



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 09:54 AM EDT

PDB ID : 4UQ8
EMDB ID: : EMD-2676
Title : Electron cryo-microscopy of bovine Complex I
Authors : Vinothkumar, K.R.; Zhu, J.; Hirst, J.
Deposited on : unknown
Resolution : 4.95 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

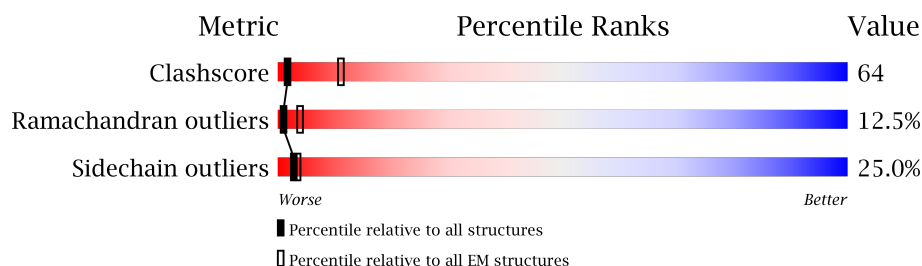
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.95 Å.

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



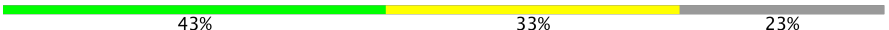










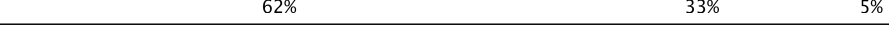





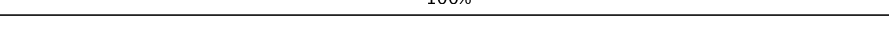
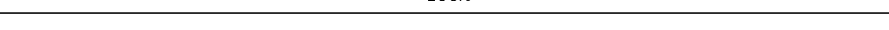
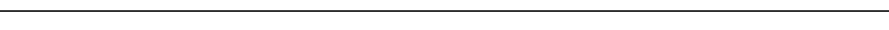

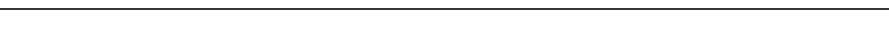
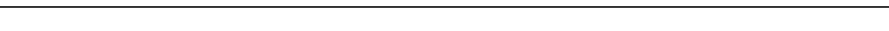


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 111 | 49% 26% 25% |
| 2 | B | 143 | 54% 43% .. |
| 3 | C | 154 | 63% 36% . |
| 4 | D | 384 | 63% 36% |
| 5 | E | 159 | 63% 37% |
| 6 | F | 411 | 49% 51% |
| 7 | G | 538 | 53% 44% .. |
| 8 | H | 313 | 57% 34% 9% |
| 9 | I | 162 | 55% 43% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 10 | J | 171 |  |
| 11 | K | 84 |  |
| 12 | L | 601 |  |
| 13 | M | 453 |  |
| 14 | N | 345 |  |
| 15 | O | 220 |  |
| 16 | P | 303 |  |
| 17 | Q | 85 |  |
| 18 | R | 47 |  |
| 19 | S | 80 |  |
| 20 | T | 75 |  |
| 21 | U | 79 |  |
| 22 | V | 71 |  |
| 23 | W | 72 |  |
| 24 | X | 79 |  |
| 25 | Y | 106 |  |
| 26 | Z | 65 |  |
| 27 | a | 29 |  |
| 28 | b | 42 |  |
| 29 | c | 27 |  |
| 29 | w | 27 |  |
| 30 | d | 39 |  |
| 31 | e | 20 |  |
| 32 | f | 30 |  |
| 32 | h | 30 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 32 | i | 30 |  100% |
| 33 | g | 22 |  100% |
| 34 | j | 24 |  100% |
| 34 | l | 24 |  100% |
| 35 | k | 28 |  100% |
| 35 | p | 28 |  100% |
| 35 | s | 28 |  100% |
| 36 | m | 34 |  100% |
| 37 | n | 59 |  100% |
| 38 | o | 21 |  100% |
| 39 | q | 25 |  100% |
| 40 | r | 26 |  100% |
| 41 | t | 57 |  100% |
| 42 | u | 43 |  35%  65% |
| 43 | v | 32 |  100% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 44 | SF4 | B | 201 | - | - | X | - |
| 44 | SF4 | I | 222 | - | - | X | - |
| 44 | SF4 | I | 223 | - | - | X | - |
| 45 | FES | G | 804 | - | - | X | - |

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 28647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1 | A | 83 | Total | C | N | O | 0 | 0 |
| | | | 415 | 249 | 83 | 83 | | |

- Molecule 2 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | B | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 719 | 429 | 143 | 143 | 4 | | |

- Molecule 3 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3 | C | 154 | Total | C | N | O | 0 | 0 |
| | | | 770 | 462 | 154 | 154 | | |

- Molecule 4 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 2, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 4 | D | 384 | Total | C | N | O | 0 | 0 |
| | | | 1920 | 1152 | 384 | 384 | | |

- Molecule 5 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 2, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | E | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 799 | 477 | 159 | 159 | 4 | | |

- Molecule 6 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 1, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | F | 411 | Total | C | N | O | S | 0 | 0 |
| | | | 2059 | 1233 | 411 | 411 | 4 | | |

- Molecule 7 is a protein called NADH-UBIQUINONE OXIDOREDUCTASE 75 KDA SUB-UNIT, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | G | 527 | Total | C | N | O | S | 0 | 0 |
| | | | 2651 | 1584 | 529 | 527 | 11 | | |

- Molecule 8 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | H | 285 | Total | C | N | O | S | 0 | 0 |
| | | | 1425 | 855 | 285 | 285 | | | |

- Molecule 9 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | I | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 486 | 162 | 162 | 8 | | |

- Molecule 10 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | J | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 655 | 393 | 131 | 131 | | | |

- Molecule 11 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11 | K | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 420 | 252 | 84 | 84 | | | |

- Molecule 12 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | L | 558 | Total | C | N | O | S | 0 | 0 |
| | | | 2790 | 1674 | 558 | 558 | | | |

- Molecule 13 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 13 | M | 439 | Total | C | N | O | 0 | 0 |
| | | | 2195 | 1317 | 439 | 439 | | |

- Molecule 14 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14 | N | 326 | Total | C | N | O | 0 | 0 |
| | | | 1630 | 978 | 326 | 326 | | |

- Molecule 15 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 10.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15 | O | 181 | Total | C | N | O | 0 | 0 |
| | | | 905 | 543 | 181 | 181 | | |

- Molecule 16 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 9, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 16 | P | 252 | Total | C | N | O | 0 | 0 |
| | | | 1260 | 756 | 252 | 252 | | |

- Molecule 17 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17 | Q | 69 | Total | C | N | O | 0 | 0 |
| | | | 345 | 207 | 69 | 69 | | |

- Molecule 18 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 18 | R | 47 | Total | C | N | O | 0 | 0 |
| | | | 235 | 141 | 47 | 47 | | |

- Molecule 19 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 19 | S | 80 | Total | C | N | O | 0 | 0 |
| | | | 400 | 240 | 80 | 80 | | |

- Molecule 20 is a protein called ACYL CARRIER PROTEIN, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 20 | T | 71 | Total | C | N | O | 0 | 0 |
| | | | 355 | 213 | 71 | 71 | | |

- Molecule 21 is a protein called NADH UBIQUