 | 1:K:111:GLU:OE2 | 2.25 | 0.69 |
| 1:L:35:SER:HB2 | 1:L:36:TYR:N | 2.07 | 0.69 |
| 3:N:81:LYS:CB | 3:N:113:PRO:CB | 2.70 | 0.69 |
| 1:E:188:SER:HA | 1:K:185:VAL:O | 1.93 | 0.69 |
| 1:G:255:SER:OG | 1:G:386:LEU:CD2 | 2.41 | 0.69 |
| 2:M:67:ILE:HG22 | 4:P:41:MET:CE | 2.20 | 0.69 |
| 1:B:254:LEU:O | 1:B:383:ARG:NH1 | 2.26 | 0.69 |
| 1:B:372:ARG:HD3 | 1:D:269:THR:HG21 | 1.73 | 0.69 |
| 1:C:98:ARG:NH2 | 1:C:111:GLU:OE2 | 2.25 | 0.69 |
| 1:D:354:GLN:HB2 | 1:D:357:ASN:HD21 | 1.56 | 0.69 |
| 1:F:80:HIS:CD2 | 1:F:83:GLU:H | 2.11 | 0.69 |
| 1:L:76:ILE:CG2 | 1:L:154:ILE:HD12 | 2.23 | 0.69 |
| 3:N:28:ARG:HH11 | 3:N:37:GLU:HG2 | 1.26 | 0.69 |
| 1:F:98:ARG:NH2 | 1:F:111:GLU:OE2 | 2.25 | 0.69 |
| 1:J:4:VAL:O | 1:J:4:VAL:HG22 | 1.93 | 0.69 |
| 1:B:9:PRO:HG3 | 1:C:34:GLN:CD | 2.12 | 0.68 |
| 1:B:395:THR:HG1 | 1:D:395:THR:N | 1.85 | 0.68 |
| 1:H:7:LEU:O | 1:H:8:THR:CB | 2.40 | 0.68 |
| 1:I:280:ASN:O | 1:I:281:LEU:HB3 | 1.91 | 0.68 |
| 1:I:4:VAL:C | 1:I:4:VAL:N | 2.46 | 0.68 |
| 1:D:382:SER:HG | 1:D:385:GLU:HG3 | 1.55 | 0.68 |
| 1:F:281:LEU:CB | 2:M:29:TYR:HE1 | 2.06 | 0.68 |
| 1:H:9:PRO:CG | 1:I:34:GLN:OE1 | 2.40 | 0.68 |
| 1:A:80:HIS:HD2 | 1:A:83:GLU:H | 1.39 | 0.68 |
| 1:D:384:THR:O | 1:D:387:VAL:HG12 | 1.89 | 0.68 |
| 1:E:187:GLN:C | 1:K:185:VAL:CA | 2.61 | 0.68 |
| 1:E:8:THR:HB | 1:E:11:GLN:CB | 2.18 | 0.68 |
| 1:G:185:VAL:HG21 | 2:M:4:ASN:C | 2.12 | 0.68 |
| 1:I:17:ASN:HB2 | 1:I:20:ALA:CB | 2.18 | 0.68 |
| 1:B:389:ALA:HB1 | 1:D:354:GLN:OE1 | 1.92 | 0.68 |
| 1:C:104:PRO:HB2 | 1:C:188:SER:HB3 | 1.75 | 0.68 |
| 1:D:281:LEU:HD21 | 1:D:385:GLU:CA | 2.24 | 0.68 |
| 1:D:384:THR:HA | 1:D:387:VAL:HG12 | 1.72 | 0.68 |
| 1:D:277:GLN:NE2 | 1:D:394:THR:HG23 | 2.06 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:80:HIS:HD2 | 1:D:83:GLU:H | 1.39 | 0.68 |
| 1:E:381:THR:C | 1:E:382:SER:CA | 2.61 | 0.68 |
| 1:J:354:GLN:HB2 | 1:J:357:ASN:HD21 | 1.56 | 0.68 |
| 1:C:80:HIS:CD2 | 1:C:83:GLU:H | 2.11 | 0.68 |
| 3:N:29:GLY:O | 3:N:30:TYR:CG | 2.46 | 0.68 |
| 3:N:60:ILE:HD13 | 3:N:97:ARG:CZ | 2.23 | 0.68 |
| 1:D:11:GLN:OE1 | 1:D:351:TYR:CE2 | 2.46 | 0.68 |
| 1:G:239:GLN:HG2 | 1:I:4:VAL:N | 2.08 | 0.68 |
| 1:J:280:ASN:O | 1:J:281:LEU:HB3 | 1.91 | 0.68 |
| 1:B:108:ARG:CZ | 1:D:314:SER:N | 2.39 | 0.68 |
| 1:H:257:LEU:HG | 1:H:383:ARG:HG2 | 1.75 | 0.68 |
| 1:F:10:ALA:CB | 2:M:26:LEU:HD23 | 2.24 | 0.68 |
| 1:B:313:PHE:O | 1:I:108:ARG:NE | 2.24 | 0.68 |
| 1:I:80:HIS:HD2 | 1:I:82:THR:H | 1.42 | 0.68 |
| 1:J:251:LEU:HD22 | 1:J:385:GLU:HB3 | 1.75 | 0.68 |
| 3:N:44:THR:O | 3:N:44:THR:HG22 | 1.93 | 0.68 |
| 1:D:106:ASN:OD1 | 1:G:238:ASP:OD2 | 2.12 | 0.68 |
| 1:H:106:ASN:HD22 | 1:H:191:ARG:HH22 | 1.42 | 0.68 |
| 1:J:28:ARG:HH21 | 1:J:253:ASP:CG | 1.96 | 0.68 |
| 1:D:80:HIS:HD2 | 1:D:82:THR:H | 1.42 | 0.67 |
| 1:I:106:ASN:HD22 | 1:I:191:ARG:HH22 | 1.42 | 0.67 |
| 1:L:56:ASP:OD2 | 3:N:11:VAL:CG1 | 2.38 | 0.67 |
| 1:F:10:ALA:HB2 | 2:M:26:LEU:HD22 | 1.73 | 0.67 |
| 1:L:108:ARG:HH12 | 3:N:89:TYR:HA | 1.47 | 0.67 |
| 1:D:185:VAL:CG1 | 1:D:186:PRO:HD3 | 2.06 | 0.67 |
| 1:D:281:LEU:HD22 | 1:D:385:GLU:C | 2.12 | 0.67 |
| 1:H:80:HIS:HD2 | 1:H:83:GLU:H | 1.39 | 0.67 |
| 4:P:12:GLY:C | 4:P:16:LEU:HD13 | 2.11 | 0.67 |
| 1:I:257:LEU:HD12 | 1:I:386:LEU:CD2 | 2.19 | 0.67 |
| 3:N:81:LYS:HB3 | 3:N:113:PRO:HG2 | 0.76 | 0.67 |
| 1:B:310:THR:HG22 | 1:B:358:VAL:HG22 | 1.77 | 0.67 |
| 1:B:358:VAL:N | 1:B:358:VAL:C | 2.47 | 0.67 |
| 1:G:309:ARG:CG | 1:G:313:PHE:O | 2.42 | 0.67 |
| 1:F:312:ASN:O | 2:M:20:PRO:HB2 | 1.95 | 0.67 |
| 1:L:353:LEU:C | 2:M:76:PRO:HD3 | 2.14 | 0.67 |
| 4:P:12:GLY:O | 4:P:16:LEU:HD12 | 1.91 | 0.67 |
| 1:D:24:ASN:CG | 1:D:252:ILE:HB | 2.14 | 0.67 |
| 1:J:184:ASN:HD22 | 1:J:247:TYR:HE1 | 1.31 | 0.67 |
| 1:K:104:PRO:HB3 | 1:K:187:GLN:CB | 2.24 | 0.67 |
| 1:L:353:LEU:CB | 2:M:76:PRO:CG | 2.72 | 0.67 |
| 3:N:27:VAL:O | 3:N:28:ARG:HG3 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:255:SER:HA | 1:A:383:ARG:HD3 | 1.65 | 0.67 |
| 1:C:185:VAL:CG2 | 1:C:247:TYR:HE1 | 2.06 | 0.67 |
| 1:D:395:THR:OG1 | 1:I:394:THR:C | 2.31 | 0.67 |
| 1:G:353:LEU:CD1 | 1:G:353:LEU:H | 2.08 | 0.67 |
| 1:I:17:ASN:HB2 | 1:I:20:ALA:HB2 | 1.72 | 0.67 |
| 3:N:23:GLY:HA3 | 3:N:109:LYS:HD2 | 1.75 | 0.67 |
| 1:A:353:LEU:H | 1:A:353:LEU:CD1 | 2.08 | 0.67 |
| 1:D:372:ARG:NH1 | 1:I:272:VAL:HG22 | 2.02 | 0.67 |
| 1:C:61:ASN:H | 1:I:189:LYS:HE2 | 1.58 | 0.67 |
| 1:K:348:LYS:NZ | 1:L:32:LEU:O | 2.20 | 0.67 |
| 1:A:255:SER:O | 1:A:383:ARG:HB2 | 1.92 | 0.67 |
| 1:D:387:VAL:HG23 | 1:I:6:GLN:NE2 | 2.08 | 0.67 |
| 3:N:32:ASP:OD1 | 3:N:99:LYS:HG2 | 1.94 | 0.67 |
| 1:F:312:ASN:CB | 2:M:20:PRO:HG2 | 2.24 | 0.67 |
| 1:A:80:HIS:HD2 | 1:A:82:THR:H | 1.42 | 0.67 |
| 1:B:108:ARG:NH1 | 1:D:314:SER:HA | 2.08 | 0.67 |
| 1:B:80:HIS:HD2 | 1:B:82:THR:H | 1.42 | 0.67 |
| 1:D:281:LEU:HD22 | 1:D:385:GLU:CA | 2.26 | 0.67 |
| 1:E:80:HIS:HD2 | 1:E:83:GLU:H | 1.43 | 0.67 |
| 1:F:35:SER:CB | 1:F:240:LEU:HD21 | 2.25 | 0.67 |
| 1:J:16:ARG:NE | 1:J:21:MET:HE3 | 2.09 | 0.67 |
| 4:P:96:ILE:CG2 | 4:P:100:LEU:CD1 | 2.45 | 0.67 |
| 1:C:80:HIS:HD2 | 1:C:83:GLU:H | 1.43 | 0.66 |
| 1:I:277:GLN:CG | 1:I:394:THR:CB | 2.65 | 0.66 |
| 1:J:21:MET:HG2 | 1:J:252:ILE:HD13 | 1.77 | 0.66 |
| 1:F:384:THR:C | 2:M:33:GLY:HA3 | 2.14 | 0.66 |
| 1:B:7:LEU:HD13 | 1:B:353:LEU:CD1 | 2.23 | 0.66 |
| 1:E:188:SER:CA | 1:K:185:VAL:O | 2.43 | 0.66 |
| 1:G:185:VAL:HG13 | 1:G:186:PRO:CD | 2.15 | 0.66 |
| 1:G:106:ASN:HD22 | 1:G:191:ARG:HH22 | 1.42 | 0.66 |
| 1:D:106:ASN:HD22 | 1:D:191:ARG:HH22 | 1.42 | 0.66 |
| 1:D:9:PRO:CB | 1:E:34:GLN:HE22 | 2.07 | 0.66 |
| 1:F:351:TYR:CE1 | 2:M:29:TYR:CZ | 2.83 | 0.66 |
| 1:G:15:LEU:HD12 | 1:G:15:LEU:N | 2.10 | 0.66 |
| 1:B:392:ILE:C | 1:B:393:SER:O | 2.34 | 0.66 |
| 1:D:281:LEU:HA | 1:D:385:GLU:OE1 | 1.95 | 0.66 |
| 1:I:11:GLN:OE1 | 1:I:351:TYR:HD2 | 1.77 | 0.66 |
| 1:L:257:LEU:C | 1:L:258:TYR:CA | 2.63 | 0.66 |
| 1:L:38:VAL:HG21 | 1:L:238:ASP:CG | 2.16 | 0.66 |
| 2:M:75:GLN:HB2 | 4:P:51:VAL:H | 1.60 | 0.66 |
| 1:L:263:SER:HB2 | 3:N:40:LYS:HE3 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:61:ASP:CA | 3:N:75:GLU:HB2 | 2.25 | 0.66 |
| 1:C:181:VAL:O | 1:C:182:LEU:HA | 1.95 | 0.66 |
| 1:D:281:LEU:CD1 | 1:D:382:SER:OG | 2.42 | 0.66 |
| 1:H:185:VAL:CG1 | 1:H:186:PRO:CD | 2.74 | 0.66 |
| 1:H:355:TYR:HE1 | 1:H:391:THR:HB | 1.60 | 0.66 |
| 1:C:60:ALA:HA | 1:I:189:LYS:NZ | 2.11 | 0.66 |
| 1:K:24:ASN:HB2 | 1:K:252:ILE:HD12 | 1.77 | 0.66 |
| 3:N:15:TYR:CB | 3:N:47:ALA:HB3 | 2.25 | 0.66 |
| 3:N:64:GLU:HB2 | 3:N:93:LEU:CA | 2.25 | 0.66 |
| 1:J:80:HIS:HD2 | 1:J:82:THR:H | 1.42 | 0.66 |
| 3:N:68:ALA:CA | 3:N:87:GLN:CD | 2.63 | 0.66 |
| 4:P:42:THR:C | 4:P:45:GLN:HG3 | 2.11 | 0.66 |
| 1:E:308:GLN:HE22 | 1:E:345:ASN:HD21 | 1.44 | 0.66 |
| 1:D:108:ARG:HH21 | 1:I:314:SER:N | 1.88 | 0.66 |
| 1:G:105:ASP:N | 2:M:7:PHE:CZ | 2.63 | 0.66 |
| 1:C:308:GLN:HE22 | 1:C:345:ASN:HD21 | 1.44 | 0.66 |
| 1:H:382:SER:HG | 1:H:385:GLU:HG3 | 1.59 | 0.66 |
| 1:H:80:HIS:HD2 | 1:H:82:THR:H | 1.42 | 0.66 |
| 1:I:311:ALA:O | 1:I:312:ASN:HB2 | 1.95 | 0.66 |
| 2:M:45:MET:CG | 2:M:48:LEU:HD11 | 2.01 | 0.66 |
| 3:N:31:PHE:CE1 | 3:N:100:PHE:CD2 | 2.84 | 0.66 |
| 3:N:62:ASN:HD22 | 3:N:95:PRO:CG | 2.08 | 0.66 |
| 3:N:64:GLU:OE1 | 3:N:93:LEU:CD2 | 2.43 | 0.66 |
| 3:N:80:ILE:HG22 | 3:N:115:PHE:O | 1.96 | 0.66 |
| 1:D:185:VAL:CG1 | 1:D:186:PRO:CD | 2.74 | 0.66 |
| 1:H:5:GLN:NE2 | 1:H:316:THR:HG21 | 2.11 | 0.66 |
| 1:J:106:ASN:HD22 | 1:J:191:ARG:HH22 | 1.42 | 0.66 |
| 1:J:383:ARG:O | 2:M:60:TYR:HD1 | 1.77 | 0.66 |
| 1:B:106:ASN:HD22 | 1:B:191:ARG:HH22 | 1.42 | 0.66 |
| 1:E:257:LEU:CG | 1:E:383:ARG:NE | 2.47 | 0.66 |
| 1:G:80:HIS:HD2 | 1:G:82:THR:H | 1.42 | 0.66 |
| 1:I:185:VAL:CG1 | 1:I:186:PRO:CD | 2.74 | 0.66 |
| 1:L:150:ALA:CA | 1:L:151:PRO:N | 2.58 | 0.66 |
| 1:L:104:PRO:CA | 1:L:189:LYS:O | 2.40 | 0.66 |
| 1:D:4:VAL:O | 1:D:313:PHE:CD1 | 2.48 | 0.65 |
| 1:K:101:TYR:CZ | 1:K:190:GLN:CG | 2.77 | 0.65 |
| 3:N:81:LYS:HD2 | 3:N:113:PRO:HB3 | 1.77 | 0.65 |
| 1:A:106:ASN:HD22 | 1:A:191:ARG:HH22 | 1.42 | 0.65 |
| 1:B:185:VAL:CG1 | 1:B:186:PRO:CD | 2.74 | 0.65 |
| 1:B:277:GLN:CB | 1:B:394:THR:CB | 2.70 | 0.65 |
| 1:E:80:HIS:HD2 | 1:E:82:THR:H | 1.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:308:GLN:HE22 | 1:F:345:ASN:HD21 | 1.44 | 0.65 |
| 1:J:385:GLU:O | 1:J:386:LEU:HD12 | 1.95 | 0.65 |
| 1:E:189:LYS:HG2 | 1:K:61:ASN:HB2 | 1.78 | 0.65 |
| 1:L:180:ALA:HB3 | 1:L:254:LEU:CD2 | 2.25 | 0.65 |
| 1:L:104:PRO:CB | 1:L:188:SER:CB | 2.74 | 0.65 |
| 1:L:61:ASN:HD21 | 1:L:189:LYS:HA | 1.59 | 0.65 |
| 2:M:21:THR:HG22 | 2:M:23:THR:N | 2.01 | 0.65 |
| 1:B:277:GLN:CG | 1:B:394:THR:CB | 2.68 | 0.65 |
| 1:F:35:SER:HB3 | 1:F:240:LEU:HD22 | 1.76 | 0.65 |
| 1:K:7:LEU:HA | 1:K:12:GLN:HE21 | 1.60 | 0.65 |
| 1:L:170:LEU:HD13 | 1:L:181:VAL:CG2 | 2.26 | 0.65 |
| 3:N:80:ILE:CG2 | 3:N:116:PHE:C | 2.60 | 0.65 |
| 1:F:80:HIS:HD2 | 1:F:83:GLU:H | 1.43 | 0.65 |
| 3:N:41:TYR:CB | 3:N:45:TYR:HB2 | 2.15 | 0.65 |
| 1:K:80:HIS:HD2 | 1:K:82:THR:H | 1.45 | 0.65 |
| 1:B:80:HIS:HD2 | 1:B:83:GLU:H | 1.39 | 0.65 |
| 1:C:280:ASN:O | 1:C:281:LEU:HB2 | 1.97 | 0.65 |
| 1:C:8:THR:HG22 | 1:C:9:PRO:CG | 2.24 | 0.65 |
| 1:E:187:GLN:O | 1:E:188:SER:O | 2.14 | 0.65 |
| 1:F:186:PRO:CD | 2:M:40:GLN:HG3 | 2.25 | 0.65 |
| 1:F:281:LEU:CA | 2:M:29:TYR:HE1 | 2.08 | 0.65 |
| 1:K:8:THR:N | 1:K:12:GLN:HE21 | 1.95 | 0.65 |
| 1:A:311:ALA:HB1 | 1:K:281:LEU:CD2 | 2.26 | 0.65 |
| 3:N:28:ARG:NH1 | 3:N:37:GLU:CB | 2.55 | 0.65 |
| 1:L:308:GLN:HE22 | 1:L:345:ASN:HD21 | 1.44 | 0.65 |
| 1:L:6:GLN:C | 1:L:7:LEU:HD13 | 2.11 | 0.65 |
| 4:P:107:LEU:O | 4:P:111:LEU:HD12 | 1.85 | 0.65 |
| 1:C:80:HIS:HD2 | 1:C:82:THR:H | 1.45 | 0.65 |
| 1:J:182:LEU:HD11 | 1:J:240:LEU:HD11 | 1.79 | 0.65 |
| 1:L:182:LEU:HD21 | 1:L:184:ASN:ND2 | 2.12 | 0.65 |
| 1:L:37:PRO:HA | 1:L:237:LEU:HA | 1.78 | 0.65 |
| 3:N:80:ILE:HG23 | 3:N:117:LEU:N | 2.12 | 0.65 |
| 1:L:279:ALA:HB1 | 3:N:43:LEU:CD1 | 2.27 | 0.65 |
| 3:N:62:ASN:CG | 3:N:95:PRO:HG2 | 2.16 | 0.65 |
| 1:B:7:LEU:HD13 | 1:B:353:LEU:HD22 | 1.78 | 0.65 |
| 1:E:191:ARG:HE | 1:K:62:VAL:CG2 | 2.10 | 0.65 |
| 1:F:15:LEU:O | 1:F:18:GLN:HB2 | 1.96 | 0.65 |
| 1:K:308:GLN:HE22 | 1:K:345:ASN:HD21 | 1.44 | 0.65 |
| 1:J:9:PRO:CG | 1:K:34:GLN:OE1 | 2.43 | 0.65 |
| 1:L:77:THR:CA | 1:L:158:ALA:O | 2.44 | 0.65 |
| 1:D:187:GLN:HB2 | 2:M:9:TYR:HE1 | 0.52 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:80:ILE:HG22 | 3:N:81:LYS:N | 2.12 | 0.65 |
| 1:J:5:GLN:N | 1:J:313:PHE:CE1 | 2.48 | 0.64 |
| 2:M:2:LEU:HD12 | 2:M:2:LEU:N | 2.12 | 0.64 |
| 1:J:239:GLN:NE2 | 2:M:72:THR:HA | 2.12 | 0.64 |
| 1:G:23:ALA:C | 1:G:24:ASN:N | 2.50 | 0.64 |
| 1:H:148:ILE:HG22 | 1:I:138:PRO:CG | 2.27 | 0.64 |
| 1:J:11:GLN:OE1 | 1:J:353:LEU:CD2 | 2.43 | 0.64 |
| 1:K:104:PRO:C | 1:K:188:SER:OG | 2.36 | 0.64 |
| 3:N:41:TYR:O | 3:N:45:TYR:HB2 | 1.97 | 0.64 |
| 4:P:96:ILE:CG2 | 4:P:100:LEU:HD22 | 2.27 | 0.64 |
| 1:L:36:TYR:HB2 | 1:L:239:GLN:HB2 | 1.80 | 0.64 |
| 1:G:385:GLU:O | 1:G:386:LEU:HD12 | 1.97 | 0.64 |
| 1:I:16:ARG:C | 1:I:18:GLN:N | 2.50 | 0.64 |
| 1:I:4:VAL:N | 1:I:5:GLN:N | 2.45 | 0.64 |
| 1:E:312:ASN:ND2 | 2:M:46:PRO:O | 2.31 | 0.64 |
| 1:J:353:LEU:HB3 | 2:M:55:VAL:HG21 | 1.79 | 0.64 |
| 3:N:37:GLU:C | 3:N:92:LEU:HB2 | 2.18 | 0.64 |
| 1:D:277:GLN:HB2 | 1:D:394:THR:OG1 | 1.96 | 0.64 |
| 1:I:11:GLN:O | 1:I:15:LEU:HD12 | 1.98 | 0.64 |
| 1:I:5:GLN:HG2 | 1:I:310:THR:OG1 | 1.97 | 0.64 |
| 1:J:11:GLN:HB3 | 1:J:15:LEU:HD11 | 1.77 | 0.64 |
| 1:J:63:GLY:HA2 | 1:J:240:LEU:HG | 1.79 | 0.64 |
| 1:I:281:LEU:HD21 | 1:I:385:GLU:C | 2.17 | 0.64 |
| 1:K:191:ARG:CA | 1:K:192:LEU:N | 2.60 | 0.64 |
| 1:L:381:THR:CA | 1:L:382:SER:N | 2.60 | 0.64 |
| 1:L:80:HIS:HD2 | 1:L:82:THR:H | 1.45 | 0.64 |
| 1:L:80:HIS:HD2 | 1:L:83:GLU:H | 1.43 | 0.64 |
| 1:F:353:LEU:CD2 | 2:M:27:LEU:N | 1.99 | 0.64 |
| 1:D:277:GLN:CB | 1:D:394:THR:OG1 | 2.46 | 0.64 |
| 4:P:24:ARG:C | 4:P:27:PRO:HD2 | 2.18 | 0.64 |
| 1:B:7:LEU:CD1 | 1:B:353:LEU:HD22 | 2.28 | 0.64 |
| 1:J:322:LYS:HE2 | 1:K:145:MET:O | 1.98 | 0.64 |
| 1:K:80:HIS:HD2 | 1:K:83:GLU:H | 1.43 | 0.64 |
| 3:N:79:ARG:O | 3:N:117:LEU:O | 2.16 | 0.64 |
| 2:M:67:ILE:HG22 | 2:M:68:GLN:N | 2.12 | 0.64 |
| 2:M:77:LEU:HD12 | 2:M:77:LEU:N | 2.13 | 0.64 |
| 4:P:12:GLY:O | 4:P:15:VAL:HG13 | 1.98 | 0.64 |
| 1:K:182:LEU:HD11 | 1:K:249:LEU:HD13 | 1.80 | 0.64 |
| 3:N:81:LYS:CB | 3:N:113:PRO:HB2 | 2.27 | 0.63 |
| 3:N:43:LEU:N | 3:N:43:LEU:HD12 | 2.14 | 0.63 |
| 4:P:7:LEU:HD12 | 4:P:7:LEU:N | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:96:ILE:HG21 | 4:P:100:LEU:CD2 | 2.28 | 0.63 |
| 1:L:279:ALA:HB1 | 3:N:42:ASP:HB2 | 1.80 | 0.63 |
| 3:N:94:VAL:HG22 | 3:N:103:ARG:HH12 | 1.60 | 0.63 |
| 4:P:100:LEU:HD12 | 4:P:100:LEU:N | 2.13 | 0.63 |
| 1:D:9:PRO:CG | 1:E:34:GLN:HE22 | 2.12 | 0.63 |
| 1:F:80:HIS:HD2 | 1:F:82:THR:H | 1.45 | 0.63 |
| 1:E:191:ARG:NE | 1:K:62:VAL:HG23 | 2.13 | 0.63 |
| 1:D:386:LEU:C | 1:I:312:ASN:CG | 2.47 | 0.63 |
| 1:D:322:LYS:HE2 | 1:E:145:MET:O | 1.97 | 0.63 |
| 1:J:21:MET:HG2 | 1:J:252:ILE:CD1 | 2.28 | 0.63 |
| 3:N:64:GLU:CG | 3:N:93:LEU:HB3 | 2.28 | 0.63 |
| 1:F:353:LEU:HD21 | 2:M:27:LEU:HD13 | 1.81 | 0.63 |
| 1:F:384:THR:O | 2:M:33:GLY:O | 2.17 | 0.63 |
| 1:K:280:ASN:O | 1:K:281:LEU:HB2 | 1.97 | 0.63 |
| 1:J:5:GLN:OE1 | 1:K:36:TYR:CD2 | 2.52 | 0.63 |
| 1:F:239:GLN:HA | 2:M:45:MET:CE | 2.25 | 0.63 |
| 1:F:239:GLN:HG3 | 2:M:45:MET:HG2 | 1.76 | 0.63 |
| 1:G:185:VAL:CG2 | 2:M:4:ASN:O | 2.36 | 0.63 |
| 1:B:272:VAL:CG2 | 1:I:372:ARG:NH1 | 2.62 | 0.63 |
| 1:L:150:ALA:C | 1:L:151:PRO:CA | 2.67 | 0.63 |
| 1:E:187:GLN:HA | 1:K:185:VAL:N | 2.12 | 0.63 |
| 1:L:75:ALA:HB1 | 1:L:159:THR:CG2 | 2.29 | 0.63 |
| 1:E:8:THR:HG21 | 1:E:11:GLN:CB | 2.29 | 0.62 |
| 1:G:239:GLN:HG2 | 1:I:4:VAL:HB | 1.81 | 0.62 |
| 3:N:49:THR:HG23 | 3:N:83:PRO:N | 2.12 | 0.62 |
| 1:A:312:ASN:ND2 | 1:K:381:THR:HG22 | 2.14 | 0.62 |
| 1:C:385:GLU:C | 1:C:386:LEU:HD12 | 2.20 | 0.62 |
| 1:E:8:THR:CG2 | 1:E:11:GLN:CB | 2.76 | 0.62 |
| 1:J:7:LEU:HD12 | 1:J:7:LEU:N | 2.14 | 0.62 |
| 1:L:78:ASN:O | 1:L:156:ALA:C | 2.36 | 0.62 |
| 3:N:57:CYS:SG | 3:N:101:VAL:CG2 | 2.81 | 0.62 |
| 1:B:17:ASN:HB3 | 1:B:20:ALA:CB | 2.25 | 0.62 |
| 1:B:277:GLN:CG | 1:B:394:THR:OG1 | 2.46 | 0.62 |
| 1:E:381:THR:CB | 1:E:382:SER:N | 2.62 | 0.62 |
| 1:I:308:GLN:HE22 | 1:I:345:ASN:ND2 | 1.97 | 0.62 |
| 3:N:69:PHE:H | 3:N:87:GLN:HE21 | 1.47 | 0.62 |
| 1:B:4:VAL:O | 1:B:4:VAL:HG22 | 1.98 | 0.62 |
| 1:D:384:THR:HA | 1:D:387:VAL:HG11 | 1.81 | 0.62 |
| 1:E:14:ALA:O | 1:E:18:GLN:HG3 | 1.99 | 0.62 |
| 1:H:384:THR:HA | 1:H:387:VAL:HG11 | 1.81 | 0.62 |
| 1:F:383:ARG:HG2 | 2:M:31:VAL:HG23 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:311:ALA:O | 1:J:312:ASN:CG | 2.38 | 0.62 |
| 1:L:56:ASP:O | 3:N:7:ASN:ND2 | 2.32 | 0.62 |
| 3:N:79:ARG:NH2 | 3:N:104:HIS:CB | 2.29 | 0.62 |
| 3:N:81:LYS:O | 3:N:115:PHE:O | 2.18 | 0.62 |
| 1:G:106:ASN:HD22 | 1:G:191:ARG:NH2 | 1.98 | 0.62 |
| 1:H:7:LEU:CG | 1:H:353:LEU:HD22 | 2.28 | 0.62 |
| 1:H:381:THR:C | 1:H:382:SER:CA | 2.68 | 0.62 |
| 1:E:51:ASN:O | 1:K:45:GLN:HG3 | 1.99 | 0.62 |
| 1:L:65:VAL:HB | 1:L:181:VAL:HB | 1.80 | 0.62 |
| 1:G:185:VAL:HG23 | 2:M:4:ASN:N | 2.14 | 0.62 |
| 3:N:64:GLU:HB3 | 3:N:93:LEU:HD22 | 1.81 | 0.62 |
| 3:N:62:ASN:CB | 3:N:95:PRO:CD | 2.78 | 0.62 |
| 1:B:11:GLN:O | 1:B:15:LEU:HD12 | 1.98 | 0.62 |
| 1:B:308:GLN:HE22 | 1:B:345:ASN:ND2 | 1.98 | 0.62 |
| 3:N:64:GLU:HB3 | 3:N:93:LEU:CB | 2.10 | 0.62 |
| 1:B:17:ASN:CB | 1:B:20:ALA:CB | 2.77 | 0.62 |
| 1:B:281:LEU:CD2 | 1:B:385:GLU:CB | 2.75 | 0.62 |
| 3:N:14:VAL:CG2 | 3:N:16:ASN:HB2 | 2.29 | 0.62 |
| 3:N:49:THR:HB | 3:N:112:VAL:HG12 | 1.66 | 0.62 |
| 1:G:185:VAL:N | 1:G:186:PRO:CD | 2.63 | 0.62 |
| 1:H:7:LEU:HD12 | 1:H:7:LEU:N | 2.15 | 0.62 |
| 1:L:177:LEU:O | 1:L:178:THR:C | 2.34 | 0.62 |
| 1:L:283:ARG:HH11 | 1:L:382:SER:HB3 | 1.63 | 0.62 |
| 3:N:44:THR:O | 3:N:44:THR:CG2 | 2.47 | 0.62 |
| 3:N:62:ASN:HB3 | 3:N:95:PRO:CD | 2.28 | 0.62 |
| 1:B:7:LEU:N | 1:B:7:LEU:HD12 | 2.15 | 0.62 |
| 1:I:281:LEU:HD21 | 1:I:385:GLU:HB3 | 1.82 | 0.62 |
| 1:I:7:LEU:HD13 | 1:I:353:LEU:CD2 | 2.30 | 0.62 |
| 1:F:351:TYR:OH | 2:M:29:TYR:CZ | 2.25 | 0.62 |
| 1:A:386:LEU:HD12 | 1:A:386:LEU:N | 2.15 | 0.61 |
| 1:B:106:ASN:HD22 | 1:B:191:ARG:NH2 | 1.98 | 0.61 |
| 1:B:387:VAL:HG23 | 1:D:313:PHE:HE1 | 1.64 | 0.61 |
| 1:C:62:VAL:N | 1:C:183:ALA:HB3 | 2.14 | 0.61 |
| 1:D:17:ASN:HB2 | 1:D:20:ALA:HB2 | 1.72 | 0.61 |
| 1:D:308:GLN:HE22 | 1:D:345:ASN:ND2 | 1.98 | 0.61 |
| 1:D:386:LEU:N | 1:D:386:LEU:HD12 | 2.15 | 0.61 |
| 1:D:7:LEU:HD12 | 1:D:7:LEU:N | 2.15 | 0.61 |
| 1:H:281:LEU:HD22 | 1:H:385:GLU:O | 2.00 | 0.61 |
| 1:J:255:SER:CA | 1:J:383:ARG:HD2 | 2.13 | 0.61 |
| 4:P:50:SER:C | 4:P:51:VAL:HG12 | 2.19 | 0.61 |
| 1:D:106:ASN:HD22 | 1:D:191:ARG:NH2 | 1.98 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:104:PRO:C | 2:M:7:PHE:CE2 | 2.73 | 0.61 |
| 1:I:7:LEU:N | 1:I:7:LEU:HD12 | 2.15 | 0.61 |
| 1:J:106:ASN:HD22 | 1:J:191:ARG:NH2 | 1.98 | 0.61 |
| 1:L:76:ILE:O | 1:L:154:ILE:HG21 | 1.99 | 0.61 |
| 2:M:1:ALA:C | 2:M:2:LEU:HD12 | 2.20 | 0.61 |
| 1:B:384:THR:HA | 1:B:387:VAL:HG11 | 1.81 | 0.61 |
| 1:D:5:GLN:NE2 | 1:E:36:TYR:CZ | 2.63 | 0.61 |
| 1:E:257:LEU:HG | 1:E:383:ARG:NE | 2.14 | 0.61 |
| 1:G:309:ARG:CG | 1:G:314:SER:HA | 2.30 | 0.61 |
| 1:I:257:LEU:HB2 | 1:I:381:THR:HG22 | 1.82 | 0.61 |
| 1:C:60:ALA:HA | 1:I:189:LYS:HZ3 | 1.65 | 0.61 |
| 1:F:185:VAL:HG22 | 2:M:38:ILE:CA | 2.29 | 0.61 |
| 1:H:5:GLN:NE2 | 1:H:316:THR:CG2 | 2.63 | 0.61 |
| 1:I:384:THR:HA | 1:I:387:VAL:HG11 | 1.81 | 0.61 |
| 1:K:17:ASN:O | 1:K:20:ALA:CB | 2.48 | 0.61 |
| 1:L:280:ASN:CG | 1:L:352:THR:CB | 2.69 | 0.61 |
| 1:G:239:GLN:CD | 1:I:313:PHE:CZ | 2.68 | 0.61 |
| 1:G:239:GLN:HG3 | 1:I:4:VAL:HA | 1.59 | 0.61 |
| 1:K:184:ASN:H | 1:K:185:VAL:HG22 | 1.63 | 0.61 |
| 3:N:50:GLN:OE1 | 3:N:52:PHE:HZ | 1.84 | 0.61 |
| 1:A:106:ASN:HD22 | 1:A:191:ARG:NH2 | 1.98 | 0.61 |
| 1:A:308:GLN:HE22 | 1:A:345:ASN:ND2 | 1.98 | 0.61 |
| 1:I:277:GLN:CD | 1:I:394:THR:OG1 | 2.31 | 0.61 |
| 1:H:5:GLN:CD | 1:I:36:TYR:CG | 2.74 | 0.61 |
| 1:L:104:PRO:O | 1:L:188:SER:OG | 2.19 | 0.61 |
| 1:F:281:LEU:CG | 2:M:29:TYR:CE1 | 2.83 | 0.61 |
| 1:B:386:LEU:HD12 | 1:B:386:LEU:N | 2.16 | 0.61 |
| 1:D:282:TYR:CD2 | 1:D:381:THR:HB | 2.36 | 0.61 |
| 1:G:309:ARG:HD3 | 1:G:314:SER:HA | 1.83 | 0.61 |
| 1:G:308:GLN:HE22 | 1:G:345:ASN:ND2 | 1.98 | 0.61 |
| 1:I:106:ASN:HD22 | 1:I:191:ARG:NH2 | 1.98 | 0.61 |
| 1:I:311:ALA:O | 1:I:312:ASN:CB | 2.43 | 0.61 |
| 1:D:387:VAL:CG2 | 1:I:6:GLN:OE1 | 2.43 | 0.61 |
| 1:L:76:ILE:CB | 1:L:154:ILE:CD1 | 2.78 | 0.61 |
| 1:A:255:SER:O | 1:A:383:ARG:CD | 2.31 | 0.61 |
| 1:B:311:ALA:HB3 | 1:I:390:GLY:C | 2.16 | 0.61 |
| 1:G:255:SER:CB | 1:G:386:LEU:HG | 2.30 | 0.61 |
| 1:H:25:LEU:O | 1:H:29:GLN:HG3 | 2.01 | 0.61 |
| 1:H:308:GLN:HE22 | 1:H:345:ASN:ND2 | 1.98 | 0.61 |
| 1:J:184:ASN:CG | 1:J:240:LEU:HD12 | 2.21 | 0.61 |
| 1:K:7:LEU:HB3 | 1:K:12:GLN:HE22 | 1.60 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:38:VAL:HB | 1:L:236:TYR:CG | 2.35 | 0.61 |
| 3:N:60:ILE:HD12 | 3:N:97:ARG:CZ | 2.28 | 0.61 |
| 3:N:37:GLU:CB | 3:N:92:LEU:HB2 | 2.31 | 0.61 |
| 1:F:185:VAL:CG2 | 2:M:37:GLY:O | 2.48 | 0.61 |
| 1:F:311:ALA:HB1 | 2:M:21:THR:CG2 | 2.22 | 0.61 |
| 1:H:106:ASN:HD22 | 1:H:191:ARG:NH2 | 1.98 | 0.61 |
| 1:I:25:LEU:O | 1:I:29:GLN:HG3 | 2.01 | 0.61 |
| 1:J:15:LEU:HD12 | 1:J:15:LEU:N | 2.16 | 0.61 |
| 1:J:9:PRO:CG | 1:K:34:GLN:HA | 2.13 | 0.61 |
| 1:A:255:SER:CA | 1:A:383:ARG:NH1 | 2.60 | 0.60 |
| 1:F:15:LEU:HD12 | 1:F:15:LEU:N | 2.16 | 0.60 |
| 1:B:25:LEU:O | 1:B:29:GLN:HG3 | 2.01 | 0.60 |
| 1:J:251:LEU:HD22 | 1:J:385:GLU:CG | 2.30 | 0.60 |
| 4:P:14:LEU:N | 4:P:14:LEU:HD12 | 2.16 | 0.60 |
| 1:D:108:ARG:NH2 | 1:I:313:PHE:C | 2.37 | 0.60 |
| 1:E:108:ARG:CD | 1:J:314:SER:HB2 | 2.29 | 0.60 |
| 1:H:382:SER:O | 1:H:386:LEU:CD1 | 2.49 | 0.60 |
| 1:E:187:GLN:CG | 1:K:184:ASN:O | 2.49 | 0.60 |
| 1:L:65:VAL:HG21 | 1:L:190:GLN:NE2 | 2.16 | 0.60 |
| 1:L:38:VAL:CG2 | 1:L:238:ASP:OD2 | 2.48 | 0.60 |
| 4:P:107:LEU:N | 4:P:107:LEU:HD12 | 2.17 | 0.60 |
| 1:A:15:LEU:HD12 | 1:A:15:LEU:N | 2.17 | 0.60 |
| 1:A:309:ARG:CG | 1:A:310:THR:O | 2.48 | 0.60 |
| 1:C:190:GLN:CA | 1:C:191:ARG:HG3 | 2.30 | 0.60 |
| 1:D:353:LEU:N | 1:D:353:LEU:HD12 | 2.17 | 0.60 |
| 1:D:281:LEU:CA | 1:D:385:GLU:OE1 | 2.44 | 0.60 |
| 1:H:311:ALA:O | 1:H:312:ASN:CB | 2.49 | 0.60 |
| 1:H:386:LEU:N | 1:H:386:LEU:HD12 | 2.16 | 0.60 |
| 1:F:383:ARG:HB3 | 2:M:31:VAL:HG22 | 1.83 | 0.60 |
| 3:N:29:GLY:O | 3:N:30:TYR:CD2 | 2.54 | 0.60 |
| 1:B:353:LEU:HD12 | 1:B:353:LEU:N | 2.17 | 0.60 |
| 1:H:281:LEU:CD2 | 1:H:385:GLU:O | 2.49 | 0.60 |
| 4:P:50:SER:O | 4:P:51:VAL:HG13 | 2.00 | 0.60 |
| 1:B:5:GLN:HG2 | 1:B:310:THR:OG1 | 2.01 | 0.60 |
| 1:C:185:VAL:N | 1:C:186:PRO:CD | 2.62 | 0.60 |
| 1:H:353:LEU:HD12 | 1:H:353:LEU:N | 2.17 | 0.60 |
| 1:J:25:LEU:O | 1:J:29:GLN:HG3 | 2.01 | 0.60 |
| 1:L:279:ALA:CB | 3:N:43:LEU:HD11 | 2.30 | 0.60 |
| 1:L:108:ARG:C | 3:N:89:TYR:OH | 2.40 | 0.60 |
| 1:D:17:ASN:C | 1:D:21:MET:N | 2.36 | 0.60 |
| 1:D:5:GLN:HG2 | 1:D:310:THR:HG21 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:5:GLN:HG2 | 1:I:310:THR:CB | 2.32 | 0.60 |
| 1:J:182:LEU:HB2 | 1:J:254:LEU:HD13 | 1.82 | 0.60 |
| 1:L:104:PRO:CB | 1:L:188:SER:O | 2.42 | 0.60 |
| 1:D:11:GLN:O | 1:D:15:LEU:HD12 | 1.98 | 0.60 |
| 1:B:264:ALA:HB3 | 1:D:272:VAL:CG1 | 2.30 | 0.60 |
| 1:F:353:LEU:CA | 2:M:26:LEU:CB | 2.77 | 0.60 |
| 1:F:382:SER:C | 1:F:383:ARG:N | 2.55 | 0.60 |
| 1:H:381:THR:HA | 1:H:382:SER:N | 2.17 | 0.60 |
| 1:I:386:LEU:HD12 | 1:I:386:LEU:N | 2.16 | 0.60 |
| 4:P:6:LEU:HD12 | 4:P:6:LEU:N | 2.16 | 0.60 |
| 1:B:257:LEU:CD2 | 1:B:383:ARG:HG2 | 2.31 | 0.60 |
| 1:F:16:ARG:C | 1:F:18:GLN:H | 2.05 | 0.60 |
| 1:H:281:LEU:HD21 | 1:H:386:LEU:CA | 2.32 | 0.60 |
| 1:H:7:LEU:HD21 | 1:H:353:LEU:CD2 | 2.15 | 0.60 |
| 1:I:384:THR:CA | 1:I:387:VAL:CG1 | 2.80 | 0.60 |
| 1:B:395:THR:HG21 | 1:I:395:THR:O | 2.01 | 0.60 |
| 1:I:7:LEU:HD13 | 1:I:353:LEU:CD1 | 2.32 | 0.60 |
| 1:J:184:ASN:ND2 | 1:J:247:TYR:CD1 | 2.70 | 0.60 |
| 1:L:15:LEU:HD12 | 1:L:15:LEU:N | 2.16 | 0.60 |
| 3:N:49:THR:CG2 | 3:N:83:PRO:N | 2.63 | 0.60 |
| 4:P:52:THR:O | 4:P:53:LEU:CD1 | 2.42 | 0.60 |
| 1:A:25:LEU:O | 1:A:29:GLN:HG3 | 2.01 | 0.60 |
| 1:E:186:PRO:O | 1:E:187:GLN:HG3 | 2.02 | 0.60 |
| 1:G:309:ARG:HG2 | 1:G:310:THR:O | 2.01 | 0.60 |
| 1:E:15:LEU:HD12 | 1:E:15:LEU:N | 2.17 | 0.59 |
| 1:G:25:LEU:O | 1:G:29:GLN:HG3 | 2.01 | 0.59 |
| 1:I:382:SER:O | 1:I:386:LEU:CD1 | 2.49 | 0.59 |
| 1:I:384:THR:C | 1:I:387:VAL:CG1 | 2.67 | 0.59 |
| 1:J:31:VAL:HG22 | 1:J:241:PRO:HG2 | 1.84 | 0.59 |
| 3:N:39:VAL:HG12 | 3:N:92:LEU:CD1 | 2.32 | 0.59 |
| 4:P:18:LEU:HD12 | 4:P:18:LEU:N | 2.16 | 0.59 |
| 1:B:354:GLN:CD | 1:I:389:ALA:HB1 | 2.21 | 0.59 |
| 1:J:353:LEU:N | 1:J:353:LEU:HD12 | 2.17 | 0.59 |
| 3:N:14:VAL:HG21 | 3:N:16:ASN:HB2 | 1.84 | 0.59 |
| 3:N:94:VAL:HG22 | 3:N:103:ARG:HH11 | 1.56 | 0.59 |
| 4:P:35:TRP:O | 4:P:36:GLU:CB | 2.47 | 0.59 |
| 1:D:15:LEU:N | 1:D:15:LEU:HD12 | 2.17 | 0.59 |
| 1:H:255:SER:O | 1:H:383:ARG:CG | 2.49 | 0.59 |
| 1:L:182:LEU:CG | 1:L:184:ASN:CG | 2.70 | 0.59 |
| 1:F:185:VAL:CB | 2:M:38:ILE:N | 2.65 | 0.59 |
| 3:N:41:TYR:CG | 3:N:45:TYR:CD2 | 2.61 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:102:TYR:CE2 | 3:N:89:TYR:CE2 | 2.90 | 0.59 |
| 3:N:37:GLU:HB3 | 3:N:92:LEU:CD2 | 2.33 | 0.59 |
| 4:P:38:PRO:N | 4:P:39:PRO:HD3 | 2.15 | 0.59 |
| 1:D:20:ALA:C | 1:D:252:ILE:HD11 | 2.23 | 0.59 |
| 1:F:382:SER:C | 1:F:383:ARG:HG3 | 2.22 | 0.59 |
| 1:J:239:GLN:HE22 | 2:M:72:THR:CA | 2.16 | 0.59 |
| 3:N:27:VAL:CG2 | 3:N:27:VAL:CA | 2.77 | 0.59 |
| 3:N:65:ASN:CB | 3:N:69:PHE:O | 2.50 | 0.59 |
| 3:N:62:ASN:HD22 | 3:N:95:PRO:CB | 2.15 | 0.59 |
| 3:N:62:ASN:HD22 | 3:N:95:PRO:HB2 | 1.66 | 0.59 |
| 1:D:255:SER:HA | 1:D:383:ARG:NH1 | 2.16 | 0.59 |
| 1:D:382:SER:O | 1:D:386:LEU:CD1 | 2.49 | 0.59 |
| 1:I:15:LEU:HD12 | 1:I:15:LEU:N | 2.17 | 0.59 |
| 1:L:7:LEU:CB | 1:L:11:GLN:HB2 | 2.24 | 0.59 |
| 4:P:111:LEU:N | 4:P:111:LEU:HD12 | 2.18 | 0.59 |
| 1:B:15:LEU:HD12 | 1:B:15:LEU:N | 2.17 | 0.59 |
| 1:D:388:ASN:OD1 | 1:I:6:GLN:CB | 2.51 | 0.59 |
| 1:H:15:LEU:N | 1:H:15:LEU:HD12 | 2.17 | 0.59 |
| 1:E:281:LEU:HD21 | 1:J:354:GLN:HE22 | 1.68 | 0.59 |
| 1:E:257:LEU:CD1 | 1:E:383:ARG:HE | 2.16 | 0.59 |
| 1:I:80:HIS:CD2 | 1:I:82:THR:H | 2.21 | 0.59 |
| 3:N:60:ILE:HD11 | 3:N:97:ARG:NH1 | 1.92 | 0.59 |
| 1:B:7:LEU:CG | 1:B:353:LEU:HD22 | 2.31 | 0.59 |
| 1:H:279:ALA:CB | 1:H:391:THR:O | 2.51 | 0.59 |
| 1:L:280:ASN:CG | 1:L:352:THR:OG1 | 2.40 | 0.59 |
| 1:L:279:ALA:CB | 3:N:43:LEU:CD1 | 2.81 | 0.59 |
| 2:M:68:GLN:N | 4:P:41:MET:CE | 2.66 | 0.59 |
| 1:C:104:PRO:C | 1:C:188:SER:OG | 2.40 | 0.58 |
| 1:F:247:TYR:CD1 | 1:F:249:LEU:HD21 | 2.38 | 0.58 |
| 1:F:281:LEU:HG | 2:M:29:TYR:HE1 | 1.64 | 0.58 |
| 1:G:23:ALA:O | 1:G:26:GLN:N | 2.36 | 0.58 |
| 1:J:186:PRO:CB | 2:M:66:GLY:HA2 | 2.33 | 0.58 |
| 1:A:80:HIS:CD2 | 1:A:82:THR:H | 2.21 | 0.58 |
| 1:B:382:SER:OG | 1:B:385:GLU:CD | 2.42 | 0.58 |
| 1:B:4:VAL:N | 1:B:5:GLN:N | 2.45 | 0.58 |
| 1:I:353:LEU:N | 1:I:353:LEU:HD12 | 2.17 | 0.58 |
| 3:N:58:ILE:HG22 | 3:N:58:ILE:O | 2.03 | 0.58 |
| 1:B:389:ALA:CA | 1:D:354:GLN:OE1 | 2.51 | 0.58 |
| 1:B:322:LYS:HE2 | 1:C:145:MET:O | 2.03 | 0.58 |
| 1:H:9:PRO:HG3 | 1:I:34:GLN:CD | 2.23 | 0.58 |
| 3:N:59:TYR:CB | 3:N:98:ALA:N | 2.66 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:181:VAL:C | 1:C:182:LEU:CB | 2.71 | 0.58 |
| 1:C:386:LEU:N | 1:C:386:LEU:HD12 | 2.18 | 0.58 |
| 1:B:108:ARG:CD | 1:D:314:SER:HB2 | 2.33 | 0.58 |
| 1:E:187:GLN:CA | 1:K:184:ASN:C | 2.70 | 0.58 |
| 1:E:310:THR:OG1 | 2:M:46:PRO:HB3 | 2.03 | 0.58 |
| 1:G:63:GLY:N | 1:G:184:ASN:HD21 | 1.95 | 0.58 |
| 1:L:78:ASN:HB3 | 1:L:154:ILE:O | 2.03 | 0.58 |
| 3:N:92:LEU:N | 3:N:92:LEU:HD12 | 2.18 | 0.58 |
| 1:B:80:HIS:CD2 | 1:B:82:THR:H | 2.21 | 0.58 |
| 1:D:4:VAL:HG11 | 1:D:313:PHE:HB3 | 1.85 | 0.58 |
| 1:J:309:ARG:CG | 1:J:310:THR:N | 2.65 | 0.58 |
| 1:K:17:ASN:O | 1:K:20:ALA:CA | 2.51 | 0.58 |
| 1:K:7:LEU:N | 1:K:7:LEU:HD12 | 2.18 | 0.58 |
| 1:L:78:ASN:HB3 | 1:L:155:ALA:C | 2.23 | 0.58 |
| 2:M:27:LEU:HD12 | 2:M:27:LEU:N | 2.19 | 0.58 |
| 1:B:389:ALA:HA | 1:D:354:GLN:OE1 | 2.04 | 0.58 |
| 1:D:9:PRO:HG3 | 1:E:34:GLN:HE22 | 1.67 | 0.58 |
| 1:G:80:HIS:CD2 | 1:G:82:THR:H | 2.22 | 0.58 |
| 1:H:382:SER:OG | 1:H:385:GLU:CD | 2.42 | 0.58 |
| 1:J:80:HIS:CD2 | 1:J:82:THR:H | 2.21 | 0.58 |
| 1:L:182:LEU:HG | 1:L:184:ASN:CG | 2.23 | 0.58 |
| 3:N:114:LEU:N | 3:N:114:LEU:HD12 | 2.19 | 0.58 |
| 1:H:80:HIS:CD2 | 1:H:82:THR:H | 2.21 | 0.58 |
| 1:I:382:SER:OG | 1:I:385:GLU:CD | 2.42 | 0.58 |
| 1:J:280:ASN:HD22 | 1:J:355:TYR:H | 1.52 | 0.58 |
| 1:K:104:PRO:CB | 1:K:187:GLN:HB3 | 2.33 | 0.58 |
| 3:N:21:GLY:H | 3:N:46:LEU:HD21 | 1.67 | 0.58 |
| 4:P:21:LEU:N | 4:P:21:LEU:HD12 | 2.17 | 0.58 |
| 1:B:281:LEU:HD21 | 1:B:385:GLU:CB | 2.34 | 0.58 |
| 1:B:311:ALA:O | 1:B:312:ASN:CB | 2.49 | 0.58 |
| 1:C:15:LEU:HD12 | 1:C:15:LEU:N | 2.19 | 0.58 |
| 1:C:43:GLU:HG3 | 1:I:52:ARG:CZ | 2.34 | 0.58 |
| 1:F:16:ARG:C | 1:F:17:ASN:CB | 2.72 | 0.58 |
| 1:G:354:GLN:HB2 | 1:G:357:ASN:CG | 2.24 | 0.58 |
| 1:H:280:ASN:HD22 | 1:H:355:TYR:H | 1.52 | 0.58 |
| 1:C:187:GLN:NE2 | 1:I:187:GLN:CG | 2.47 | 0.58 |
| 1:L:109:HIS:CE1 | 1:L:257:LEU:HD22 | 2.39 | 0.58 |
| 2:M:6:GLN:C | 2:M:8:PRO:HD3 | 2.15 | 0.58 |
| 3:N:93:LEU:N | 3:N:93:LEU:HD12 | 2.19 | 0.58 |
| 1:F:103:ASP:HB2 | 1:F:104:PRO:CD | 2.34 | 0.58 |
| 1:F:353:LEU:CD2 | 2:M:27:LEU:HD13 | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:183:ALA:CA | 1:L:184:ASN:N | 2.67 | 0.58 |
| 1:L:34:GLN:CB | 1:L:241:PRO:HB3 | 2.34 | 0.58 |
| 3:N:31:PHE:CD2 | 3:N:100:PHE:CD1 | 2.67 | 0.58 |
| 1:C:7:LEU:HD12 | 1:C:7:LEU:N | 2.18 | 0.58 |
| 1:G:107:GLN:HG2 | 1:G:383:ARG:HH21 | 1.69 | 0.58 |
| 3:N:68:ALA:HB3 | 3:N:87:GLN:CD | 2.22 | 0.58 |
| 1:B:384:THR:CA | 1:B:387:VAL:CG1 | 2.80 | 0.57 |
| 1:L:265:GLN:CD | 3:N:40:LYS:HZ2 | 2.04 | 0.57 |
| 3:N:46:LEU:HD12 | 3:N:46:LEU:N | 2.17 | 0.57 |
| 4:P:36:GLU:C | 4:P:38:PRO:HD3 | 2.25 | 0.57 |
| 1:D:382:SER:OG | 1:D:385:GLU:CD | 2.42 | 0.57 |
| 1:F:386:LEU:N | 1:F:386:LEU:HD12 | 2.19 | 0.57 |
| 1:K:103:ASP:HB2 | 1:K:104:PRO:CD | 2.34 | 0.57 |
| 1:L:111:GLU:CD | 3:N:89:TYR:HB3 | 2.21 | 0.57 |
| 1:C:103:ASP:HB2 | 1:C:104:PRO:CD | 2.34 | 0.57 |
| 1:J:386:LEU:HD12 | 1:J:386:LEU:N | 2.19 | 0.57 |
| 1:E:189:LYS:CE | 1:K:61:ASN:HB2 | 2.32 | 0.57 |
| 3:N:68:ALA:CB | 3:N:87:GLN:CG | 2.71 | 0.57 |
| 1:B:382:SER:O | 1:B:386:LEU:CD1 | 2.49 | 0.57 |
| 1:G:354:GLN:CD | 1:G:357:ASN:HD21 | 2.08 | 0.57 |
| 1:I:277:GLN:CB | 1:I:394:THR:CB | 2.82 | 0.57 |
| 1:I:280:ASN:HD22 | 1:I:355:TYR:H | 1.51 | 0.57 |
| 3:N:62:ASN:CG | 3:N:95:PRO:O | 2.42 | 0.57 |
| 4:P:37:GLY:N | 4:P:38:PRO:CD | 2.68 | 0.57 |
| 1:B:17:ASN:O | 1:B:21:MET:N | 2.34 | 0.57 |
| 1:B:280:ASN:HD22 | 1:B:355:TYR:H | 1.52 | 0.57 |
| 1:L:103:ASP:HB2 | 1:L:104:PRO:CD | 2.34 | 0.57 |
| 1:B:5:GLN:OE1 | 1:B:310:THR:HG21 | 1.95 | 0.57 |
| 1:E:8:THR:HG21 | 1:E:11:GLN:HG3 | 0.69 | 0.57 |
| 1:F:247:TYR:HD1 | 1:F:249:LEU:HD21 | 1.69 | 0.57 |
| 1:A:269:THR:HG22 | 1:K:263:SER:HB2 | 1.86 | 0.57 |
| 1:K:308:GLN:HE22 | 1:K:345:ASN:ND2 | 2.03 | 0.57 |
| 2:M:3:ILE:HA | 2:M:9:TYR:CD2 | 2.39 | 0.57 |
| 1:D:384:THR:CA | 1:D:387:VAL:CG1 | 2.80 | 0.57 |
| 1:F:35:SER:HB2 | 1:F:240:LEU:CD2 | 2.30 | 0.57 |
| 1:J:313:PHE:HE2 | 1:K:238:ASP:CG | 2.08 | 0.57 |
| 1:L:65:VAL:HG21 | 1:L:190:GLN:HE22 | 1.70 | 0.57 |
| 3:N:52:PHE:HB2 | 3:N:75:GLU:OE2 | 2.04 | 0.57 |
| 1:D:258:TYR:HB2 | 1:D:380:PHE:HE2 | 1.70 | 0.57 |
| 1:B:387:VAL:HG23 | 1:D:313:PHE:CE1 | 2.40 | 0.57 |
| 1:G:185:VAL:N | 1:G:186:PRO:HD2 | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:4:VAL:N | 1:J:313:PHE:HZ | 2.01 | 0.57 |
| 1:L:312:ASN:HB2 | 2:M:73:PHE:CE2 | 2.31 | 0.57 |
| 1:E:103:ASP:HB2 | 1:E:104:PRO:CD | 2.34 | 0.57 |
| 1:J:184:ASN:OD1 | 1:J:240:LEU:CD1 | 2.52 | 0.57 |
| 1:J:384:THR:HB | 2:M:62:ALA:HA | 1.86 | 0.57 |
| 1:E:187:GLN:NE2 | 1:K:247:TYR:OH | 2.37 | 0.57 |
| 1:L:182:LEU:CD2 | 1:L:184:ASN:HD21 | 2.18 | 0.57 |
| 1:F:239:GLN:NE2 | 2:M:45:MET:HG2 | 2.18 | 0.57 |
| 3:N:57:CYS:CB | 3:N:101:VAL:HG23 | 2.34 | 0.57 |
| 4:P:12:GLY:O | 4:P:15:VAL:HG12 | 2.03 | 0.57 |
| 1:G:182:LEU:HD23 | 2:M:4:ASN:HB3 | 1.84 | 0.57 |
| 1:A:354:GLN:CD | 1:A:357:ASN:HD21 | 2.08 | 0.56 |
| 1:B:17:ASN:N | 1:B:18:GLN:N | 2.53 | 0.56 |
| 1:E:280:ASN:O | 1:E:281:LEU:HB2 | 2.04 | 0.56 |
| 1:E:7:LEU:N | 1:E:7:LEU:HD12 | 2.20 | 0.56 |
| 1:F:7:LEU:N | 1:F:7:LEU:HD12 | 2.21 | 0.56 |
| 1:K:8:THR:O | 1:K:12:GLN:HG3 | 2.05 | 0.56 |
| 1:L:38:VAL:CG2 | 1:L:238:ASP:CG | 2.73 | 0.56 |
| 1:F:383:ARG:HB3 | 2:M:31:VAL:CG2 | 2.35 | 0.56 |
| 1:D:187:GLN:CB | 2:M:9:TYR:CD1 | 2.63 | 0.56 |
| 1:B:17:ASN:C | 1:B:18:GLN:N | 2.59 | 0.56 |
| 1:D:311:ALA:O | 1:D:312:ASN:CB | 2.49 | 0.56 |
| 1:D:391:THR:HG22 | 1:D:392:ILE:N | 2.20 | 0.56 |
| 1:F:281:LEU:CG | 2:M:29:TYR:HE1 | 2.17 | 0.56 |
| 1:J:310:THR:HG22 | 1:J:358:VAL:HG22 | 1.87 | 0.56 |
| 1:K:7:LEU:C | 1:K:12:GLN:NE2 | 2.58 | 0.56 |
| 1:J:9:PRO:CG | 1:K:34:GLN:CD | 2.73 | 0.56 |
| 4:P:10:VAL:HG22 | 4:P:14:LEU:HD11 | 1.87 | 0.56 |
| 4:P:53:LEU:N | 4:P:53:LEU:HD12 | 2.19 | 0.56 |
| 1:D:277:GLN:HG3 | 1:D:394:THR:CG2 | 2.35 | 0.56 |
| 1:K:15:LEU:HD12 | 1:K:15:LEU:N | 2.20 | 0.56 |
| 3:N:68:ALA:CB | 3:N:87:GLN:CD | 2.73 | 0.56 |
| 4:P:16:LEU:HD12 | 4:P:16:LEU:N | 2.20 | 0.56 |
| 4:P:39:PRO:HG2 | 4:P:42:THR:OG1 | 2.06 | 0.56 |
| 1:C:181:VAL:C | 1:C:182:LEU:HA | 2.25 | 0.56 |
| 1:D:277:GLN:H | 1:D:394:THR:HG1 | 1.50 | 0.56 |
| 1:E:308:GLN:HE22 | 1:E:345:ASN:ND2 | 2.03 | 0.56 |
| 1:G:382:SER:C | 1:G:383:ARG:HG3 | 2.25 | 0.56 |
| 1:L:308:GLN:HE22 | 1:L:345:ASN:ND2 | 2.03 | 0.56 |
| 3:N:105:LEU:N | 3:N:105:LEU:HD12 | 2.20 | 0.56 |
| 1:A:354:GLN:HB2 | 1:A:357:ASN:CG | 2.25 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:63:GLY:CA | 1:D:184:ASN:ND2 | 2.68 | 0.56 |
| 1:F:308:GLN:HE22 | 1:F:345:ASN:ND2 | 2.03 | 0.56 |
| 1:H:391:THR:HG22 | 1:H:392:ILE:N | 2.20 | 0.56 |
| 3:N:64:GLU:CG | 3:N:93:LEU:CB | 2.84 | 0.56 |
| 4:P:16:LEU:O | 4:P:20:TRP:CD1 | 2.49 | 0.56 |
| 4:P:96:ILE:HG21 | 4:P:100:LEU:HD22 | 1.87 | 0.56 |
| 1:I:391:THR:HG22 | 1:I:392:ILE:N | 2.20 | 0.56 |
| 1:J:281:LEU:HD13 | 2:M:58:GLN:HG2 | 1.87 | 0.56 |
| 1:F:383:ARG:CA | 2:M:31:VAL:HG22 | 2.36 | 0.56 |
| 1:F:185:VAL:HG22 | 2:M:37:GLY:O | 2.05 | 0.56 |
| 1:F:280:ASN:O | 1:F:281:LEU:HB2 | 2.04 | 0.56 |
| 1:H:17:ASN:HB3 | 1:H:20:ALA:CB | 2.36 | 0.56 |
| 1:K:348:LYS:NZ | 1:L:35:SER:O | 2.38 | 0.56 |
| 3:N:40:LYS:O | 3:N:45:TYR:CE2 | 2.59 | 0.56 |
| 1:I:6:GLN:C | 1:I:7:LEU:N | 2.59 | 0.56 |
| 1:D:187:GLN:NE2 | 2:M:9:TYR:HA | 2.20 | 0.56 |
| 1:B:392:ILE:CG2 | 1:B:393:SER:N | 2.63 | 0.56 |
| 1:E:311:ALA:O | 1:E:312:ASN:CG | 2.44 | 0.56 |
| 1:F:353:LEU:HD22 | 2:M:27:LEU:CA | 2.24 | 0.56 |
| 3:N:81:LYS:HD3 | 3:N:113:PRO:HG3 | 0.61 | 0.56 |
| 3:N:48:ASP:O | 3:N:86:LYS:HE3 | 2.06 | 0.56 |
| 4:P:37:GLY:N | 4:P:38:PRO:HD3 | 2.20 | 0.56 |
| 1:B:5:GLN:HG2 | 1:B:310:THR:HG21 | 1.75 | 0.56 |
| 1:F:311:ALA:O | 1:F:312:ASN:CG | 2.44 | 0.56 |
| 3:N:25:GLN:CG | 3:N:107:SER:OG | 2.51 | 0.56 |
| 1:G:185:VAL:CG2 | 2:M:4:ASN:CA | 2.84 | 0.56 |
| 1:C:352:THR:O | 1:C:353:LEU:CB | 2.54 | 0.55 |
| 1:D:7:LEU:HD13 | 1:D:353:LEU:CD2 | 2.35 | 0.55 |
| 1:F:247:TYR:OH | 2:M:43:GLN:NE2 | 2.37 | 0.55 |
| 1:L:151:PRO:HD2 | 1:L:162:LEU:CD2 | 2.34 | 0.55 |
| 3:N:57:CYS:SG | 3:N:101:VAL:HA | 2.46 | 0.55 |
| 1:B:358:VAL:HG13 | 1:B:358:VAL:HA | 1.83 | 0.55 |
| 1:J:4:VAL:N | 1:J:313:PHE:CZ | 2.74 | 0.55 |
| 1:E:189:LYS:HZ1 | 1:K:61:ASN:CG | 2.07 | 0.55 |
| 1:L:282:TYR:OH | 3:N:42:ASP:OD2 | 2.23 | 0.55 |
| 1:L:6:GLN:O | 1:L:7:LEU:CG | 2.55 | 0.55 |
| 1:C:15:LEU:HD12 | 1:C:15:LEU:H | 1.72 | 0.55 |
| 1:B:264:ALA:CB | 1:D:272:VAL:HG11 | 2.33 | 0.55 |
| 1:D:9:PRO:CG | 1:E:34:GLN:NE2 | 2.63 | 0.55 |
| 1:D:395:THR:HA | 1:I:395:THR:C | 2.26 | 0.55 |
| 1:L:104:PRO:HB3 | 1:L:188:SER:CA | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:77:THR:CG2 | 1:L:158:ALA:O | 2.51 | 0.55 |
| 1:L:182:LEU:HD21 | 1:L:184:ASN:OD1 | 2.06 | 0.55 |
| 1:B:391:THR:HG22 | 1:B:392:ILE:N | 2.20 | 0.55 |
| 1:E:352:THR:O | 1:E:353:LEU:HB2 | 2.07 | 0.55 |
| 1:L:59:PRO:HD2 | 1:L:190:GLN:O | 2.06 | 0.55 |
| 2:M:48:LEU:HD12 | 2:M:48:LEU:N | 2.21 | 0.55 |
| 3:N:21:GLY:O | 3:N:46:LEU:HD22 | 2.06 | 0.55 |
| 4:P:14:LEU:HD12 | 4:P:14:LEU:H | 1.72 | 0.55 |
| 4:P:24:ARG:HA | 4:P:27:PRO:HG2 | 1.88 | 0.55 |
| 1:D:311:ALA:O | 1:D:312:ASN:HB2 | 2.07 | 0.55 |
| 1:F:352:THR:O | 1:F:353:LEU:HB2 | 2.07 | 0.55 |
| 1:H:281:LEU:CD2 | 1:H:385:GLU:HB3 | 2.35 | 0.55 |
| 1:I:257:LEU:HD21 | 1:I:383:ARG:HG2 | 1.88 | 0.55 |
| 1:K:80:HIS:CD2 | 1:K:82:THR:H | 2.25 | 0.55 |
| 1:B:41:GLN:HG2 | 1:K:106:ASN:HD21 | 1.72 | 0.55 |
| 1:D:280:ASN:HD22 | 1:D:355:TYR:H | 1.51 | 0.55 |
| 1:F:352:THR:O | 1:F:353:LEU:CB | 2.55 | 0.55 |
| 1:K:8:THR:N | 1:K:12:GLN:NE2 | 2.54 | 0.55 |
| 1:L:34:GLN:HB3 | 1:L:241:PRO:HB3 | 1.89 | 0.55 |
| 3:N:37:GLU:HB3 | 3:N:92:LEU:CB | 2.36 | 0.55 |
| 1:B:6:GLN:C | 1:B:7:LEU:N | 2.59 | 0.55 |
| 1:D:80:HIS:CD2 | 1:D:82:THR:H | 2.22 | 0.55 |
| 1:E:280:ASN:CB | 1:E:352:THR:OG1 | 2.54 | 0.55 |
| 1:E:352:THR:O | 1:E:353:LEU:CB | 2.54 | 0.55 |
| 1:G:35:SER:O | 1:I:348:LYS:HE3 | 2.07 | 0.55 |
| 3:N:50:GLN:OE1 | 3:N:52:PHE:CZ | 2.60 | 0.55 |
| 1:B:311:ALA:O | 1:B:312:ASN:HB2 | 2.07 | 0.55 |
| 1:C:308:GLN:HE22 | 1:C:345:ASN:ND2 | 2.03 | 0.55 |
| 1:E:312:ASN:OD1 | 2:M:47:PHE:CZ | 2.60 | 0.55 |
| 1:G:23:ALA:O | 1:G:24:ASN:C | 2.45 | 0.55 |
| 1:L:352:THR:O | 1:L:353:LEU:HB2 | 2.06 | 0.55 |
| 1:F:383:ARG:CB | 2:M:31:VAL:HG22 | 2.32 | 0.55 |
| 3:N:49:THR:CB | 3:N:83:PRO:HA | 2.32 | 0.55 |
| 1:A:255:SER:CA | 1:A:383:ARG:NE | 2.54 | 0.55 |
| 1:B:272:VAL:HG23 | 1:I:372:ARG:NH1 | 2.22 | 0.55 |
| 1:C:181:VAL:O | 1:C:182:LEU:CA | 2.54 | 0.55 |
| 1:F:10:ALA:CB | 2:M:26:LEU:CD2 | 2.78 | 0.55 |
| 1:K:283:ARG:HD3 | 1:K:381:THR:HA | 1.89 | 0.55 |
| 1:L:352:THR:O | 1:L:353:LEU:CB | 2.54 | 0.55 |
| 3:N:117:LEU:HD12 | 3:N:117:LEU:N | 2.22 | 0.55 |
| 1:A:387:VAL:HG22 | 1:A:388:ASN:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:352:THR:O | 1:C:353:LEU:HB2 | 2.07 | 0.55 |
| 1:F:280:ASN:CB | 1:F:352:THR:OG1 | 2.54 | 0.55 |
| 1:F:356:GLY:CA | 2:M:23:THR:CG2 | 2.78 | 0.55 |
| 1:I:5:GLN:CG | 1:I:310:THR:CG2 | 2.72 | 0.55 |
| 1:J:241:PRO:HB2 | 1:J:248:ILE:HB | 1.89 | 0.55 |
| 1:E:106:ASN:CG | 1:K:62:VAL:HG13 | 2.27 | 0.55 |
| 1:L:102:TYR:CZ | 3:N:13:PRO:HG3 | 2.42 | 0.55 |
| 1:L:278:TYR:O | 1:L:280:ASN:OD1 | 2.24 | 0.55 |
| 1:D:281:LEU:HG | 1:D:381:THR:OG1 | 2.07 | 0.54 |
| 1:L:182:LEU:CD2 | 1:L:184:ASN:ND2 | 2.70 | 0.54 |
| 1:L:85:VAL:O | 1:L:153:THR:HG22 | 2.07 | 0.54 |
| 4:P:52:THR:HG22 | 4:P:53:LEU:N | 2.23 | 0.54 |
| 1:B:15:LEU:O | 1:B:16:ARG:HB2 | 2.08 | 0.54 |
| 1:B:272:VAL:HG21 | 1:I:372:ARG:HH11 | 1.72 | 0.54 |
| 1:K:352:THR:O | 1:K:353:LEU:CB | 2.55 | 0.54 |
| 3:N:80:ILE:HG21 | 3:N:116:PHE:CD2 | 2.40 | 0.54 |
| 1:A:24:ASN:N | 1:A:25:LEU:N | 2.53 | 0.54 |
| 1:C:186:PRO:C | 1:C:187:GLN:HG3 | 2.22 | 0.54 |
| 1:G:239:GLN:CG | 1:I:4:VAL:CB | 2.85 | 0.54 |
| 1:G:386:LEU:HD12 | 1:G:386:LEU:N | 2.23 | 0.54 |
| 1:H:384:THR:CA | 1:H:387:VAL:CG1 | 2.80 | 0.54 |
| 1:B:17:ASN:CA | 1:B:20:ALA:H | 2.21 | 0.54 |
| 1:E:264:ALA:CB | 1:J:272:VAL:CG1 | 2.86 | 0.54 |
| 1:F:35:SER:HB2 | 1:F:240:LEU:HD23 | 1.84 | 0.54 |
| 1:H:311:ALA:O | 1:H:312:ASN:HB2 | 2.07 | 0.54 |
| 1:J:184:ASN:OD1 | 1:J:240:LEU:HD12 | 2.08 | 0.54 |
| 1:F:185:VAL:CB | 2:M:38:ILE:O | 2.55 | 0.54 |
| 1:L:353:LEU:O | 2:M:75:GLN:HB3 | 2.07 | 0.54 |
| 4:P:96:ILE:HG21 | 4:P:100:LEU:CG | 2.36 | 0.54 |
| 1:B:17:ASN:CA | 1:B:18:GLN:N | 2.69 | 0.54 |
| 1:B:189:LYS:NZ | 1:E:60:ALA:HA | 2.22 | 0.54 |
| 1:F:16:ARG:C | 1:F:17:ASN:CA | 2.75 | 0.54 |
| 1:B:272:VAL:HG21 | 1:I:372:ARG:NH1 | 2.22 | 0.54 |
| 1:J:281:LEU:CD1 | 2:M:58:GLN:HG2 | 2.38 | 0.54 |
| 1:J:383:ARG:N | 2:M:60:TYR:CE1 | 2.75 | 0.54 |
| 1:K:352:THR:O | 1:K:353:LEU:HB2 | 2.06 | 0.54 |
| 4:P:106:SER:OG | 4:P:107:LEU:HD12 | 2.07 | 0.54 |
| 1:A:309:ARG:CG | 1:A:313:PHE:O | 2.55 | 0.54 |
| 1:C:15:LEU:CD1 | 1:C:15:LEU:H | 2.21 | 0.54 |
| 1:K:104:PRO:HB2 | 1:K:187:GLN:HB3 | 1.88 | 0.54 |
| 1:L:7:LEU:CB | 1:L:11:GLN:HB3 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:265:GLN:HG2 | 3:N:40:LYS:NZ | 2.14 | 0.54 |
| 3:N:39:VAL:HG12 | 3:N:92:LEU:HD13 | 1.88 | 0.54 |
| 1:I:282:TYR:CE2 | 1:I:386:LEU:HG | 2.43 | 0.54 |
| 1:J:251:LEU:HD22 | 1:J:385:GLU:CB | 2.37 | 0.54 |
| 4:P:12:GLY:HA2 | 4:P:15:VAL:CG1 | 2.37 | 0.54 |
| 1:D:282:TYR:CD2 | 1:D:381:THR:CB | 2.91 | 0.54 |
| 1:F:80:HIS:CD2 | 1:F:82:THR:H | 2.25 | 0.54 |
| 1:H:384:THR:C | 1:H:387:VAL:CG1 | 2.67 | 0.54 |
| 1:K:32:LEU:HD11 | 1:K:175:THR:O | 2.08 | 0.54 |
| 1:K:102:TYR:O | 1:K:190:GLN:CG | 2.56 | 0.54 |
| 3:N:13:PRO:CD | 3:N:68:ALA:HB1 | 2.27 | 0.54 |
| 3:N:82:CYS:SG | 3:N:116:PHE:CZ | 2.92 | 0.54 |
| 1:D:7:LEU:CG | 1:D:353:LEU:HD22 | 2.36 | 0.54 |
| 1:F:25:LEU:O | 1:F:29:GLN:HG3 | 2.08 | 0.54 |
| 1:J:16:ARG:CD | 1:J:21:MET:CE | 2.79 | 0.54 |
| 1:L:35:SER:C | 1:L:36:TYR:N | 2.61 | 0.54 |
| 1:E:186:PRO:O | 1:K:184:ASN:O | 2.25 | 0.53 |
| 1:H:17:ASN:HB3 | 1:H:20:ALA:HB2 | 1.89 | 0.53 |
| 1:I:281:LEU:CG | 1:I:385:GLU:HB3 | 2.35 | 0.53 |
| 1:J:8:THR:HG23 | 1:J:9:PRO:HD3 | 1.79 | 0.53 |
| 1:K:101:TYR:CZ | 1:K:190:GLN:HG2 | 2.41 | 0.53 |
| 1:L:15:LEU:HD12 | 1:L:15:LEU:H | 1.72 | 0.53 |
| 1:A:312:ASN:HD22 | 1:K:381:THR:HG22 | 1.73 | 0.53 |
| 1:D:282:TYR:CZ | 1:D:386:LEU:HG | 2.31 | 0.53 |
| 1:F:281:LEU:HG | 2:M:29:TYR:CD1 | 2.42 | 0.53 |
| 1:I:5:GLN:OE1 | 1:I:310:THR:HG22 | 1.99 | 0.53 |
| 1:A:354:GLN:NE2 | 1:K:386:LEU:O | 2.41 | 0.53 |
| 1:A:255:SER:CA | 1:A:383:ARG:CZ | 2.86 | 0.53 |
| 1:F:353:LEU:CD2 | 2:M:26:LEU:HA | 2.39 | 0.53 |
| 1:I:15:LEU:O | 1:I:16:ARG:HB2 | 2.08 | 0.53 |
| 1:K:8:THR:H | 1:K:12:GLN:HE21 | 1.55 | 0.53 |
| 1:L:77:THR:CB | 1:L:158:ALA:O | 2.56 | 0.53 |
| 4:P:12:GLY:HA2 | 4:P:15:VAL:HG12 | 1.89 | 0.53 |
| 1:D:187:GLN:HA | 1:G:187:GLN:NE2 | 2.13 | 0.53 |
| 1:G:309:ARG:HE | 1:G:314:SER:HA | 1.69 | 0.53 |
| 1:L:7:LEU:HD12 | 1:L:7:LEU:N | 2.21 | 0.53 |
| 1:D:384:THR:C | 1:D:387:VAL:CG1 | 2.67 | 0.53 |
| 1:H:279:ALA:HB2 | 1:H:391:THR:O | 2.08 | 0.53 |
| 1:E:189:LYS:HZ3 | 1:K:61:ASN:HB2 | 1.57 | 0.53 |
| 1:B:41:GLN:CG | 1:K:106:ASN:ND2 | 2.71 | 0.53 |
| 1:C:80:HIS:CD2 | 1:C:82:THR:H | 2.25 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:187:GLN:O | 1:K:186:PRO:CD | 2.54 | 0.53 |
| 1:E:98:ARG:HH12 | 1:J:318:LYS:NZ | 2.06 | 0.53 |
| 1:B:108:ARG:NE | 1:D:313:PHE:O | 2.42 | 0.53 |
| 1:D:258:TYR:HB2 | 1:D:380:PHE:CE2 | 2.43 | 0.53 |
| 1:H:15:LEU:O | 1:H:16:ARG:HB2 | 2.08 | 0.53 |
| 1:H:392:ILE:HG22 | 1:H:393:SER:CA | 2.32 | 0.53 |
| 1:J:5:GLN:HE22 | 1:K:38:VAL:HG22 | 1.73 | 0.53 |
| 1:K:25:LEU:O | 1:K:29:GLN:HG3 | 2.08 | 0.53 |
| 1:L:78:ASN:HB3 | 1:L:155:ALA:O | 2.08 | 0.53 |
| 3:N:80:ILE:HG22 | 3:N:81:LYS:H | 1.71 | 0.53 |
| 1:A:280:ASN:HD22 | 1:A:355:TYR:H | 1.57 | 0.53 |
| 1:G:185:VAL:CG1 | 1:G:186:PRO:CD | 2.77 | 0.53 |
| 1:L:311:ALA:O | 1:L:312:ASN:CB | 2.54 | 0.53 |
| 1:B:355:TYR:OH | 1:B:392:ILE:C | 2.47 | 0.53 |
| 1:B:6:GLN:HB2 | 1:I:387:VAL:O | 2.09 | 0.53 |
| 1:E:25:LEU:O | 1:E:29:GLN:HG3 | 2.08 | 0.53 |
| 1:H:355:TYR:HE2 | 1:H:394:THR:CB | 2.21 | 0.53 |
| 1:B:6:GLN:CB | 1:I:388:ASN:HA | 2.31 | 0.53 |
| 1:I:355:TYR:CE2 | 1:I:394:THR:OG1 | 2.48 | 0.53 |
| 1:L:15:LEU:CD1 | 1:L:15:LEU:H | 2.22 | 0.53 |
| 1:L:75:ALA:HB1 | 1:L:159:THR:HG23 | 1.90 | 0.53 |
| 2:M:67:ILE:CG2 | 2:M:68:GLN:N | 2.72 | 0.53 |
| 3:N:49:THR:HG21 | 3:N:83:PRO:CA | 2.30 | 0.53 |
| 1:F:354:GLN:CA | 2:M:26:LEU:CD2 | 2.85 | 0.53 |
| 1:K:282:TYR:CA | 1:K:381:THR:CG2 | 2.86 | 0.53 |
| 2:M:68:GLN:O | 4:P:41:MET:CE | 2.57 | 0.53 |
| 4:P:14:LEU:CD1 | 4:P:14:LEU:H | 2.22 | 0.53 |
| 1:B:358:VAL:HG23 | 1:B:358:VAL:CA | 2.26 | 0.52 |
| 1:C:104:PRO:CG | 1:C:188:SER:O | 2.57 | 0.52 |
| 1:L:8:THR:O | 1:L:12:GLN:HG3 | 2.08 | 0.52 |
| 1:J:386:LEU:HD11 | 2:M:62:ALA:HB3 | 1.88 | 0.52 |
| 3:N:41:TYR:CG | 3:N:45:TYR:CE2 | 2.90 | 0.52 |
| 1:B:277:GLN:CA | 1:B:394:THR:OG1 | 2.50 | 0.52 |
| 1:D:15:LEU:O | 1:D:16:ARG:HB2 | 2.07 | 0.52 |
| 1:E:108:ARG:NH1 | 1:J:314:SER:CA | 2.71 | 0.52 |
| 1:E:8:THR:CG2 | 1:E:11:GLN:N | 2.58 | 0.52 |
| 1:F:15:LEU:O | 1:F:17:ASN:OD1 | 2.26 | 0.52 |
| 1:C:14:ALA:O | 1:C:17:ASN:CG | 2.48 | 0.52 |
| 1:C:184:ASN:OD1 | 1:C:185:VAL:HB | 2.08 | 0.52 |
| 1:C:279:ALA:O | 1:C:280:ASN:O | 2.28 | 0.52 |
| 1:E:80:HIS:CD2 | 1:E:82:THR:H | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:I:17:ASN:C | 1:I:21:MET:N | 2.47 | 0.52 |
| 1:B:6:GLN:HB3 | 1:I:388:ASN:CG | 2.28 | 0.52 |
| 1:J:307:SER:HB2 | 1:J:318:LYS:HA | 1.90 | 0.52 |
| 1:L:25:LEU:O | 1:L:29:GLN:HG3 | 2.08 | 0.52 |
| 1:F:239:GLN:OE1 | 2:M:45:MET:CE | 2.57 | 0.52 |
| 3:N:60:ILE:CB | 3:N:97:ARG:HD2 | 2.39 | 0.52 |
| 1:C:25:LEU:O | 1:C:29:GLN:HG3 | 2.08 | 0.52 |
| 1:L:102:TYR:OH | 3:N:13:PRO:HG3 | 2.10 | 0.52 |
| 1:L:80:HIS:CD2 | 1:L:82:THR:H | 2.25 | 0.52 |
| 3:N:62:ASN:HB2 | 3:N:95:PRO:CG | 2.38 | 0.52 |
| 3:N:80:ILE:CG2 | 3:N:115:PHE:O | 2.54 | 0.52 |
| 1:A:310:THR:OG1 | 1:A:313:PHE:HB2 | 2.09 | 0.52 |
| 1:E:312:ASN:HB2 | 2:M:46:PRO:HA | 1.90 | 0.52 |
| 1:D:307:SER:OG | 1:D:315:ASP:HB3 | 2.10 | 0.52 |
| 1:E:182:LEU:HG | 1:E:184:ASN:N | 2.25 | 0.52 |
| 1:H:316:THR:HB | 1:I:36:TYR:HE2 | 1.75 | 0.52 |
| 1:I:305:TYR:CZ | 1:I:318:LYS:HE3 | 2.45 | 0.52 |
| 3:N:71:ILE:HD11 | 3:N:85:GLY:HA3 | 1.92 | 0.52 |
| 1:B:305:TYR:CZ | 1:B:318:LYS:HE3 | 2.45 | 0.52 |
| 1:D:281:LEU:CD2 | 1:D:386:LEU:N | 2.55 | 0.52 |
| 1:I:307:SER:OG | 1:I:315:ASP:HB3 | 2.10 | 0.52 |
| 1:H:319:LEU:HD21 | 1:I:39:ILE:HG23 | 1.92 | 0.52 |
| 3:N:80:ILE:CG2 | 3:N:116:PHE:CG | 2.82 | 0.52 |
| 3:N:80:ILE:HD13 | 3:N:116:PHE:CA | 2.38 | 0.52 |
| 1:H:307:SER:OG | 1:H:315:ASP:HB3 | 2.10 | 0.52 |
| 1:H:148:ILE:HG22 | 1:I:138:PRO:CD | 2.40 | 0.52 |
| 1:E:187:GLN:CA | 1:K:185:VAL:CA | 2.69 | 0.52 |
| 2:M:26:LEU:N | 2:M:26:LEU:HD12 | 2.24 | 0.52 |
| 1:D:305:TYR:CZ | 1:D:318:LYS:HE3 | 2.45 | 0.52 |
| 1:F:280:ASN:HB3 | 1:F:352:THR:OG1 | 2.10 | 0.52 |
| 1:D:187:GLN:O | 1:G:187:GLN:HG3 | 2.07 | 0.52 |
| 1:G:305:TYR:CZ | 1:G:318:LYS:HE3 | 2.45 | 0.52 |
| 1:H:106:ASN:ND2 | 1:H:191:ARG:NH2 | 2.56 | 0.52 |
| 1:K:101:TYR:OH | 1:K:190:GLN:HG2 | 2.07 | 0.52 |
| 1:L:65:VAL:HG21 | 1:L:190:GLN:CD | 2.30 | 0.52 |
| 1:B:255:SER:O | 1:B:383:ARG:HG3 | 2.10 | 0.52 |
| 1:B:313:PHE:HE1 | 1:I:387:VAL:CG2 | 2.20 | 0.52 |
| 1:H:305:TYR:CZ | 1:H:318:LYS:HE3 | 2.45 | 0.52 |
| 1:K:279:ALA:O | 1:K:280:ASN:O | 2.27 | 0.52 |
| 1:K:283:ARG:N | 1:K:381:THR:HG1 | 1.89 | 0.52 |
| 3:N:64:GLU:OE1 | 3:N:93:LEU:CG | 2.58 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:305:TYR:CZ | 1:A:318:LYS:HE3 | 2.45 | 0.51 |
| 1:F:392:ILE:CD1 | 2:M:40:GLN:HA | 2.40 | 0.51 |
| 4:P:12:GLY:CA | 4:P:15:VAL:HG12 | 2.41 | 0.51 |
| 1:B:281:LEU:CD2 | 1:B:385:GLU:O | 2.58 | 0.51 |
| 1:C:14:ALA:C | 1:C:17:ASN:ND2 | 2.63 | 0.51 |
| 1:E:7:LEU:O | 1:E:8:THR:CB | 2.57 | 0.51 |
| 1:H:352:THR:HB | 1:H:357:ASN:HB2 | 1.92 | 0.51 |
| 1:L:312:ASN:OD1 | 2:M:73:PHE:CE2 | 2.56 | 0.51 |
| 1:L:353:LEU:O | 2:M:75:GLN:CB | 2.58 | 0.51 |
| 1:D:264:ALA:HB3 | 1:I:272:VAL:CG1 | 2.39 | 0.51 |
| 1:E:279:ALA:O | 1:E:280:ASN:O | 2.28 | 0.51 |
| 1:E:280:ASN:HB3 | 1:E:352:THR:OG1 | 2.10 | 0.51 |
| 1:J:352:THR:HB | 1:J:357:ASN:HB2 | 1.92 | 0.51 |
| 1:L:38:VAL:HB | 1:L:236:TYR:CD1 | 2.45 | 0.51 |
| 4:P:106:SER:HB2 | 4:P:110:TYR:HE2 | 1.73 | 0.51 |
| 1:C:184:ASN:OD1 | 1:C:185:VAL:CG2 | 2.58 | 0.51 |
| 1:E:264:ALA:HB3 | 1:J:272:VAL:CG1 | 2.41 | 0.51 |
| 1:E:311:ALA:C | 2:M:47:PHE:HE1 | 2.13 | 0.51 |
| 3:N:13:PRO:CD | 3:N:69:PHE:CE1 | 2.93 | 0.51 |
| 1:L:102:TYR:OH | 3:N:68:ALA:HB2 | 2.10 | 0.51 |
| 3:N:79:ARG:C | 3:N:80:ILE:HG13 | 2.30 | 0.51 |
| 3:N:62:ASN:CB | 3:N:95:PRO:HD2 | 2.40 | 0.51 |
| 4:P:52:THR:HG22 | 4:P:53:LEU:H | 1.76 | 0.51 |
| 1:G:255:SER:HB3 | 1:G:386:LEU:HG | 1.93 | 0.51 |
| 1:J:305:TYR:CZ | 1:J:318:LYS:HE3 | 2.45 | 0.51 |
| 1:J:239:GLN:HE22 | 2:M:72:THR:HA | 1.74 | 0.51 |
| 3:N:13:PRO:N | 3:N:69:PHE:HZ | 2.04 | 0.51 |
| 4:P:11:GLY:O | 4:P:15:VAL:HG12 | 2.10 | 0.51 |
| 1:A:307:SER:OG | 1:A:315:ASP:HB3 | 2.10 | 0.51 |
| 1:G:309:ARG:HG3 | 1:G:314:SER:HA | 1.92 | 0.51 |
| 1:D:389:ALA:HB1 | 1:I:354:GLN:HE22 | 1.51 | 0.51 |
| 1:J:5:GLN:NE2 | 1:K:38:VAL:CG2 | 2.69 | 0.51 |
| 3:N:41:TYR:C | 3:N:45:TYR:CD2 | 2.65 | 0.51 |
| 1:A:312:ASN:HD21 | 1:K:281:LEU:CB | 2.14 | 0.51 |
| 1:F:11:GLN:HB3 | 1:F:15:LEU:HD11 | 1.93 | 0.51 |
| 1:K:312:ASN:O | 1:K:313:PHE:HB2 | 2.11 | 0.51 |
| 1:A:62:VAL:HA | 1:A:184:ASN:CG | 2.16 | 0.51 |
| 1:B:307:SER:OG | 1:B:315:ASP:HB3 | 2.10 | 0.51 |
| 1:F:353:LEU:CD2 | 2:M:27:LEU:CD1 | 2.88 | 0.51 |
| 3:N:65:ASN:ND2 | 3:N:85:GLY:C | 2.63 | 0.51 |
| 3:N:62:ASN:HB3 | 3:N:95:PRO:HD2 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:61:ASN:HB3 | 1:C:183:ALA:HB1 | 1.93 | 0.51 |
| 1:I:308:GLN:NE2 | 1:I:345:ASN:HD21 | 2.07 | 0.51 |
| 1:J:186:PRO:HB3 | 2:M:66:GLY:CA | 2.41 | 0.51 |
| 3:N:80:ILE:CB | 3:N:117:LEU:H | 2.24 | 0.51 |
| 3:N:62:ASN:HB2 | 3:N:95:PRO:CD | 2.40 | 0.51 |
| 3:N:49:THR:HG21 | 3:N:82:CYS:C | 2.27 | 0.51 |
| 3:N:64:GLU:HB3 | 3:N:93:LEU:CD2 | 2.40 | 0.51 |
| 1:A:281:LEU:HD11 | 1:A:382:SER:OG | 2.10 | 0.51 |
| 1:A:387:VAL:CG2 | 1:A:388:ASN:N | 2.74 | 0.51 |
| 1:A:49:PRO:HG3 | 1:A:228:ILE:HD12 | 1.93 | 0.51 |
| 1:B:106:ASN:ND2 | 1:B:191:ARG:NH2 | 2.56 | 0.51 |
| 1:F:11:GLN:HA | 1:F:14:ALA:HB3 | 1.92 | 0.51 |
| 1:F:279:ALA:O | 1:F:280:ASN:O | 2.28 | 0.51 |
| 1:J:49:PRO:HG3 | 1:J:228:ILE:HD12 | 1.93 | 0.51 |
| 1:E:108:ARG:HH11 | 1:J:314:SER:HB2 | 1.76 | 0.51 |
| 1:L:177:LEU:O | 1:L:179:GLY:N | 2.44 | 0.51 |
| 1:L:74:ALA:O | 1:L:161:GLU:HA | 2.10 | 0.51 |
| 1:L:353:LEU:HB3 | 2:M:76:PRO:CG | 2.41 | 0.51 |
| 1:H:392:ILE:O | 1:H:393:SER:C | 2.49 | 0.50 |
| 1:L:108:ARG:NH1 | 3:N:89:TYR:C | 2.59 | 0.50 |
| 1:C:186:PRO:C | 1:C:187:GLN:CG | 2.76 | 0.50 |
| 1:C:312:ASN:O | 1:C:313:PHE:HB2 | 2.11 | 0.50 |
| 1:C:64:ILE:HG12 | 1:C:182:LEU:CD1 | 2.40 | 0.50 |
| 1:G:15:LEU:CD1 | 1:G:15:LEU:N | 2.73 | 0.50 |
| 1:G:49:PRO:HG3 | 1:G:228:ILE:HD12 | 1.93 | 0.50 |
| 2:M:18:PRO:O | 2:M:20:PRO:HD3 | 2.11 | 0.50 |
| 2:M:67:ILE:HG23 | 4:P:41:MET:CE | 2.40 | 0.50 |
| 1:C:185:VAL:CG2 | 1:C:247:TYR:CE1 | 2.92 | 0.50 |
| 1:F:311:ALA:HB3 | 2:M:23:THR:CG2 | 2.41 | 0.50 |
| 1:I:352:THR:HB | 1:I:357:ASN:HB2 | 1.92 | 0.50 |
| 4:P:21:LEU:H | 4:P:21:LEU:HD12 | 1.75 | 0.50 |
| 1:C:14:ALA:HA | 1:C:17:ASN:HD21 | 1.70 | 0.50 |
| 1:G:307:SER:OG | 1:G:315:ASP:HB3 | 2.10 | 0.50 |
| 1:H:280:ASN:ND2 | 1:H:355:TYR:HB2 | 2.27 | 0.50 |
| 1:I:13:ALA:O | 1:I:16:ARG:HG2 | 2.12 | 0.50 |
| 1:K:108:ARG:HD2 | 1:K:111:GLU:OE1 | 2.12 | 0.50 |
| 1:D:280:ASN:ND2 | 1:D:355:TYR:HB2 | 2.27 | 0.50 |
| 1:D:352:THR:HB | 1:D:357:ASN:HB2 | 1.92 | 0.50 |
| 1:D:49:PRO:HG3 | 1:D:228:ILE:HD12 | 1.93 | 0.50 |
| 1:D:52:ARG:CZ | 1:G:43:GLU:HG3 | 2.41 | 0.50 |
| 1:F:392:ILE:O | 1:F:393:SER:C | 2.48 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:16:ARG:HH11 | 1:J:21:MET:HE1 | 1.65 | 0.50 |
| 1:J:387:VAL:C | 1:J:388:ASN:OD1 | 2.45 | 0.50 |
| 3:N:79:ARG:NH2 | 3:N:104:HIS:O | 2.45 | 0.50 |
| 3:N:30:TYR:O | 3:N:101:VAL:HG12 | 2.11 | 0.50 |
| 1:A:280:ASN:ND2 | 1:A:355:TYR:HB2 | 2.27 | 0.50 |
| 1:B:189:LYS:HE2 | 1:E:61:ASN:H | 1.77 | 0.50 |
| 1:H:319:LEU:HD21 | 1:I:39:ILE:CG2 | 2.42 | 0.50 |
| 1:F:353:LEU:CD1 | 2:M:27:LEU:O | 2.50 | 0.50 |
| 1:B:49:PRO:HG3 | 1:B:228:ILE:HD12 | 1.94 | 0.50 |
| 1:B:311:ALA:HB2 | 1:I:391:THR:HA | 1.93 | 0.50 |
| 1:C:7:LEU:H | 1:C:7:LEU:HD12 | 1.77 | 0.50 |
| 1:H:63:GLY:CA | 1:H:184:ASN:ND2 | 2.67 | 0.50 |
| 3:N:14:VAL:CG2 | 3:N:16:ASN:CB | 2.89 | 0.50 |
| 1:B:13:ALA:O | 1:B:16:ARG:HG2 | 2.12 | 0.50 |
| 1:F:239:GLN:HG2 | 2:M:45:MET:HG3 | 1.81 | 0.50 |
| 1:G:145:MET:O | 1:I:322:LYS:HE2 | 2.12 | 0.50 |
| 1:G:280:ASN:HD22 | 1:G:355:TYR:H | 1.57 | 0.50 |
| 1:J:180:ALA:O | 1:J:254:LEU:HD23 | 2.12 | 0.50 |
| 1:J:351:TYR:OH | 2:M:58:GLN:NE2 | 2.42 | 0.50 |
| 1:J:9:PRO:HG3 | 1:K:34:GLN:CA | 2.13 | 0.50 |
| 1:F:356:GLY:HA2 | 2:M:23:THR:HG22 | 1.89 | 0.50 |
| 1:F:353:LEU:HB3 | 2:M:26:LEU:HB3 | 1.94 | 0.50 |
| 1:C:185:VAL:HG23 | 1:C:247:TYR:HE1 | 1.75 | 0.50 |
| 1:G:280:ASN:ND2 | 1:G:355:TYR:HB2 | 2.27 | 0.50 |
| 1:H:281:LEU:HD22 | 1:H:385:GLU:C | 2.28 | 0.50 |
| 1:J:7:LEU:HD11 | 1:J:352:THR:O | 2.12 | 0.50 |
| 4:P:37:GLY:CA | 4:P:39:PRO:HD2 | 2.37 | 0.50 |
| 1:B:280:ASN:ND2 | 1:B:355:TYR:HB2 | 2.27 | 0.49 |
| 1:B:389:ALA:CB | 1:D:354:GLN:NE2 | 2.69 | 0.49 |
| 1:I:257:LEU:HG | 1:I:383:ARG:CG | 2.37 | 0.49 |
| 1:I:280:ASN:ND2 | 1:I:355:TYR:HB2 | 2.27 | 0.49 |
| 4:P:21:LEU:H | 4:P:21:LEU:CD1 | 2.25 | 0.49 |
| 1:D:106:ASN:ND2 | 1:D:191:ARG:NH2 | 2.56 | 0.49 |
| 1:D:13:ALA:O | 1:D:16:ARG:HG2 | 2.12 | 0.49 |
| 1:D:386:LEU:O | 1:I:312:ASN:CG | 2.48 | 0.49 |
| 1:H:355:TYR:HE2 | 1:H:394:THR:OG1 | 1.93 | 0.49 |
| 1:J:280:ASN:ND2 | 1:J:355:TYR:HB2 | 2.27 | 0.49 |
| 1:G:185:VAL:CB | 2:M:4:ASN:CB | 2.43 | 0.49 |
| 1:H:14:ALA:O | 1:H:16:ARG:HG3 | 2.13 | 0.49 |
| 1:F:108:ARG:HD2 | 1:F:111:GLU:OE1 | 2.12 | 0.49 |
| 1:G:185:VAL:H | 1:G:186:PRO:HD2 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:307:SER:OG | 1:J:315:ASP:HB3 | 2.12 | 0.49 |
| 3:N:80:ILE:CG2 | 3:N:116:PHE:CD2 | 2.96 | 0.49 |
| 1:B:372:ARG:HH11 | 1:D:272:VAL:HG21 | 1.78 | 0.49 |
| 1:D:14:ALA:O | 1:D:16:ARG:HG3 | 2.13 | 0.49 |
| 1:F:353:LEU:HD12 | 2:M:29:TYR:OH | 2.11 | 0.49 |
| 1:G:103:ASP:HB2 | 1:G:104:PRO:CD | 2.43 | 0.49 |
| 1:L:353:LEU:CG | 2:M:76:PRO:HG3 | 2.42 | 0.49 |
| 4:P:10:VAL:CG2 | 4:P:14:LEU:HD11 | 2.42 | 0.49 |
| 4:P:18:LEU:HD12 | 4:P:18:LEU:H | 1.78 | 0.49 |
| 1:B:187:GLN:CB | 1:E:186:PRO:HA | 2.38 | 0.49 |
| 1:C:64:ILE:HG12 | 1:C:182:LEU:HD13 | 1.95 | 0.49 |
| 1:E:98:ARG:NH1 | 1:J:318:LYS:NZ | 2.61 | 0.49 |
| 1:I:277:GLN:HG3 | 1:I:394:THR:HB | 1.90 | 0.49 |
| 1:E:106:ASN:CB | 1:K:62:VAL:HG13 | 2.42 | 0.49 |
| 1:L:109:HIS:O | 3:N:89:TYR:HE1 | 1.95 | 0.49 |
| 1:B:103:ASP:HB2 | 1:B:104:PRO:CD | 2.43 | 0.49 |
| 1:B:354:GLN:CD | 1:I:389:ALA:CB | 2.79 | 0.49 |
| 1:E:108:ARG:HD2 | 1:E:111:GLU:OE1 | 2.12 | 0.49 |
| 1:G:308:GLN:NE2 | 1:G:345:ASN:HD21 | 2.07 | 0.49 |
| 1:I:49:PRO:HG3 | 1:I:228:ILE:HD12 | 1.93 | 0.49 |
| 3:N:13:PRO:CA | 3:N:69:PHE:CZ | 2.91 | 0.49 |
| 4:P:1:MET:SD | 4:P:3:LYS:HE3 | 2.52 | 0.49 |
| 1:B:14:ALA:O | 1:B:16:ARG:HG3 | 2.13 | 0.49 |
| 1:B:391:THR:HG22 | 1:B:392:ILE:H | 1.77 | 0.49 |
| 1:C:108:ARG:HD2 | 1:C:111:GLU:OE1 | 2.12 | 0.49 |
| 1:H:49:PRO:HG3 | 1:H:228:ILE:HD12 | 1.93 | 0.49 |
| 1:H:391:THR:HG22 | 1:H:392:ILE:H | 1.77 | 0.49 |
| 1:E:189:LYS:CG | 1:K:61:ASN:HB2 | 2.41 | 0.49 |
| 2:M:2:LEU:N | 2:M:2:LEU:CD1 | 2.75 | 0.49 |
| 1:E:312:ASN:ND2 | 2:M:46:PRO:HA | 2.27 | 0.49 |
| 1:A:103:ASP:HB2 | 1:A:104:PRO:CD | 2.43 | 0.49 |
| 1:E:8:THR:CB | 1:E:11:GLN:CB | 2.86 | 0.49 |
| 1:F:392:ILE:O | 1:F:393:SER:O | 2.29 | 0.49 |
| 1:H:103:ASP:HB2 | 1:H:104:PRO:CD | 2.43 | 0.49 |
| 1:K:104:PRO:HA | 1:K:188:SER:OG | 2.12 | 0.49 |
| 1:L:35:SER:C | 1:L:36:TYR:HA | 2.33 | 0.49 |
| 3:N:68:ALA:CA | 3:N:87:GLN:NE2 | 2.61 | 0.49 |
| 1:F:353:LEU:HD12 | 2:M:29:TYR:CE2 | 2.46 | 0.49 |
| 1:H:257:LEU:HD12 | 1:H:386:LEU:HD22 | 1.95 | 0.49 |
| 1:B:354:GLN:NE2 | 1:I:389:ALA:HB1 | 2.24 | 0.49 |
| 1:K:308:GLN:NE2 | 1:K:345:ASN:HD21 | 2.10 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:182:LEU:CD2 | 1:L:184:ASN:OD1 | 2.60 | 0.49 |
| 1:L:76:ILE:HB | 1:L:154:ILE:HD11 | 1.93 | 0.49 |
| 1:D:103:ASP:HB2 | 1:D:104:PRO:CD | 2.43 | 0.48 |
| 1:D:281:LEU:HD11 | 1:D:385:GLU:HB2 | 1.14 | 0.48 |
| 1:D:388:ASN:OD1 | 1:I:6:GLN:HB3 | 2.12 | 0.48 |
| 1:H:308:GLN:NE2 | 1:H:345:ASN:HD21 | 2.07 | 0.48 |
| 1:J:183:ALA:O | 1:J:184:ASN:C | 2.50 | 0.48 |
| 4:P:111:LEU:H | 4:P:111:LEU:HD12 | 1.77 | 0.48 |
| 1:B:372:ARG:NH1 | 1:D:272:VAL:HG21 | 2.28 | 0.48 |
| 1:E:311:ALA:HB1 | 2:M:47:PHE:CE1 | 2.45 | 0.48 |
| 1:I:277:GLN:CB | 1:I:394:THR:HB | 2.43 | 0.48 |
| 1:K:103:ASP:HA | 1:K:190:GLN:CG | 2.26 | 0.48 |
| 1:A:308:GLN:NE2 | 1:A:345:ASN:HD21 | 2.07 | 0.48 |
| 1:B:357:ASN:O | 1:B:358:VAL:CA | 2.61 | 0.48 |
| 1:D:391:THR:HG22 | 1:D:392:ILE:H | 1.77 | 0.48 |
| 3:N:71:ILE:CD1 | 3:N:85:GLY:HA3 | 2.43 | 0.48 |
| 4:P:18:LEU:CD1 | 4:P:18:LEU:H | 2.26 | 0.48 |
| 1:D:11:GLN:CD | 1:D:351:TYR:CE2 | 2.87 | 0.48 |
| 1:G:251:LEU:CD1 | 1:G:388:ASN:CG | 2.70 | 0.48 |
| 1:I:386:LEU:HD12 | 1:I:386:LEU:H | 1.79 | 0.48 |
| 3:N:80:ILE:CG2 | 3:N:81:LYS:N | 2.76 | 0.48 |
| 1:L:52:ARG:CZ | 3:N:8:GLN:HG2 | 2.42 | 0.48 |
| 1:E:107:GLN:HG2 | 1:E:383:ARG:CZ | 2.44 | 0.48 |
| 1:D:187:GLN:HB3 | 1:G:187:GLN:HG3 | 1.95 | 0.48 |
| 1:I:391:THR:HG22 | 1:I:392:ILE:H | 1.77 | 0.48 |
| 3:N:21:GLY:N | 3:N:46:LEU:HD21 | 2.27 | 0.48 |
| 3:N:23:GLY:HA3 | 3:N:109:LYS:CD | 2.40 | 0.48 |
| 1:A:312:ASN:ND2 | 1:K:381:THR:CG2 | 2.76 | 0.48 |
| 1:B:272:VAL:HG23 | 1:I:372:ARG:HH12 | 1.77 | 0.48 |
| 1:E:15:LEU:HD12 | 1:E:15:LEU:H | 1.77 | 0.48 |
| 1:I:103:ASP:HB2 | 1:I:104:PRO:CD | 2.42 | 0.48 |
| 2:M:15:ILE:N | 2:M:16:PRO:HD3 | 2.25 | 0.48 |
| 3:N:92:LEU:O | 3:N:93:LEU:HD12 | 2.14 | 0.48 |
| 4:P:12:GLY:C | 4:P:15:VAL:HG12 | 2.34 | 0.48 |
| 1:H:392:ILE:HG22 | 1:H:393:SER:CB | 2.44 | 0.48 |
| 1:I:120:VAL:HG21 | 1:I:260:LEU:HD13 | 1.96 | 0.48 |
| 1:L:182:LEU:CD1 | 1:L:184:ASN:HD21 | 2.09 | 0.48 |
| 1:C:104:PRO:HB3 | 1:C:188:SER:CA | 2.44 | 0.48 |
| 1:C:186:PRO:O | 1:C:187:GLN:CG | 2.26 | 0.48 |
| 1:E:8:THR:O | 1:E:12:GLN:CG | 2.56 | 0.48 |
| 1:I:14:ALA:O | 1:I:16:ARG:HG3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:76:ILE:HG22 | 1:L:154:ILE:HD12 | 1.96 | 0.48 |
| 1:L:280:ASN:O | 1:L:281:LEU:HD13 | 2.14 | 0.48 |
| 3:N:112:VAL:HG23 | 3:N:113:PRO:HD2 | 0.48 | 0.48 |
| 1:B:102:TYR:CE2 | 1:B:108:ARG:HG3 | 2.49 | 0.48 |
| 1:F:15:LEU:CA | 1:F:17:ASN:OD1 | 2.61 | 0.48 |
| 1:F:353:LEU:HD21 | 2:M:27:LEU:HB2 | 1.95 | 0.48 |
| 1:G:120:VAL:HG21 | 1:G:260:LEU:HD13 | 1.96 | 0.48 |
| 2:M:77:LEU:H | 2:M:77:LEU:HD12 | 1.79 | 0.48 |
| 1:L:102:TYR:HE2 | 3:N:13:PRO:HG3 | 1.77 | 0.48 |
| 3:N:39:VAL:CG1 | 3:N:92:LEU:HD11 | 2.44 | 0.48 |
| 1:L:52:ARG:HH12 | 3:N:8:GLN:HG2 | 1.79 | 0.48 |
| 4:P:100:LEU:CD1 | 4:P:100:LEU:N | 2.76 | 0.48 |
| 1:A:314:SER:OG | 1:A:315:ASP:CA | 2.35 | 0.47 |
| 1:C:184:ASN:N | 1:C:185:VAL:O | 2.47 | 0.47 |
| 1:D:102:TYR:CE2 | 1:D:108:ARG:HG3 | 2.49 | 0.47 |
| 1:E:186:PRO:O | 1:E:187:GLN:CG | 2.62 | 0.47 |
| 1:E:281:LEU:HD12 | 1:E:281:LEU:N | 2.29 | 0.47 |
| 3:N:21:GLY:O | 3:N:46:LEU:CD2 | 2.63 | 0.47 |
| 4:P:26:ARG:N | 4:P:27:PRO:HD2 | 2.30 | 0.47 |
| 1:B:7:LEU:CD1 | 1:B:7:LEU:N | 2.77 | 0.47 |
| 1:C:7:LEU:H | 1:C:7:LEU:CD1 | 2.26 | 0.47 |
| 1:D:387:VAL:HG22 | 1:D:388:ASN:OD1 | 2.15 | 0.47 |
| 1:D:5:GLN:OE1 | 1:E:36:TYR:CZ | 2.67 | 0.47 |
| 1:G:239:GLN:CG | 1:I:4:VAL:HB | 2.44 | 0.47 |
| 1:J:102:TYR:CE2 | 1:J:108:ARG:HG3 | 2.49 | 0.47 |
| 1:J:120:VAL:HG21 | 1:J:260:LEU:HD13 | 1.96 | 0.47 |
| 1:A:309:ARG:HG2 | 1:A:310:THR:N | 2.29 | 0.47 |
| 1:F:239:GLN:OE1 | 2:M:45:MET:HE1 | 2.15 | 0.47 |
| 1:J:16:ARG:HH11 | 1:J:21:MET:CE | 2.21 | 0.47 |
| 1:J:28:ARG:NE | 1:J:253:ASP:OD2 | 2.41 | 0.47 |
| 1:L:102:TYR:CZ | 3:N:89:TYR:CE2 | 3.02 | 0.47 |
| 4:P:52:THR:CA | 4:P:53:LEU:HD12 | 2.38 | 0.47 |
| 1:A:120:VAL:HG21 | 1:A:260:LEU:HD13 | 1.96 | 0.47 |
| 1:B:386:LEU:HD12 | 1:B:386:LEU:H | 1.79 | 0.47 |
| 1:C:281:LEU:HD12 | 1:C:281:LEU:N | 2.29 | 0.47 |
| 1:D:120:VAL:HG21 | 1:D:260:LEU:HD13 | 1.96 | 0.47 |
| 3:N:112:VAL:CG2 | 3:N:113:PRO:CG | 2.82 | 0.47 |
| 1:E:308:GLN:NE2 | 1:E:345:ASN:HD21 | 2.11 | 0.47 |
| 1:F:281:LEU:N | 1:F:281:LEU:HD12 | 2.29 | 0.47 |
| 1:G:239:GLN:CG | 1:I:313:PHE:CZ | 2.96 | 0.47 |
| 1:I:102:TYR:CE2 | 1:I:108:ARG:HG3 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:103:ASP:HB2 | 1:J:104:PRO:CD | 2.43 | 0.47 |
| 1:L:59:PRO:HB2 | 1:L:190:GLN:HB2 | 1.95 | 0.47 |
| 3:N:39:VAL:CG1 | 3:N:92:LEU:CD1 | 2.92 | 0.47 |
| 4:P:107:LEU:CD1 | 4:P:107:LEU:H | 2.27 | 0.47 |
| 1:B:120:VAL:HG21 | 1:B:260:LEU:HD13 | 1.96 | 0.47 |
| 1:C:61:ASN:C | 1:C:183:ALA:CB | 2.83 | 0.47 |
| 1:D:24:ASN:HB2 | 1:D:252:ILE:HG13 | 1.97 | 0.47 |
| 1:G:23:ALA:O | 1:G:25:LEU:N | 2.48 | 0.47 |
| 1:H:102:TYR:CE2 | 1:H:108:ARG:HG3 | 2.49 | 0.47 |
| 1:H:7:LEU:CD1 | 1:H:7:LEU:N | 2.77 | 0.47 |
| 1:I:255:SER:O | 1:I:383:ARG:HG3 | 2.15 | 0.47 |
| 1:I:386:LEU:CD1 | 1:I:386:LEU:H | 2.28 | 0.47 |
| 1:J:182:LEU:HD21 | 1:J:249:LEU:HD11 | 1.93 | 0.47 |
| 1:K:281:LEU:N | 1:K:281:LEU:HD12 | 2.29 | 0.47 |
| 1:L:36:TYR:CB | 1:L:239:GLN:HB2 | 2.44 | 0.47 |
| 1:F:255:SER:CA | 2:M:35:ILE:HD11 | 2.45 | 0.47 |
| 4:P:111:LEU:CD1 | 4:P:111:LEU:H | 2.28 | 0.47 |
| 1:D:386:LEU:H | 1:D:386:LEU:CD1 | 2.28 | 0.47 |
| 1:D:391:THR:OG1 | 1:I:356:GLY:C | 2.45 | 0.47 |
| 1:G:107:GLN:HG2 | 1:G:383:ARG:NH2 | 2.30 | 0.47 |
| 1:I:279:ALA:CB | 1:I:391:THR:O | 2.63 | 0.47 |
| 2:M:77:LEU:CD1 | 2:M:77:LEU:N | 2.77 | 0.47 |
| 3:N:60:ILE:CG2 | 3:N:62:ASN:OD1 | 2.61 | 0.47 |
| 3:N:79:ARG:O | 3:N:80:ILE:HG13 | 2.15 | 0.47 |
| 1:L:102:TYR:CZ | 3:N:89:TYR:HE2 | 2.32 | 0.47 |
| 3:N:59:TYR:CE1 | 3:N:98:ALA:HA | 2.11 | 0.47 |
| 1:A:314:SER:OG | 1:A:315:ASP:CB | 2.62 | 0.47 |
| 1:E:187:GLN:HG2 | 1:K:184:ASN:C | 2.35 | 0.47 |
| 1:G:102:TYR:CE2 | 1:G:108:ARG:HG3 | 2.49 | 0.47 |
| 1:G:316:THR:HG21 | 1:H:36:TYR:CE2 | 2.50 | 0.47 |
| 1:I:7:LEU:CD1 | 1:I:7:LEU:N | 2.77 | 0.47 |
| 1:J:240:LEU:HA | 1:J:240:LEU:HD22 | 1.80 | 0.47 |
| 4:P:6:LEU:N | 4:P:6:LEU:CD1 | 2.78 | 0.47 |
| 1:A:102:TYR:CE2 | 1:A:108:ARG:HG3 | 2.49 | 0.47 |
| 1:B:389:ALA:CB | 1:D:354:GLN:CD | 2.83 | 0.47 |
| 1:E:8:THR:CB | 1:E:11:GLN:CG | 2.92 | 0.47 |
| 1:E:15:LEU:CD1 | 1:E:15:LEU:H | 2.26 | 0.47 |
| 1:E:182:LEU:HG | 1:E:183:ALA:C | 2.35 | 0.47 |
| 1:H:17:ASN:O | 1:H:20:ALA:N | 2.47 | 0.47 |
| 1:H:120:VAL:HG21 | 1:H:260:LEU:HD13 | 1.96 | 0.47 |
| 1:B:311:ALA:HB2 | 1:I:390:GLY:O | 2.06 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:38:VAL:O | 1:L:236:TYR:CA | 2.59 | 0.47 |
| 3:N:30:TYR:O | 3:N:101:VAL:CG1 | 2.63 | 0.47 |
| 1:L:193:LYS:HZ3 | 3:N:68:ALA:HA | 1.80 | 0.47 |
| 1:H:386:LEU:CD1 | 1:H:386:LEU:H | 2.28 | 0.47 |
| 1:J:182:LEU:CD2 | 1:J:249:LEU:CD1 | 2.75 | 0.47 |
| 1:L:281:LEU:N | 1:L:281:LEU:HD12 | 2.29 | 0.47 |
| 2:M:3:ILE:HA | 2:M:9:TYR:CE2 | 2.49 | 0.47 |
| 1:B:63:GLY:CA | 1:B:184:ASN:ND2 | 2.67 | 0.47 |
| 1:D:282:TYR:CD2 | 1:D:381:THR:OG1 | 2.68 | 0.47 |
| 1:D:275:VAL:O | 1:D:394:THR:HG21 | 2.14 | 0.47 |
| 1:F:15:LEU:N | 1:F:15:LEU:CD1 | 2.78 | 0.47 |
| 1:L:15:LEU:CD1 | 1:L:15:LEU:N | 2.78 | 0.47 |
| 1:L:279:ALA:C | 3:N:43:LEU:CD1 | 2.71 | 0.47 |
| 1:L:76:ILE:HB | 1:L:154:ILE:HD12 | 1.91 | 0.47 |
| 4:P:107:LEU:HD12 | 4:P:107:LEU:H | 1.78 | 0.47 |
| 1:A:316:THR:HG21 | 1:B:36:TYR:CE2 | 2.50 | 0.46 |
| 1:E:322:LYS:HE2 | 1:F:145:MET:O | 2.15 | 0.46 |
| 1:F:392:ILE:HD12 | 2:M:40:GLN:HA | 1.97 | 0.46 |
| 1:I:7:LEU:HD22 | 1:I:353:LEU:HD21 | 1.93 | 0.46 |
| 1:L:37:PRO:HA | 1:L:237:LEU:CA | 2.44 | 0.46 |
| 3:N:112:VAL:O | 3:N:114:LEU:HD11 | 2.13 | 0.46 |
| 1:A:63:GLY:N | 1:A:184:ASN:HD21 | 1.95 | 0.46 |
| 1:A:386:LEU:CD1 | 1:A:386:LEU:N | 2.78 | 0.46 |
| 3:N:79:ARG:CZ | 3:N:104:HIS:O | 2.63 | 0.46 |
| 3:N:80:ILE:CG2 | 3:N:117:LEU:N | 2.77 | 0.46 |
| 3:N:80:ILE:HG12 | 3:N:117:LEU:C | 2.32 | 0.46 |
| 3:N:94:VAL:HG22 | 3:N:103:ARG:CZ | 2.37 | 0.46 |
| 1:C:190:GLN:CB | 1:C:191:ARG:HG3 | 2.46 | 0.46 |
| 1:D:187:GLN:CA | 1:G:187:GLN:HE21 | 2.14 | 0.46 |
| 1:I:15:LEU:HD12 | 1:I:15:LEU:H | 1.80 | 0.46 |
| 1:A:310:THR:O | 1:A:311:ALA:C | 2.54 | 0.46 |
| 1:A:255:SER:HB2 | 1:A:383:ARG:HB2 | 1.97 | 0.46 |
| 1:H:387:VAL:HG22 | 1:H:388:ASN:OD1 | 2.14 | 0.46 |
| 1:I:281:LEU:HD13 | 1:I:385:GLU:HB3 | 1.81 | 0.46 |
| 1:L:79:ASN:HA | 1:L:157:GLY:H | 1.80 | 0.46 |
| 1:F:386:LEU:HD12 | 2:M:33:GLY:O | 2.13 | 0.46 |
| 3:N:19:ASP:OD2 | 3:N:110:LYS:HA | 2.15 | 0.46 |
| 4:P:6:LEU:HB3 | 4:P:7:LEU:CD1 | 2.41 | 0.46 |
| 1:B:386:LEU:H | 1:B:386:LEU:CD1 | 2.28 | 0.46 |
| 1:D:59:PRO:HD2 | 1:D:190:GLN:HB2 | 1.98 | 0.46 |
| 1:I:277:GLN:HB2 | 1:I:394:THR:HB | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:43:LEU:N | 3:N:43:LEU:CD1 | 2.77 | 0.46 |
| 1:G:59:PRO:HD2 | 1:G:190:GLN:HB2 | 1.98 | 0.46 |
| 1:H:185:VAL:HG22 | 1:H:185:VAL:O | 2.16 | 0.46 |
| 1:J:184:ASN:HD21 | 1:J:240:LEU:CD1 | 2.12 | 0.46 |
| 1:K:316:THR:HG21 | 1:L:36:TYR:CE2 | 2.51 | 0.46 |
| 1:L:39:ILE:HG23 | 1:L:39:ILE:O | 2.15 | 0.46 |
| 1:E:257:LEU:HD11 | 1:E:383:ARG:HE | 1.81 | 0.46 |
| 1:G:255:SER:HB2 | 2:M:6:GLN:NE2 | 2.31 | 0.46 |
| 1:H:386:LEU:HD12 | 1:H:386:LEU:H | 1.79 | 0.46 |
| 2:M:23:THR:HA | 2:M:25:PRO:HD2 | 1.97 | 0.46 |
| 4:P:96:ILE:HB | 4:P:100:LEU:HB2 | 1.98 | 0.46 |
| 1:D:21:MET:CA | 1:D:252:ILE:CD1 | 2.89 | 0.46 |
| 1:F:184:ASN:O | 1:F:186:PRO:HD3 | 2.16 | 0.46 |
| 1:F:281:LEU:HA | 2:M:29:TYR:CZ | 2.51 | 0.46 |
| 1:H:59:PRO:HD2 | 1:H:190:GLN:HB2 | 1.98 | 0.46 |
| 1:I:185:VAL:H | 1:I:186:PRO:HD2 | 1.49 | 0.46 |
| 1:I:59:PRO:HD2 | 1:I:190:GLN:HB2 | 1.98 | 0.46 |
| 1:K:15:LEU:HD12 | 1:K:15:LEU:H | 1.80 | 0.46 |
| 1:K:322:LYS:HE2 | 1:L:145:MET:O | 2.16 | 0.46 |
| 1:L:308:GLN:NE2 | 1:L:345:ASN:HD21 | 2.11 | 0.46 |
| 4:P:22:TRP:O | 4:P:26:ARG:HG3 | 2.16 | 0.46 |
| 1:B:353:LEU:CD1 | 1:B:353:LEU:N | 2.79 | 0.46 |
| 1:E:108:ARG:HH11 | 1:J:314:SER:CB | 2.29 | 0.46 |
| 1:E:12:GLN:O | 1:E:16:ARG:HG3 | 2.16 | 0.46 |
| 1:F:312:ASN:CG | 2:M:20:PRO:HG2 | 2.36 | 0.46 |
| 1:G:239:GLN:HG2 | 1:I:4:VAL:CB | 2.46 | 0.46 |
| 1:K:282:TYR:CA | 1:K:381:THR:HG21 | 2.38 | 0.46 |
| 1:E:106:ASN:HB2 | 1:K:62:VAL:HG13 | 1.98 | 0.46 |
| 1:L:182:LEU:HD21 | 1:L:184:ASN:CG | 2.36 | 0.46 |
| 1:F:240:LEU:N | 2:M:43:GLN:OE1 | 2.49 | 0.46 |
| 3:N:14:VAL:HG22 | 3:N:16:ASN:HB2 | 1.97 | 0.46 |
| 3:N:15:TYR:CD2 | 3:N:47:ALA:HB2 | 2.50 | 0.46 |
| 3:N:27:VAL:CG2 | 3:N:27:VAL:C | 2.84 | 0.46 |
| 3:N:65:ASN:HD21 | 3:N:71:ILE:CD1 | 2.07 | 0.46 |
| 3:N:71:ILE:HD12 | 3:N:85:GLY:N | 2.31 | 0.46 |
| 4:P:18:LEU:CD1 | 4:P:18:LEU:N | 2.79 | 0.46 |
| 1:A:24:ASN:O | 1:A:26:GLN:N | 2.45 | 0.46 |
| 1:B:59:PRO:HD2 | 1:B:190:GLN:HB2 | 1.98 | 0.46 |
| 1:D:7:LEU:CD1 | 1:D:7:LEU:N | 2.77 | 0.46 |
| 1:G:35:SER:C | 1:G:36:TYR:HA | 2.35 | 0.46 |
| 1:H:353:LEU:N | 1:H:353:LEU:CD1 | 2.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:386:LEU:N | 1:H:386:LEU:CD1 | 2.78 | 0.46 |
| 1:A:14:ALA:O | 1:A:18:GLN:HG3 | 2.15 | 0.45 |
| 1:A:59:PRO:HD2 | 1:A:190:GLN:HB2 | 1.98 | 0.45 |
| 1:B:108:ARG:HH21 | 1:D:313:PHE:C | 2.03 | 0.45 |
| 1:B:7:LEU:HD13 | 1:B:353:LEU:CD2 | 2.44 | 0.45 |
| 1:D:15:LEU:H | 1:D:15:LEU:HD12 | 1.80 | 0.45 |
| 1:D:187:GLN:HG3 | 2:M:9:TYR:CE1 | 2.33 | 0.45 |
| 1:D:7:LEU:CD1 | 1:D:353:LEU:HD13 | 2.30 | 0.45 |
| 1:G:23:ALA:C | 1:G:26:GLN:HB3 | 2.36 | 0.45 |
| 1:J:391:THR:HB | 4:P:41:MET:HE2 | 1.97 | 0.45 |
| 1:J:7:LEU:CD1 | 1:J:7:LEU:N | 2.77 | 0.45 |
| 1:L:12:GLN:O | 1:L:16:ARG:HG3 | 2.16 | 0.45 |
| 2:M:77:LEU:CD1 | 2:M:77:LEU:H | 2.29 | 0.45 |
| 1:B:372:ARG:NH1 | 1:D:272:VAL:CG2 | 2.79 | 0.45 |
| 1:E:15:LEU:O | 1:E:19:GLN:HG3 | 2.16 | 0.45 |
| 1:D:5:GLN:CD | 1:E:36:TYR:CD2 | 2.87 | 0.45 |
| 1:I:257:LEU:HB2 | 1:I:381:THR:CG2 | 2.47 | 0.45 |
| 1:I:353:LEU:N | 1:I:353:LEU:CD1 | 2.79 | 0.45 |
| 1:I:386:LEU:CD1 | 1:I:386:LEU:N | 2.78 | 0.45 |
| 1:J:31:VAL:O | 1:J:35:SER:CB | 2.63 | 0.45 |
| 1:K:34:GLN:O | 1:K:35:SER:N | 2.48 | 0.45 |
| 1:B:386:LEU:N | 1:B:386:LEU:CD1 | 2.78 | 0.45 |
| 1:E:311:ALA:O | 2:M:47:PHE:CD1 | 2.69 | 0.45 |
| 1:I:255:SER:HA | 1:I:383:ARG:HD2 | 1.97 | 0.45 |
| 1:J:15:LEU:CD1 | 1:J:15:LEU:N | 2.78 | 0.45 |
| 1:A:310:THR:HA | 1:A:357:ASN:O | 2.17 | 0.45 |
| 1:B:185:VAL:O | 1:B:185:VAL:HG22 | 2.16 | 0.45 |
| 1:C:8:THR:O | 1:C:12:GLN:HG3 | 2.17 | 0.45 |
| 1:C:8:THR:HG22 | 1:C:9:PRO:N | 2.25 | 0.45 |
| 1:D:386:LEU:H | 1:D:386:LEU:HD12 | 1.79 | 0.45 |
| 1:J:353:LEU:CD1 | 1:J:353:LEU:N | 2.79 | 0.45 |
| 1:J:5:GLN:OE1 | 1:K:36:TYR:HD2 | 1.97 | 0.45 |
| 3:N:101:VAL:CG2 | 3:N:102:ALA:N | 2.80 | 0.45 |
| 3:N:14:VAL:HG22 | 3:N:16:ASN:CB | 2.46 | 0.45 |
| 3:N:80:ILE:CG2 | 3:N:81:LYS:H | 2.30 | 0.45 |
| 1:B:63:GLY:HA2 | 1:B:184:ASN:HD21 | 1.81 | 0.45 |
| 1:D:353:LEU:N | 1:D:353:LEU:CD1 | 2.79 | 0.45 |
| 1:D:386:LEU:N | 1:D:386:LEU:CD1 | 2.78 | 0.45 |
| 1:E:106:ASN:OD1 | 1:K:62:VAL:HG21 | 2.16 | 0.45 |
| 1:L:186:PRO:O | 1:L:187:GLN:CB | 2.54 | 0.45 |
| 1:L:312:ASN:ND2 | 2:M:73:PHE:CD2 | 2.76 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:308:GLN:NE2 | 1:C:345:ASN:HD21 | 2.11 | 0.45 |
| 1:D:83:GLU:HB3 | 1:D:218:ALA:HB3 | 1.99 | 0.45 |
| 1:D:388:ASN:OD1 | 1:I:6:GLN:CD | 2.47 | 0.45 |
| 1:E:15:LEU:CD1 | 1:E:15:LEU:N | 2.80 | 0.45 |
| 1:I:106:ASN:ND2 | 1:I:191:ARG:NH2 | 2.56 | 0.45 |
| 1:I:13:ALA:O | 1:I:16:ARG:CG | 2.65 | 0.45 |
| 1:D:264:ALA:HB3 | 1:I:272:VAL:HG13 | 1.98 | 0.45 |
| 1:J:5:GLN:N | 1:J:313:PHE:HZ | 1.99 | 0.45 |
| 1:K:310:THR:HG22 | 1:K:358:VAL:HG22 | 1.99 | 0.45 |
| 1:L:38:VAL:HG11 | 1:L:236:TYR:CZ | 2.52 | 0.45 |
| 2:M:62:ALA:C | 2:M:63:ILE:HG13 | 2.37 | 0.45 |
| 3:N:37:GLU:HB2 | 3:N:92:LEU:HB2 | 1.90 | 0.45 |
| 1:A:106:ASN:ND2 | 1:A:191:ARG:NH2 | 2.56 | 0.45 |
| 1:B:15:LEU:CD1 | 1:B:15:LEU:H | 2.30 | 0.45 |
| 1:B:15:LEU:H | 1:B:15:LEU:HD12 | 1.80 | 0.45 |
| 1:B:15:LEU:CD1 | 1:B:15:LEU:N | 2.80 | 0.45 |
| 1:E:182:LEU:CD2 | 1:E:184:ASN:OD1 | 2.41 | 0.45 |
| 1:H:15:LEU:CD1 | 1:H:15:LEU:H | 2.30 | 0.45 |
| 1:J:384:THR:CG2 | 2:M:62:ALA:HA | 2.46 | 0.45 |
| 3:N:41:TYR:O | 3:N:45:TYR:HD2 | 2.00 | 0.45 |
| 3:N:46:LEU:CD1 | 3:N:46:LEU:N | 2.79 | 0.45 |
| 1:D:21:MET:N | 1:D:252:ILE:HD11 | 2.31 | 0.45 |
| 1:E:187:GLN:HB3 | 1:E:188:SER:H | 1.13 | 0.45 |
| 1:G:211:LEU:HD21 | 1:G:374:LEU:HD13 | 1.99 | 0.45 |
| 1:J:5:GLN:HE22 | 1:K:38:VAL:HG21 | 1.77 | 0.45 |
| 1:L:76:ILE:CG2 | 1:L:154:ILE:CD1 | 2.94 | 0.45 |
| 1:L:61:ASN:ND2 | 1:L:189:LYS:HA | 2.28 | 0.45 |
| 1:F:351:TYR:HE1 | 2:M:29:TYR:OH | 1.84 | 0.45 |
| 3:N:69:PHE:HB2 | 3:N:85:GLY:O | 2.16 | 0.45 |
| 1:B:13:ALA:O | 1:B:16:ARG:CG | 2.65 | 0.45 |
| 1:B:4:VAL:N | 1:B:5:GLN:H | 2.13 | 0.45 |
| 1:D:185:VAL:HG22 | 1:D:185:VAL:O | 2.16 | 0.45 |
| 1:G:83:GLU:HB3 | 1:G:218:ALA:HB3 | 1.99 | 0.45 |
| 1:I:11:GLN:CD | 1:I:351:TYR:HD2 | 2.21 | 0.45 |
| 4:P:107:LEU:N | 4:P:107:LEU:CD1 | 2.79 | 0.45 |
| 4:P:21:LEU:N | 4:P:21:LEU:CD1 | 2.80 | 0.45 |
| 1:D:15:LEU:CD1 | 1:D:15:LEU:H | 2.30 | 0.45 |
| 1:B:52:ARG:NH2 | 1:E:43:GLU:HG3 | 2.31 | 0.45 |
| 1:H:211:LEU:HD21 | 1:H:374:LEU:HD13 | 1.99 | 0.45 |
| 1:I:185:VAL:O | 1:I:185:VAL:HG22 | 2.16 | 0.45 |
| 1:I:257:LEU:HD23 | 1:I:383:ARG:HG2 | 1.92 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:211:LEU:HD21 | 1:A:374:LEU:HD13 | 1.99 | 0.44 |
| 1:D:211:LEU:HD21 | 1:D:374:LEU:HD13 | 1.99 | 0.44 |
| 1:F:310:THR:HG22 | 1:F:358:VAL:HG22 | 1.99 | 0.44 |
| 1:H:15:LEU:N | 1:H:15:LEU:CD1 | 2.80 | 0.44 |
| 1:H:281:LEU:HD21 | 1:H:386:LEU:HD12 | 1.99 | 0.44 |
| 1:L:310:THR:HG22 | 1:L:358:VAL:HG22 | 1.99 | 0.44 |
| 1:L:35:SER:CB | 1:L:36:TYR:N | 2.78 | 0.44 |
| 4:P:14:LEU:N | 4:P:14:LEU:CD1 | 2.79 | 0.44 |
| 4:P:16:LEU:CD1 | 4:P:16:LEU:H | 2.30 | 0.44 |
| 1:A:255:SER:C | 1:A:383:ARG:NE | 2.69 | 0.44 |
| 1:G:314:SER:C | 1:G:315:ASP:CG | 2.76 | 0.44 |
| 1:H:15:LEU:HD12 | 1:H:15:LEU:H | 1.80 | 0.44 |
| 1:I:15:LEU:CD1 | 1:I:15:LEU:N | 2.80 | 0.44 |
| 1:I:83:GLU:HB3 | 1:I:218:ALA:HB3 | 1.99 | 0.44 |
| 1:J:31:VAL:O | 1:J:35:SER:HB3 | 2.17 | 0.44 |
| 1:J:83:GLU:HB3 | 1:J:218:ALA:HB3 | 1.99 | 0.44 |
| 1:D:255:SER:O | 1:D:383:ARG:HD2 | 2.17 | 0.44 |
| 1:E:310:THR:HG22 | 1:E:358:VAL:HG22 | 1.99 | 0.44 |
| 1:F:239:GLN:CG | 2:M:45:MET:HE1 | 1.97 | 0.44 |
| 1:J:59:PRO:HD2 | 1:J:190:GLN:HB2 | 1.98 | 0.44 |
| 1:K:102:TYR:O | 1:K:190:GLN:HG2 | 2.18 | 0.44 |
| 4:P:16:LEU:H | 4:P:16:LEU:HD12 | 1.81 | 0.44 |
| 1:B:211:LEU:HD21 | 1:B:374:LEU:HD13 | 1.99 | 0.44 |
| 1:B:308:GLN:NE2 | 1:B:345:ASN:HD21 | 2.07 | 0.44 |
| 1:B:384:THR:C | 1:B:387:VAL:CG1 | 2.67 | 0.44 |
| 1:B:7:LEU:HD13 | 1:B:353:LEU:CG | 2.47 | 0.44 |
| 1:C:187:GLN:HG3 | 1:I:187:GLN:HB2 | 1.44 | 0.44 |
| 1:D:277:GLN:HG3 | 1:D:394:THR:HG23 | 1.99 | 0.44 |
| 1:D:4:VAL:CG1 | 1:D:313:PHE:CB | 2.87 | 0.44 |
| 1:B:52:ARG:CZ | 1:E:43:GLU:HG3 | 2.47 | 0.44 |
| 1:G:239:GLN:NE2 | 1:I:4:VAL:HG23 | 2.33 | 0.44 |
| 1:H:5:GLN:OE1 | 1:I:36:TYR:CZ | 2.70 | 0.44 |
| 1:K:280:ASN:CG | 1:K:352:THR:OG1 | 2.56 | 0.44 |
| 1:L:65:VAL:CG2 | 1:L:190:GLN:HE22 | 2.30 | 0.44 |
| 2:M:3:ILE:HA | 2:M:9:TYR:HD2 | 1.81 | 0.44 |
| 1:G:255:SER:CB | 2:M:6:GLN:NE2 | 2.80 | 0.44 |
| 1:D:13:ALA:O | 1:D:16:ARG:CG | 2.65 | 0.44 |
| 1:H:255:SER:HA | 1:H:383:ARG:CZ | 2.48 | 0.44 |
| 1:I:15:LEU:CD1 | 1:I:15:LEU:H | 2.30 | 0.44 |
| 1:J:383:ARG:CB | 1:J:384:THR:N | 2.75 | 0.44 |
| 1:K:15:LEU:CD1 | 1:K:15:LEU:H | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:104:PRO:C | 1:L:188:SER:HG | 2.19 | 0.44 |
| 4:P:4:LYS:HB3 | 4:P:6:LEU:HD13 | 1.99 | 0.44 |
| 1:A:15:LEU:CD1 | 1:A:15:LEU:N | 2.79 | 0.44 |
| 4:P:26:ARG:N | 4:P:27:PRO:CD | 2.80 | 0.44 |
| 1:B:83:GLU:HB3 | 1:B:218:ALA:HB3 | 1.99 | 0.44 |
| 1:D:15:LEU:CD1 | 1:D:15:LEU:N | 2.80 | 0.44 |
| 1:D:254:LEU:O | 1:D:383:ARG:CZ | 2.65 | 0.44 |
| 1:G:61:ASN:HB3 | 1:G:183:ALA:O | 2.18 | 0.44 |
| 1:H:355:TYR:CE2 | 1:H:394:THR:CB | 3.00 | 0.44 |
| 1:H:83:GLU:HB3 | 1:H:218:ALA:HB3 | 1.99 | 0.44 |
| 3:N:50:GLN:HB2 | 3:N:52:PHE:HE1 | 1.83 | 0.44 |
| 3:N:65:ASN:ND2 | 3:N:71:ILE:HB | 2.32 | 0.44 |
| 3:N:63:ALA:HB2 | 3:N:73:VAL:HG21 | 1.79 | 0.44 |
| 3:N:71:ILE:CD1 | 3:N:85:GLY:CA | 2.96 | 0.44 |
| 3:N:37:GLU:HB3 | 3:N:92:LEU:HD23 | 2.00 | 0.44 |
| 4:P:26:ARG:HB2 | 4:P:27:PRO:CD | 2.42 | 0.44 |
| 1:A:61:ASN:HB3 | 1:A:183:ALA:O | 2.18 | 0.44 |
| 1:C:103:ASP:HB2 | 1:C:104:PRO:HD2 | 2.00 | 0.44 |
| 1:G:106:ASN:ND2 | 1:G:191:ARG:NH2 | 2.56 | 0.44 |
| 1:E:187:GLN:CB | 1:K:184:ASN:O | 2.66 | 0.44 |
| 4:P:15:VAL:O | 4:P:19:ILE:HG13 | 2.18 | 0.44 |
| 1:A:83:GLU:HB3 | 1:A:218:ALA:HB3 | 1.99 | 0.44 |
| 1:B:185:VAL:O | 1:B:185:VAL:CG2 | 2.65 | 0.44 |
| 1:B:307:SER:HB2 | 1:B:318:LYS:HA | 2.00 | 0.44 |
| 1:E:151:PRO:HD2 | 1:E:162:LEU:HD22 | 2.00 | 0.44 |
| 2:M:67:ILE:HG23 | 4:P:41:MET:HE3 | 1.98 | 0.44 |
| 3:N:61:ASP:H | 3:N:75:GLU:HB2 | 1.83 | 0.44 |
| 1:A:270:PRO:HD2 | 1:K:264:ALA:O | 2.18 | 0.43 |
| 1:B:277:GLN:HG3 | 1:B:394:THR:HG21 | 1.12 | 0.43 |
| 1:D:61:ASN:HB3 | 1:D:183:ALA:O | 2.18 | 0.43 |
| 1:D:185:VAL:O | 1:D:185:VAL:CG2 | 2.65 | 0.43 |
| 1:E:316:THR:HG21 | 1:F:36:TYR:CE2 | 2.52 | 0.43 |
| 1:F:308:GLN:NE2 | 1:F:345:ASN:HD21 | 2.11 | 0.43 |
| 1:H:148:ILE:HG22 | 1:I:138:PRO:HD2 | 2.00 | 0.43 |
| 1:K:12:GLN:HA | 1:K:15:LEU:HD13 | 1.99 | 0.43 |
| 2:M:4:ASN:O | 2:M:7:PHE:C | 2.54 | 0.43 |
| 3:N:114:LEU:CD1 | 3:N:114:LEU:N | 2.81 | 0.43 |
| 3:N:92:LEU:N | 3:N:92:LEU:CD1 | 2.80 | 0.43 |
| 1:A:381:THR:HG23 | 1:A:382:SER:N | 2.31 | 0.43 |
| 1:D:189:LYS:HE2 | 1:G:61:ASN:H | 1.83 | 0.43 |
| 1:I:211:LEU:HD21 | 1:I:374:LEU:HD13 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:15:ILE:O | 2:M:15:ILE:CG2 | 2.66 | 0.43 |
| 1:C:280:ASN:CG | 1:C:352:THR:OG1 | 2.56 | 0.43 |
| 1:G:247:TYR:OH | 2:M:2:LEU:HD22 | 2.11 | 0.43 |
| 1:H:185:VAL:CG2 | 1:H:185:VAL:O | 2.65 | 0.43 |
| 1:I:279:ALA:HB2 | 1:I:391:THR:O | 2.17 | 0.43 |
| 1:K:188:SER:OG | 1:K:189:LYS:N | 2.44 | 0.43 |
| 1:K:7:LEU:N | 1:K:7:LEU:CD1 | 2.80 | 0.43 |
| 3:N:81:LYS:HB2 | 3:N:113:PRO:CB | 2.32 | 0.43 |
| 1:B:61:ASN:HB3 | 1:B:183:ALA:O | 2.18 | 0.43 |
| 1:C:15:LEU:CD1 | 1:C:15:LEU:N | 2.81 | 0.43 |
| 1:C:310:THR:HG22 | 1:C:358:VAL:HG22 | 1.99 | 0.43 |
| 1:I:260:LEU:HA | 1:I:377:TYR:O | 2.19 | 0.43 |
| 1:K:282:TYR:CA | 1:K:381:THR:HG1 | 2.19 | 0.43 |
| 2:M:27:LEU:CD1 | 2:M:27:LEU:N | 2.81 | 0.43 |
| 3:N:105:LEU:N | 3:N:105:LEU:CD1 | 2.81 | 0.43 |
| 1:A:307:SER:HB2 | 1:A:318:LYS:HA | 2.00 | 0.43 |
| 1:C:43:GLU:HG3 | 1:I:52:ARG:NH1 | 2.32 | 0.43 |
| 1:C:7:LEU:N | 1:C:7:LEU:CD1 | 2.80 | 0.43 |
| 1:F:182:LEU:HD11 | 1:F:184:ASN:ND2 | 2.34 | 0.43 |
| 1:H:36:TYR:HA | 1:H:37:PRO:HD3 | 1.83 | 0.43 |
| 1:H:5:GLN:NE2 | 1:H:316:THR:HG22 | 2.34 | 0.43 |
| 1:I:61:ASN:HB3 | 1:I:183:ALA:O | 2.18 | 0.43 |
| 1:I:63:GLY:CA | 1:I:184:ASN:ND2 | 2.68 | 0.43 |
| 1:I:63:GLY:HA2 | 1:I:184:ASN:HD21 | 1.81 | 0.43 |
| 1:J:211:LEU:HD21 | 1:J:374:LEU:HD13 | 1.99 | 0.43 |
| 1:E:189:LYS:CD | 1:K:61:ASN:HB2 | 2.49 | 0.43 |
| 1:G:185:VAL:HG23 | 2:M:4:ASN:HB2 | 1.91 | 0.43 |
| 1:D:187:GLN:HE22 | 2:M:9:TYR:HB3 | 1.47 | 0.43 |
| 1:D:307:SER:HB2 | 1:D:318:LYS:HA | 2.00 | 0.43 |
| 1:E:103:ASP:HB2 | 1:E:104:PRO:HD2 | 1.99 | 0.43 |
| 1:E:184:ASN:O | 1:E:186:PRO:HD2 | 2.18 | 0.43 |
| 1:G:239:GLN:NE2 | 1:I:4:VAL:HB | 2.34 | 0.43 |
| 1:I:102:TYR:HB2 | 1:I:191:ARG:HB2 | 2.01 | 0.43 |
| 1:I:355:TYR:OH | 1:I:393:SER:N | 2.52 | 0.43 |
| 1:J:61:ASN:HB3 | 1:J:183:ALA:O | 2.18 | 0.43 |
| 1:K:184:ASN:HD22 | 1:K:249:LEU:HD11 | 1.84 | 0.43 |
| 1:B:260:LEU:HA | 1:B:377:TYR:O | 2.19 | 0.43 |
| 1:D:102:TYR:HB2 | 1:D:191:ARG:HB2 | 2.01 | 0.43 |
| 1:B:108:ARG:HH12 | 1:D:314:SER:HA | 1.84 | 0.43 |
| 1:D:308:GLN:NE2 | 1:D:345:ASN:HD21 | 2.07 | 0.43 |
| 1:G:307:SER:HB2 | 1:G:318:LYS:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:260:LEU:HA | 1:J:377:TYR:O | 2.19 | 0.43 |
| 1:K:103:ASP:HB2 | 1:K:104:PRO:HD2 | 1.99 | 0.43 |
| 1:B:41:GLN:CG | 1:K:106:ASN:HD21 | 2.29 | 0.43 |
| 1:K:151:PRO:HD2 | 1:K:162:LEU:HD22 | 2.00 | 0.43 |
| 1:K:15:LEU:CD1 | 1:K:15:LEU:N | 2.82 | 0.43 |
| 1:K:24:ASN:OD1 | 1:K:252:ILE:HB | 2.18 | 0.43 |
| 1:L:103:ASP:HB2 | 1:L:104:PRO:HD2 | 2.00 | 0.43 |
| 1:L:6:GLN:CB | 1:L:7:LEU:HD12 | 2.48 | 0.43 |
| 3:N:58:ILE:O | 3:N:58:ILE:CG2 | 2.66 | 0.43 |
| 3:N:93:LEU:N | 3:N:93:LEU:CD1 | 2.81 | 0.43 |
| 4:P:16:LEU:CD1 | 4:P:16:LEU:N | 2.82 | 0.43 |
| 1:L:150:ALA:HA | 1:L:151:PRO:N | 2.32 | 0.43 |
| 1:A:102:TYR:HB2 | 1:A:191:ARG:HB2 | 2.01 | 0.43 |
| 1:H:5:GLN:CD | 1:I:36:TYR:CD1 | 2.91 | 0.43 |
| 1:F:353:LEU:HD23 | 2:M:26:LEU:HA | 2.01 | 0.43 |
| 3:N:112:VAL:HG22 | 3:N:113:PRO:CG | 2.42 | 0.43 |
| 3:N:61:ASP:N | 3:N:75:GLU:HB2 | 2.34 | 0.43 |
| 4:P:24:ARG:O | 4:P:28:ALA:CA | 2.65 | 0.43 |
| 1:D:260:LEU:HA | 1:D:377:TYR:O | 2.19 | 0.43 |
| 1:J:386:LEU:CD1 | 1:J:386:LEU:N | 2.82 | 0.43 |
| 1:L:265:GLN:HE22 | 3:N:40:LYS:HE3 | 1.55 | 0.43 |
| 3:N:71:ILE:HD12 | 3:N:85:GLY:CA | 2.49 | 0.43 |
| 1:D:11:GLN:NE2 | 1:D:351:TYR:CD2 | 2.69 | 0.42 |
| 1:I:185:VAL:O | 1:I:185:VAL:CG2 | 2.65 | 0.42 |
| 1:J:102:TYR:HB2 | 1:J:191:ARG:HB2 | 2.01 | 0.42 |
| 2:M:75:GLN:HB3 | 2:M:76:PRO:HD2 | 2.00 | 0.42 |
| 3:N:101:VAL:HG22 | 3:N:102:ALA:N | 2.34 | 0.42 |
| 1:A:260:LEU:HA | 1:A:377:TYR:O | 2.19 | 0.42 |
| 1:C:151:PRO:HD2 | 1:C:162:LEU:HD22 | 2.00 | 0.42 |
| 1:C:386:LEU:N | 1:C:386:LEU:CD1 | 2.80 | 0.42 |
| 1:F:386:LEU:N | 1:F:386:LEU:CD1 | 2.81 | 0.42 |
| 1:G:102:TYR:HB2 | 1:G:191:ARG:HB2 | 2.01 | 0.42 |
| 1:G:260:LEU:HA | 1:G:377:TYR:O | 2.19 | 0.42 |
| 1:H:102:TYR:HB2 | 1:H:191:ARG:HB2 | 2.01 | 0.42 |
| 1:H:61:ASN:HB3 | 1:H:183:ALA:O | 2.18 | 0.42 |
| 1:I:307:SER:HB2 | 1:I:318:LYS:HA | 2.00 | 0.42 |
| 1:J:32:LEU:HD23 | 1:J:237:LEU:HD13 | 2.01 | 0.42 |
| 1:F:281:LEU:HA | 2:M:29:TYR:OH | 2.19 | 0.42 |
| 1:G:185:VAL:HG21 | 2:M:4:ASN:CA | 2.48 | 0.42 |
| 1:B:277:GLN:HG3 | 1:B:394:THR:CB | 2.33 | 0.42 |
| 1:E:188:SER:OG | 1:E:189:LYS:C | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:7:LEU:CD1 | 1:E:7:LEU:N | 2.82 | 0.42 |
| 1:F:151:PRO:HD2 | 1:F:162:LEU:HD22 | 2.00 | 0.42 |
| 2:M:48:LEU:N | 2:M:48:LEU:CD1 | 2.82 | 0.42 |
| 2:M:59:THR:O | 2:M:60:TYR:CG | 2.72 | 0.42 |
| 1:J:247:TYR:OH | 2:M:68:GLN:HA | 2.19 | 0.42 |
| 3:N:23:GLY:CA | 3:N:109:LYS:HD2 | 2.45 | 0.42 |
| 1:A:242:VAL:HG22 | 1:A:247:TYR:CD2 | 2.55 | 0.42 |
| 1:B:102:TYR:HB2 | 1:B:191:ARG:HB2 | 2.01 | 0.42 |
| 1:C:185:VAL:H | 1:C:186:PRO:CD | 2.31 | 0.42 |
| 1:C:185:VAL:H | 1:C:186:PRO:HD3 | 1.84 | 0.42 |
| 1:C:284:TYR:HB2 | 1:C:350:ILE:HB | 2.01 | 0.42 |
| 1:E:189:LYS:HZ2 | 1:K:61:ASN:ND2 | 2.10 | 0.42 |
| 1:H:16:ARG:C | 1:H:17:ASN:OD1 | 2.58 | 0.42 |
| 1:H:320:ASP:OD2 | 1:I:233:TYR:OH | 2.27 | 0.42 |
| 1:J:5:GLN:NE2 | 1:K:38:VAL:HG21 | 2.34 | 0.42 |
| 1:K:8:THR:HG21 | 1:K:11:GLN:NE2 | 2.35 | 0.42 |
| 2:M:4:ASN:HA | 2:M:5:PRO:HD2 | 1.86 | 0.42 |
| 3:N:28:ARG:NH1 | 3:N:37:GLU:OE1 | 2.51 | 0.42 |
| 1:L:193:LYS:NZ | 3:N:68:ALA:HA | 2.34 | 0.42 |
| 3:N:68:ALA:CA | 3:N:87:GLN:HG2 | 2.49 | 0.42 |
| 1:G:255:SER:HB2 | 2:M:6:GLN:HE22 | 1.85 | 0.42 |
| 1:G:36:TYR:HA | 1:G:37:PRO:HD3 | 1.83 | 0.42 |
| 1:H:307:SER:HB2 | 1:H:318:LYS:HA | 2.00 | 0.42 |
| 1:L:284:TYR:HB2 | 1:L:350:ILE:HB | 2.01 | 0.42 |
| 3:N:65:ASN:HD21 | 3:N:85:GLY:N | 2.17 | 0.42 |
| 3:N:71:ILE:CD1 | 3:N:85:GLY:N | 2.83 | 0.42 |
| 1:C:187:GLN:HG2 | 1:I:187:GLN:HB3 | 1.09 | 0.42 |
| 1:D:7:LEU:HD13 | 1:D:353:LEU:CG | 2.49 | 0.42 |
| 1:E:182:LEU:CG | 1:E:183:ALA:N | 2.83 | 0.42 |
| 1:E:182:LEU:HG | 1:E:183:ALA:N | 2.35 | 0.42 |
| 1:G:255:SER:HG | 1:G:386:LEU:HD21 | 1.77 | 0.42 |
| 1:H:9:PRO:CB | 1:I:34:GLN:NE2 | 2.61 | 0.42 |
| 1:K:284:TYR:HB2 | 1:K:350:ILE:HB | 2.02 | 0.42 |
| 3:N:45:TYR:C | 3:N:46:LEU:CD1 | 2.63 | 0.42 |
| 1:A:15:LEU:HD12 | 1:A:15:LEU:H | 1.84 | 0.42 |
| 1:C:181:VAL:O | 1:C:182:LEU:N | 2.53 | 0.42 |
| 1:F:242:VAL:HG22 | 1:F:247:TYR:CD2 | 2.55 | 0.42 |
| 1:G:242:VAL:HG22 | 1:G:247:TYR:CD2 | 2.55 | 0.42 |
| 1:H:242:VAL:HG22 | 1:H:247:TYR:CD2 | 2.55 | 0.42 |
| 1:H:260:LEU:HA | 1:H:377:TYR:O | 2.19 | 0.42 |
| 1:K:311:ALA:O | 1:K:312:ASN:CG | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:66:ASP:CA | 3:N:87:GLN:NE2 | 2.72 | 0.42 |
| 4:P:100:LEU:O | 4:P:101:ASN:C | 2.56 | 0.42 |
| 1:B:108:ARG:HH12 | 1:D:314:SER:CA | 2.28 | 0.42 |
| 1:E:275:VAL:HG22 | 1:E:361:VAL:HG22 | 2.02 | 0.42 |
| 1:F:98:ARG:HE | 1:F:98:ARG:HB3 | 1.69 | 0.42 |
| 1:I:4:VAL:N | 1:I:5:GLN:H | 2.13 | 0.42 |
| 1:J:182:LEU:CD1 | 1:J:240:LEU:HD11 | 2.49 | 0.42 |
| 1:L:280:ASN:O | 1:L:281:LEU:HB2 | 2.20 | 0.42 |
| 1:L:353:LEU:HB3 | 2:M:76:PRO:HG2 | 2.01 | 0.42 |
| 1:L:35:SER:CA | 1:L:36:TYR:N | 2.82 | 0.42 |
| 1:F:353:LEU:CB | 2:M:26:LEU:HA | 2.50 | 0.42 |
| 1:F:185:VAL:HG11 | 2:M:38:ILE:N | 2.06 | 0.42 |
| 1:K:17:ASN:O | 1:K:21:MET:N | 2.48 | 0.42 |
| 1:K:182:LEU:HD11 | 1:K:184:ASN:ND2 | 2.35 | 0.42 |
| 1:K:184:ASN:N | 1:K:185:VAL:HG22 | 2.33 | 0.42 |
| 1:K:369:GLN:O | 1:K:370:ASN:HB2 | 2.20 | 0.42 |
| 1:L:242:VAL:HG22 | 1:L:247:TYR:CD2 | 2.55 | 0.42 |
| 1:G:105:ASP:OD1 | 2:M:7:PHE:CE1 | 2.67 | 0.42 |
| 3:N:12:THR:HG23 | 3:N:68:ALA:O | 2.20 | 0.42 |
| 1:C:242:VAL:HG22 | 1:C:247:TYR:CD2 | 2.55 | 0.41 |
| 1:C:275:VAL:HG22 | 1:C:361:VAL:HG22 | 2.02 | 0.41 |
| 1:D:242:VAL:HG22 | 1:D:247:TYR:CD2 | 2.55 | 0.41 |
| 1:E:108:ARG:HD3 | 1:J:313:PHE:O | 2.19 | 0.41 |
| 1:E:107:GLN:HG2 | 1:E:383:ARG:NH2 | 2.35 | 0.41 |
| 1:H:355:TYR:OH | 1:H:392:ILE:C | 2.58 | 0.41 |
| 1:I:391:THR:CG2 | 1:I:392:ILE:N | 2.83 | 0.41 |
| 3:N:66:ASP:HB2 | 3:N:87:GLN:CD | 2.40 | 0.41 |
| 1:B:242:VAL:HG22 | 1:B:247:TYR:CD2 | 2.55 | 0.41 |
| 1:D:16:ARG:C | 1:D:17:ASN:OD1 | 2.58 | 0.41 |
| 1:E:98:ARG:NH1 | 1:J:318:LYS:HZ1 | 2.18 | 0.41 |
| 1:D:52:ARG:NH2 | 1:G:43:GLU:HG3 | 2.35 | 0.41 |
| 1:H:391:THR:CG2 | 1:H:392:ILE:N | 2.83 | 0.41 |
| 1:I:242:VAL:HG22 | 1:I:247:TYR:CD2 | 2.55 | 0.41 |
| 1:J:36:TYR:HA | 1:J:37:PRO:HD3 | 1.83 | 0.41 |
| 1:K:275:VAL:HG22 | 1:K:361:VAL:HG22 | 2.02 | 0.41 |
| 2:M:68:GLN:O | 4:P:41:MET:HE1 | 2.21 | 0.41 |
| 1:B:24:ASN:CG | 1:B:252:ILE:HB | 2.41 | 0.41 |
| 1:F:284:TYR:HB2 | 1:F:350:ILE:HB | 2.01 | 0.41 |
| 1:F:369:GLN:O | 1:F:370:ASN:HB2 | 2.20 | 0.41 |
| 1:J:182:LEU:HB2 | 1:J:254:LEU:CD1 | 2.49 | 0.41 |
| 2:M:72:THR:CG2 | 4:P:44:ASN:HB3 | 2.27 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:15:LEU:CD1 | 1:A:15:LEU:H | 2.32 | 0.41 |
| 1:B:11:GLN:CD | 1:B:351:TYR:CD2 | 2.79 | 0.41 |
| 1:B:260:LEU:HD22 | 1:B:378:GLU:HG2 | 2.03 | 0.41 |
| 1:C:369:GLN:O | 1:C:370:ASN:HB2 | 2.20 | 0.41 |
| 1:D:391:THR:CG2 | 1:D:392:ILE:N | 2.83 | 0.41 |
| 1:L:35:SER:OG | 1:L:237:LEU:HD13 | 2.21 | 0.41 |
| 1:L:369:GLN:O | 1:L:370:ASN:HB2 | 2.20 | 0.41 |
| 4:P:111:LEU:CD1 | 4:P:111:LEU:N | 2.80 | 0.41 |
| 4:P:45:GLN:N | 4:P:46:PRO:HD3 | 2.35 | 0.41 |
| 1:C:182:LEU:HD11 | 1:C:184:ASN:ND2 | 2.35 | 0.41 |
| 1:D:4:VAL:HG22 | 1:D:4:VAL:O | 2.13 | 0.41 |
| 1:F:103:ASP:HB2 | 1:F:104:PRO:HD2 | 2.00 | 0.41 |
| 1:G:260:LEU:HD22 | 1:G:378:GLU:HG2 | 2.02 | 0.41 |
| 1:H:89:ASP:HA | 1:I:140:LYS:HD2 | 2.02 | 0.41 |
| 1:E:264:ALA:CB | 1:J:272:VAL:HG11 | 2.50 | 0.41 |
| 1:L:111:GLU:HB2 | 3:N:89:TYR:CD1 | 2.56 | 0.41 |
| 1:L:11:GLN:C | 1:L:15:LEU:CD1 | 2.53 | 0.41 |
| 1:L:275:VAL:HG22 | 1:L:361:VAL:HG22 | 2.02 | 0.41 |
| 1:L:7:LEU:CD1 | 1:L:7:LEU:N | 2.83 | 0.41 |
| 1:F:386:LEU:N | 2:M:33:GLY:O | 2.53 | 0.41 |
| 3:N:66:ASP:CB | 3:N:87:GLN:CD | 2.89 | 0.41 |
| 1:A:309:ARG:CG | 1:A:310:THR:N | 2.84 | 0.41 |
| 1:B:257:LEU:HG | 1:B:383:ARG:CG | 2.31 | 0.41 |
| 1:F:386:LEU:HD22 | 2:M:34:ARG:HG2 | 2.02 | 0.41 |
| 3:N:91:PRO:O | 3:N:92:LEU:CD1 | 2.50 | 0.41 |
| 1:C:102:TYR:O | 1:C:190:GLN:CG | 2.61 | 0.41 |
| 1:C:311:ALA:O | 1:C:312:ASN:CG | 2.58 | 0.41 |
| 1:E:242:VAL:HG22 | 1:E:247:TYR:CD2 | 2.55 | 0.41 |
| 1:E:285:LEU:HD23 | 1:E:349:PRO:HG3 | 2.03 | 0.41 |
| 1:I:17:ASN:HB2 | 1:I:20:ALA:HB3 | 1.95 | 0.41 |
| 1:I:260:LEU:HD22 | 1:I:378:GLU:HG2 | 2.03 | 0.41 |
| 1:I:392:ILE:O | 1:I:393:SER:O | 2.39 | 0.41 |
| 1:K:12:GLN:CA | 1:K:15:LEU:HD13 | 2.51 | 0.41 |
| 1:L:7:LEU:C | 1:L:11:GLN:HB2 | 2.41 | 0.41 |
| 3:N:117:LEU:N | 3:N:117:LEU:CD1 | 2.83 | 0.41 |
| 1:A:311:ALA:C | 1:A:313:PHE:H | 2.24 | 0.41 |
| 1:A:352:THR:OG1 | 1:A:354:GLN:O | 2.36 | 0.41 |
| 1:C:162:LEU:HD23 | 1:C:162:LEU:N | 2.36 | 0.41 |
| 1:E:106:ASN:OD1 | 1:K:62:VAL:CG2 | 2.69 | 0.41 |
| 1:F:16:ARG:C | 1:F:18:GLN:N | 2.73 | 0.41 |
| 1:F:278:TYR:O | 1:F:280:ASN:OD1 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:6:GLN:HB3 | 1:J:7:LEU:HA | 2.02 | 0.41 |
| 1:K:8:THR:HG21 | 1:K:11:GLN:HG3 | 2.02 | 0.41 |
| 1:L:162:LEU:HD23 | 1:L:162:LEU:N | 2.36 | 0.41 |
| 1:L:14:ALA:O | 1:L:18:GLN:HG3 | 2.20 | 0.41 |
| 1:L:61:ASN:HD21 | 1:L:189:LYS:CA | 2.29 | 0.41 |
| 1:B:24:ASN:OD1 | 1:B:252:ILE:HB | 2.21 | 0.41 |
| 1:C:14:ALA:HB3 | 1:C:15:LEU:HD12 | 2.03 | 0.41 |
| 1:E:278:TYR:O | 1:E:280:ASN:OD1 | 2.39 | 0.41 |
| 1:F:83:GLU:HB3 | 1:F:218:ALA:HB3 | 2.03 | 0.41 |
| 1:G:309:ARG:CG | 1:G:314:SER:C | 2.82 | 0.41 |
| 1:G:386:LEU:CD1 | 1:G:386:LEU:N | 2.84 | 0.41 |
| 1:I:355:TYR:OH | 1:I:392:ILE:C | 2.59 | 0.41 |
| 1:K:242:VAL:HG22 | 1:K:247:TYR:CD2 | 2.55 | 0.41 |
| 1:L:310:THR:O | 1:L:312:ASN:N | 2.54 | 0.41 |
| 2:M:41:ALA:O | 2:M:42:ARG:CB | 2.51 | 0.41 |
| 1:E:284:TYR:HB2 | 1:E:350:ILE:HB | 2.01 | 0.41 |
| 1:B:52:ARG:NH1 | 1:E:43:GLU:HG3 | 2.36 | 0.41 |
| 1:F:7:LEU:N | 1:F:7:LEU:CD1 | 2.83 | 0.41 |
| 1:I:281:LEU:HD21 | 1:I:385:GLU:CB | 2.49 | 0.41 |
| 1:D:387:VAL:O | 1:I:6:GLN:HB2 | 2.21 | 0.41 |
| 1:K:17:ASN:C | 1:K:20:ALA:H | 2.17 | 0.41 |
| 1:L:280:ASN:ND2 | 1:L:352:THR:HG21 | 2.35 | 0.41 |
| 3:N:60:ILE:HB | 3:N:97:ARG:HD2 | 2.01 | 0.41 |
| 1:B:79:ASN:O | 1:B:79:ASN:CG | 2.60 | 0.41 |
| 1:C:182:LEU:HD22 | 1:C:254:LEU:HD13 | 2.03 | 0.41 |
| 1:C:352:THR:O | 1:C:353:LEU:HG | 2.21 | 0.41 |
| 1:D:63:GLY:HA2 | 1:D:184:ASN:HD21 | 1.81 | 0.41 |
| 1:F:311:ALA:HB1 | 2:M:23:THR:OG1 | 2.20 | 0.41 |
| 1:F:275:VAL:HG22 | 1:F:361:VAL:HG22 | 2.02 | 0.41 |
| 1:H:382:SER:HG | 1:H:385:GLU:CG | 2.26 | 0.41 |
| 1:H:394:THR:HG22 | 1:H:395:THR:O | 2.20 | 0.41 |
| 1:H:9:PRO:CD | 1:I:34:GLN:OE1 | 2.69 | 0.41 |
| 3:N:60:ILE:CD1 | 3:N:97:ARG:NE | 2.64 | 0.41 |
| 3:N:49:THR:HG23 | 3:N:82:CYS:C | 2.22 | 0.41 |
| 1:C:280:ASN:CB | 1:C:352:THR:OG1 | 2.69 | 0.40 |
| 1:C:83:GLU:HB3 | 1:C:218:ALA:HB3 | 2.03 | 0.40 |
| 1:D:264:ALA:CB | 1:I:272:VAL:CG1 | 2.98 | 0.40 |
| 1:F:162:LEU:HD23 | 1:F:162:LEU:N | 2.36 | 0.40 |
| 1:K:83:GLU:HB3 | 1:K:218:ALA:HB3 | 2.03 | 0.40 |
| 1:D:260:LEU:HD22 | 1:D:378:GLU:HG2 | 2.03 | 0.40 |
| 1:F:285:LEU:HD23 | 1:F:349:PRO:HG3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:260:LEU:HD22 | 1:H:378:GLU:HG2 | 2.03 | 0.40 |
| 1:H:9:PRO:HD3 | 1:I:34:GLN:OE1 | 2.21 | 0.40 |
| 1:B:269:THR:CG2 | 1:I:372:ARG:HD3 | 2.12 | 0.40 |
| 1:E:187:GLN:CA | 1:K:185:VAL:N | 2.81 | 0.40 |
| 1:K:280:ASN:CB | 1:K:352:THR:OG1 | 2.69 | 0.40 |
| 1:J:354:GLN:HG2 | 2:M:54:ALA:O | 2.21 | 0.40 |
| 4:P:56:ALA:HB3 | 4:P:100:LEU:HD23 | 2.03 | 0.40 |
| 1:D:79:ASN:O | 1:D:79:ASN:CG | 2.60 | 0.40 |
| 1:F:39:ILE:HG23 | 1:F:39:ILE:O | 2.22 | 0.40 |
| 1:H:79:ASN:CG | 1:H:79:ASN:O | 2.60 | 0.40 |
| 1:J:16:ARG:NE | 1:J:21:MET:CE | 2.77 | 0.40 |
| 1:J:384:THR:HG22 | 2:M:62:ALA:HB1 | 1.82 | 0.40 |
| 1:K:352:THR:O | 1:K:353:LEU:HG | 2.22 | 0.40 |
| 1:L:35:SER:C | 1:L:36:TYR:CA | 2.89 | 0.40 |
| 3:N:47:ALA:C | 3:N:48:ASP:OD1 | 2.56 | 0.40 |
| 1:C:285:LEU:HD23 | 1:C:349:PRO:HG3 | 2.03 | 0.40 |
| 1:E:83:GLU:HB3 | 1:E:218:ALA:HB3 | 2.03 | 0.40 |
| 1:E:264:ALA:CB | 1:J:272:VAL:HG13 | 2.51 | 0.40 |
| 1:F:16:ARG:HB2 | 1:F:17:ASN:HD22 | 1.47 | 0.40 |
| 1:F:312:ASN:O | 1:F:313:PHE:HB2 | 2.21 | 0.40 |
| 1:F:353:LEU:HD22 | 2:M:26:LEU:CA | 2.52 | 0.40 |
| 1:G:23:ALA:N | 1:G:24:ASN:N | 2.69 | 0.40 |
| 1:G:79:ASN:O | 1:G:79:ASN:CG | 2.60 | 0.40 |
| 1:J:106:ASN:ND2 | 1:J:191:ARG:NH2 | 2.56 | 0.40 |
| 1:J:79:ASN:O | 1:J:79:ASN:CG | 2.60 | 0.40 |
| 1:K:285:LEU:HD23 | 1:K:349:PRO:HG3 | 2.03 | 0.40 |
| 1:L:183:ALA:C | 1:L:184:ASN:CA | 2.90 | 0.40 |
| 1:F:281:LEU:N | 1:F:281:LEU:CD1 | 2.85 | 0.40 |
| 1:F:352:THR:O | 1:F:353:LEU:HG | 2.21 | 0.40 |
| 1:J:353:LEU:O | 2:M:55:VAL:HG23 | 2.21 | 0.40 |
| 2:M:15:ILE:O | 2:M:15:ILE:HG22 | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 378/395 (96%) | 358 (95%) | 14 (4%) | 6 (2%) | 9 | 45 |
| 1 | B | 386/395 (98%) | 366 (95%) | 11 (3%) | 9 (2%) | 6 | 37 |
| 1 | C | 379/395 (96%) | 356 (94%) | 18 (5%) | 5 (1%) | 12 | 48 |
| 1 | D | 388/395 (98%) | 368 (95%) | 13 (3%) | 7 (2%) | 8 | 42 |
| 1 | E | 376/395 (95%) | 354 (94%) | 17 (4%) | 5 (1%) | 12 | 48 |
| 1 | F | 382/395 (97%) | 359 (94%) | 18 (5%) | 5 (1%) | 12 | 48 |
| 1 | G | 371/395 (94%) | 354 (95%) | 12 (3%) | 5 (1%) | 12 | 48 |
| 1 | H | 390/395 (99%) | 368 (94%) | 15 (4%) | 7 (2%) | 8 | 42 |
| 1 | I | 386/395 (98%) | 367 (95%) | 11 (3%) | 8 (2%) | 7 | 39 |
| 1 | J | 384/395 (97%) | 364 (95%) | 13 (3%) | 7 (2%) | 8 | 42 |
| 1 | K | 380/395 (96%) | 350 (92%) | 25 (7%) | 5 (1%) | 12 | 48 |
| 1 | L | 373/395 (94%) | 348 (93%) | 17 (5%) | 8 (2%) | 7 | 39 |
| 2 | M | 81/83 (98%) | 65 (80%) | 8 (10%) | 8 (10%) | 0 | 10 |
| 3 | N | 112/126 (89%) | 94 (84%) | 6 (5%) | 12 (11%) | 0 | 8 |
| 4 | P | 76/117 (65%) | 57 (75%) | 11 (14%) | 8 (10%) | 0 | 8 |
| All | All | 4842/5066 (96%) | 4528 (94%) | 209 (4%) | 105 (2%) | 6 | 38 |

All (105) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 186 | PRO |
| 1 | A | 244 | GLN |
| 1 | A | 353 | LEU |
| 1 | B | 8 | THR |
| 1 | B | 186 | PRO |
| 1 | B | 312 | ASN |
| 1 | B | 353 | LEU |
| 1 | B | 393 | SER |
| 1 | C | 185 | VAL |
| 1 | C | 187 | GLN |
| 1 | C | 244 | GLN |
| 1 | D | 8 | THR |
| 1 | D | 186 | PRO |
| 1 | D | 312 | ASN |
| 1 | D | 353 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 393 | SER |
| 1 | E | 8 | THR |
| 1 | E | 187 | GLN |
| 1 | E | 188 | SER |
| 1 | E | 280 | ASN |
| 1 | F | 247 | TYR |
| 1 | F | 248 | ILE |
| 1 | F | 280 | ASN |
| 1 | G | 186 | PRO |
| 1 | G | 244 | GLN |
| 1 | G | 353 | LEU |
| 1 | H | 8 | THR |
| 1 | H | 186 | PRO |
| 1 | H | 312 | ASN |
| 1 | H | 353 | LEU |
| 1 | I | 8 | THR |
| 1 | I | 186 | PRO |
| 1 | I | 312 | ASN |
| 1 | I | 353 | LEU |
| 1 | J | 186 | PRO |
| 1 | J | 314 | SER |
| 1 | J | 353 | LEU |
| 1 | K | 188 | SER |
| 1 | K | 244 | GLN |
| 1 | L | 187 | GLN |
| 1 | L | 312 | ASN |
| 1 | L | 313 | PHE |
| 2 | M | 12 | PRO |
| 2 | M | 51 | PRO |
| 3 | N | 6 | PRO |
| 3 | N | 13 | PRO |
| 3 | N | 28 | ARG |
| 3 | N | 91 | PRO |
| 3 | N | 95 | PRO |
| 3 | N | 111 | SER |
| 4 | P | 46 | PRO |
| 4 | P | 50 | SER |
| 4 | P | 54 | PRO |
| 1 | A | 385 | GLU |
| 1 | B | 16 | ARG |
| 1 | B | 314 | SER |
| 1 | C | 311 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 314 | SER |
| 1 | E | 311 | ALA |
| 1 | F | 311 | ALA |
| 1 | F | 393 | SER |
| 1 | G | 314 | SER |
| 1 | H | 314 | SER |
| 1 | I | 16 | ARG |
| 1 | J | 312 | ASN |
| 1 | K | 311 | ALA |
| 1 | L | 7 | LEU |
| 1 | L | 8 | THR |
| 3 | N | 24 | PRO |
| 3 | N | 27 | VAL |
| 3 | N | 55 | VAL |
| 4 | P | 31 | VAL |
| 4 | P | 36 | GLU |
| 1 | A | 311 | ALA |
| 1 | C | 281 | LEU |
| 1 | G | 382 | SER |
| 1 | I | 314 | SER |
| 1 | J | 239 | GLN |
| 1 | K | 281 | LEU |
| 1 | L | 281 | LEU |
| 2 | M | 81 | GLN |
| 3 | N | 83 | PRO |
| 3 | N | 100 | PHE |
| 1 | A | 312 | ASN |
| 1 | J | 185 | VAL |
| 1 | J | 187 | GLN |
| 2 | M | 15 | ILE |
| 4 | P | 39 | PRO |
| 1 | I | 393 | SER |
| 1 | L | 311 | ALA |
| 2 | M | 24 | MET |
| 2 | M | 41 | ALA |
| 4 | P | 51 | VAL |
| 1 | B | 392 | ILE |
| 1 | L | 237 | LEU |
| 4 | P | 45 | GLN |
| 1 | B | 185 | VAL |
| 1 | D | 185 | VAL |
| 1 | H | 185 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 392 | ILE |
| 1 | I | 185 | VAL |
| 2 | M | 25 | PRO |
| 2 | M | 46 | PRO |
| 1 | K | 185 | VAL |
| 3 | N | 80 | ILE |

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 312/326 (96%) | 310 (99%) | 2 (1%) | 86 | 92 |
| 1 | B | 324/326 (99%) | 322 (99%) | 2 (1%) | 86 | 92 |
| 1 | C | 318/326 (98%) | 315 (99%) | 3 (1%) | 78 | 87 |
| 1 | D | 324/326 (99%) | 323 (100%) | 1 (0%) | 92 | 95 |
| 1 | E | 312/326 (96%) | 308 (99%) | 4 (1%) | 69 | 82 |
| 1 | F | 319/326 (98%) | 317 (99%) | 2 (1%) | 86 | 92 |
| 1 | G | 311/326 (95%) | 310 (100%) | 1 (0%) | 92 | 95 |
| 1 | H | 324/326 (99%) | 323 (100%) | 1 (0%) | 92 | 95 |
| 1 | I | 324/326 (99%) | 322 (99%) | 2 (1%) | 86 | 92 |
| 1 | J | 321/326 (98%) | 318 (99%) | 3 (1%) | 78 | 87 |
| 1 | K | 317/326 (97%) | 312 (98%) | 5 (2%) | 62 | 79 |
| 1 | L | 313/326 (96%) | 309 (99%) | 4 (1%) | 69 | 82 |
| 2 | M | 66/66 (100%) | 66 (100%) | 0 | 100 | 100 |
| 3 | N | 92/102 (90%) | 92 (100%) | 0 | 100 | 100 |
| 4 | P | 65/94 (69%) | 65 (100%) | 0 | 100 | 100 |
| All | All | 4042/4174 (97%) | 4012 (99%) | 30 (1%) | 84 | 90 |

All (30) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 310 | THR |
| 1 | A | 315 | ASP |
| 1 | B | 4 | VAL |
| 1 | B | 315 | ASP |
| 1 | C | 162 | LEU |
| 1 | C | 186 | PRO |
| 1 | C | 355 | TYR |
| 1 | D | 315 | ASP |
| 1 | E | 162 | LEU |
| 1 | E | 186 | PRO |
| 1 | E | 188 | SER |
| 1 | E | 355 | TYR |
| 1 | F | 162 | LEU |
| 1 | F | 355 | TYR |
| 1 | G | 315 | ASP |
| 1 | H | 315 | ASP |
| 1 | I | 4 | VAL |
| 1 | I | 315 | ASP |
| 1 | J | 240 | LEU |
| 1 | J | 241 | PRO |
| 1 | J | 315 | ASP |
| 1 | K | 162 | LEU |
| 1 | K | 185 | VAL |
| 1 | K | 186 | PRO |
| 1 | K | 188 | SER |
| 1 | K | 355 | TYR |
| 1 | L | 37 | PRO |
| 1 | L | 162 | LEU |
| 1 | L | 237 | LEU |
| 1 | L | 355 | TYR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 41 | GLN |
| 1 | A | 61 | ASN |
| 1 | A | 79 | ASN |
| 1 | A | 80 | HIS |
| 1 | A | 106 | ASN |
| 1 | A | 190 | GLN |
| 1 | A | 200 | ASN |
| 1 | A | 280 | ASN |
| 1 | A | 312 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 345 | ASN |
| 1 | A | 357 | ASN |
| 1 | B | 17 | ASN |
| 1 | B | 41 | GLN |
| 1 | B | 61 | ASN |
| 1 | B | 79 | ASN |
| 1 | B | 80 | HIS |
| 1 | B | 106 | ASN |
| 1 | B | 190 | GLN |
| 1 | B | 200 | ASN |
| 1 | B | 265 | GLN |
| 1 | B | 280 | ASN |
| 1 | B | 345 | ASN |
| 1 | B | 357 | ASN |
| 1 | C | 17 | ASN |
| 1 | C | 41 | GLN |
| 1 | C | 80 | HIS |
| 1 | C | 187 | GLN |
| 1 | C | 190 | GLN |
| 1 | C | 271 | ASN |
| 1 | C | 345 | ASN |
| 1 | C | 354 | GLN |
| 1 | D | 5 | GLN |
| 1 | D | 41 | GLN |
| 1 | D | 61 | ASN |
| 1 | D | 79 | ASN |
| 1 | D | 80 | HIS |
| 1 | D | 106 | ASN |
| 1 | D | 187 | GLN |
| 1 | D | 190 | GLN |
| 1 | D | 200 | ASN |
| 1 | D | 277 | GLN |
| 1 | D | 280 | ASN |
| 1 | D | 345 | ASN |
| 1 | D | 357 | ASN |
| 1 | E | 41 | GLN |
| 1 | E | 80 | HIS |
| 1 | E | 187 | GLN |
| 1 | E | 271 | ASN |
| 1 | E | 345 | ASN |
| 1 | E | 354 | GLN |
| 1 | F | 41 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | F | 80 | HIS |
| 1 | F | 271 | ASN |
| 1 | F | 345 | ASN |
| 1 | F | 354 | GLN |
| 1 | G | 18 | GLN |
| 1 | G | 41 | GLN |
| 1 | G | 61 | ASN |
| 1 | G | 79 | ASN |
| 1 | G | 80 | HIS |
| 1 | G | 106 | ASN |
| 1 | G | 187 | GLN |
| 1 | G | 190 | GLN |
| 1 | G | 200 | ASN |
| 1 | G | 239 | GLN |
| 1 | G | 280 | ASN |
| 1 | G | 345 | ASN |
| 1 | G | 357 | ASN |
| 1 | H | 5 | GLN |
| 1 | H | 41 | GLN |
| 1 | H | 61 | ASN |
| 1 | H | 79 | ASN |
| 1 | H | 80 | HIS |
| 1 | H | 106 | ASN |
| 1 | H | 190 | GLN |
| 1 | H | 200 | ASN |
| 1 | H | 265 | GLN |
| 1 | H | 280 | ASN |
| 1 | H | 345 | ASN |
| 1 | I | 17 | ASN |
| 1 | I | 33 | GLN |
| 1 | I | 41 | GLN |
| 1 | I | 61 | ASN |
| 1 | I | 80 | HIS |
| 1 | I | 106 | ASN |
| 1 | I | 190 | GLN |
| 1 | I | 200 | ASN |
| 1 | I | 280 | ASN |
| 1 | I | 345 | ASN |
| 1 | I | 354 | GLN |
| 1 | I | 357 | ASN |
| 1 | J | 5 | GLN |
| 1 | J | 41 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 61 | ASN |
| 1 | J | 79 | ASN |
| 1 | J | 80 | HIS |
| 1 | J | 106 | ASN |
| 1 | J | 190 | GLN |
| 1 | J | 200 | ASN |
| 1 | J | 280 | ASN |
| 1 | J | 345 | ASN |
| 1 | J | 357 | ASN |
| 1 | K | 12 | GLN |
| 1 | K | 41 | GLN |
| 1 | K | 61 | ASN |
| 1 | K | 80 | HIS |
| 1 | K | 106 | ASN |
| 1 | K | 271 | ASN |
| 1 | K | 345 | ASN |
| 1 | K | 354 | GLN |
| 1 | L | 41 | GLN |
| 1 | L | 80 | HIS |
| 1 | L | 190 | GLN |
| 1 | L | 271 | ASN |
| 1 | L | 345 | ASN |
| 1 | L | 354 | GLN |
| 2 | M | 6 | GLN |
| 2 | M | 43 | GLN |
| 2 | M | 58 | GLN |
| 3 | N | 50 | GLN |
| 3 | N | 62 | ASN |
| 3 | N | 65 | ASN |
| 3 | N | 87 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | I | 15 |
| 1 | D | 14 |
| 1 | B | 14 |
| 1 | J | 11 |
| 1 | H | 9 |
| 3 | N | 9 |
| 1 | F | 9 |
| 1 | L | 8 |
| 1 | G | 7 |
| 1 | K | 7 |
| 1 | C | 6 |
| 1 | A | 6 |
| 2 | M | 5 |
| 4 | P | 4 |
| 1 | E | 3 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | J | 383:ARG | C | 384:THR | N | 3.74 |
| 1 | C | 190:GLN | C | 191:ARG | N | 3.53 |
| 1 | D | 17:ASN | C | 18:GLN | N | 3.14 |
| 1 | I | 17:ASN | C | 18:GLN | N | 3.14 |
| 1 | L | 35:SER | C | 36:TYR | N | 2.61 |
| 1 | B | 6:GLN | C | 7:LEU | N | 2.59 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | B | 17:ASN | C | 18:GLN | N | 2.59 |
| 1 | I | 6:GLN | C | 7:LEU | N | 2.59 |
| 1 | F | 382:SER | C | 383:ARG | N | 2.55 |
| 1 | G | 23:ALA | C | 24:ASN | N | 2.50 |
| 1 | J | 34:GLN | C | 35:SER | N | 2.45 |
| 1 | L | 183:ALA | C | 184:ASN | N | 2.27 |
| 1 | C | 181:VAL | C | 182:LEU | N | 2.23 |
| 1 | K | 34:GLN | C | 35:SER | N | 2.20 |
| 1 | F | 16:ARG | C | 17:ASN | N | 2.18 |
| 1 | A | 24:ASN | C | 25:LEU | N | 1.98 |
| 1 | L | 381:THR | C | 382:SER | N | 1.96 |
| 1 | L | 150:ALA | C | 151:PRO | N | 1.94 |
| 1 | H | 381:THR | C | 382:SER | N | 1.83 |
| 1 | K | 191:ARG | C | 192:LEU | N | 1.78 |
| 1 | G | 35:SER | C | 36:TYR | N | 1.76 |
| 1 | E | 381:THR | C | 382:SER | N | 1.72 |
| 1 | I | 392:ILE | C | 393:SER | N | 1.71 |
| 1 | L | 257:LEU | C | 258:TYR | N | 1.71 |
| 1 | G | 382:SER | C | 383:ARG | N | 1.70 |
| 1 | B | 8:THR | C | 9:PRO | N | 1.69 |
| 1 | I | 8:THR | C | 9:PRO | N | 1.69 |
| 1 | J | 384:THR | C | 385:GLU | N | 1.69 |
| 1 | N | 55:VAL | C | 56:GLN | N | 1.66 |
| 1 | J | 187:GLN | C | 188:SER | N | 1.61 |
| 1 | B | 392:ILE | C | 393:SER | N | 1.60 |
| 1 | N | 16:ASN | C | 17:GLY | N | 1.60 |
| 1 | K | 279:ALA | C | 280:ASN | N | 1.20 |
| 1 | M | 67:ILE | C | 68:GLN | N | 1.20 |
| 1 | N | 18:CYS | C | 19:ASP | N | 1.20 |
| 1 | N | 54:GLY | C | 55:VAL | N | 1.20 |
| 1 | C | 279:ALA | C | 280:ASN | N | 1.19 |
| 1 | D | 26:GLN | C | 27:ALA | N | 1.19 |
| 1 | F | 393:SER | C | 394:THR | N | 1.19 |
| 1 | M | 11:GLY | C | 12:PRO | N | 1.19 |
| 1 | P | 4:LYS | C | 5:LYS | N | 1.18 |
| 1 | P | 33:SER | C | 34:ASN | N | 1.18 |
| 1 | D | 357:ASN | C | 358:VAL | N | 1.17 |
| 1 | D | 380:PHE | C | 381:THR | N | 1.17 |
| 1 | H | 357:ASN | C | 358:VAL | N | 1.17 |
| 1 | I | 357:ASN | C | 358:VAL | N | 1.17 |
| 1 | J | 184:ASN | C | 185:VAL | N | 1.17 |
| 1 | J | 357:ASN | C | 358:VAL | N | 1.17 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | F | 391:THR | C | 392:ILE | N | 1.16 |
| 1 | M | 41:ALA | C | 42:ARG | N | 1.16 |
| 1 | P | 32:ALA | C | 33:SER | N | 1.15 |
| 1 | B | 389:ALA | C | 390:GLY | N | 1.14 |
| 1 | D | 389:ALA | C | 390:GLY | N | 1.14 |
| 1 | H | 389:ALA | C | 390:GLY | N | 1.14 |
| 1 | I | 389:ALA | C | 390:GLY | N | 1.14 |
| 1 | D | 356:GLY | C | 357:ASN | N | 1.13 |
| 1 | H | 356:GLY | C | 357:ASN | N | 1.13 |
| 1 | I | 356:GLY | C | 357:ASN | N | 1.13 |
| 1 | J | 356:GLY | C | 357:ASN | N | 1.13 |
| 1 | L | 161:GLU | C | 162:LEU | N | 1.13 |
| 1 | C | 311:ALA | C | 312:ASN | N | 1.12 |
| 1 | K | 311:ALA | C | 312:ASN | N | 1.12 |
| 1 | L | 311:ALA | C | 312:ASN | N | 1.12 |
| 1 | N | 27:VAL | C | 28:ARG | N | 1.12 |
| 1 | P | 31:VAL | C | 32:ALA | N | 1.12 |
| 1 | B | 245:ASN | C | 246:GLY | N | 1.11 |
| 1 | D | 245:ASN | C | 246:GLY | N | 1.11 |
| 1 | H | 245:ASN | C | 246:GLY | N | 1.11 |
| 1 | I | 245:ASN | C | 246:GLY | N | 1.11 |
| 1 | M | 46:PRO | C | 47:PHE | N | 1.11 |
| 1 | N | 65:ASN | C | 66:ASP | N | 1.10 |
| 1 | A | 356:GLY | C | 357:ASN | N | 1.09 |
| 1 | E | 279:ALA | C | 280:ASN | N | 1.09 |
| 1 | F | 279:ALA | C | 280:ASN | N | 1.09 |
| 1 | G | 356:GLY | C | 357:ASN | N | 1.09 |
| 1 | M | 64:GLY | C | 65:THR | N | 1.09 |
| 1 | N | 17:GLY | C | 18:CYS | N | 1.09 |
| 1 | D | 392:ILE | C | 393:SER | N | 1.08 |
| 1 | B | 357:ASN | C | 358:VAL | N | 1.07 |
| 1 | J | 250:PRO | C | 251:LEU | N | 1.07 |
| 1 | J | 313:PHE | C | 314:SER | N | 1.07 |
| 1 | B | 185:VAL | C | 186:PRO | N | 1.04 |
| 1 | D | 185:VAL | C | 186:PRO | N | 1.04 |
| 1 | H | 185:VAL | C | 186:PRO | N | 1.04 |
| 1 | I | 185:VAL | C | 186:PRO | N | 1.04 |
| 1 | A | 183:ALA | C | 184:ASN | N | 1.03 |
| 1 | F | 247:TYR | C | 248:ILE | N | 1.03 |
| 1 | G | 183:ALA | C | 184:ASN | N | 1.03 |
| 1 | N | 57:CYS | C | 58:ILE | N | 1.03 |
| 1 | B | 394:THR | C | 395:THR | N | 1.00 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | D | 394:THR | C | 395:THR | N | 1.00 |
| 1 | I | 394:THR | C | 395:THR | N | 1.00 |
| 1 | N | 111:SER | C | 112:VAL | N | 1.00 |
| 1 | B | 352:THR | C | 353:LEU | N | 0.99 |
| 1 | D | 352:THR | C | 353:LEU | N | 0.99 |
| 1 | H | 352:THR | C | 353:LEU | N | 0.99 |
| 1 | I | 352:THR | C | 353:LEU | N | 0.99 |
| 1 | J | 352:THR | C | 353:LEU | N | 0.99 |
| 1 | E | 311:ALA | C | 312:ASN | N | 0.98 |
| 1 | F | 311:ALA | C | 312:ASN | N | 0.98 |
| 1 | I | 313:PHE | C | 314:SER | N | 0.98 |
| 1 | B | 16:ARG | C | 17:ASN | N | 0.95 |
| 1 | I | 16:ARG | C | 17:ASN | N | 0.95 |
| 1 | J | 256:THR | C | 257:LEU | N | 0.95 |
| 1 | L | 312:ASN | C | 313:PHE | N | 0.94 |
| 1 | A | 381:THR | C | 382:SER | N | 0.93 |
| 1 | K | 380:PHE | C | 381:THR | N | 0.92 |
| 1 | A | 243:GLY | C | 244:GLN | N | 0.91 |
| 1 | B | 311:ALA | C | 312:ASN | N | 0.91 |
| 1 | D | 311:ALA | C | 312:ASN | N | 0.91 |
| 1 | D | 313:PHE | C | 314:SER | N | 0.91 |
| 1 | G | 243:GLY | C | 244:GLN | N | 0.91 |
| 1 | H | 311:ALA | C | 312:ASN | N | 0.91 |
| 1 | H | 313:PHE | C | 314:SER | N | 0.91 |
| 1 | B | 313:PHE | C | 314:SER | N | 0.90 |
| 1 | I | 311:ALA | C | 312:ASN | N | 0.90 |
| 1 | C | 243:GLY | C | 244:GLN | N | 0.88 |
| 1 | K | 243:GLY | C | 244:GLN | N | 0.88 |
| 1 | I | 7:LEU | C | 8:THR | N | 0.86 |
| 1 | B | 7:LEU | C | 8:THR | N | 0.85 |
| 1 | D | 7:LEU | C | 8:THR | N | 0.85 |
| 1 | F | 239:GLN | C | 240:LEU | N | 0.76 |
| 1 | C | 186:PRO | C | 187:GLN | N | 0.71 |
| 1 | G | 313:PHE | C | 314:SER | N | 0.71 |
| 1 | F | 186:PRO | C | 187:GLN | N | 0.67 |
| 1 | K | 186:PRO | C | 187:GLN | N | 0.63 |
| 1 | A | 313:PHE | C | 314:SER | N | 0.51 |

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.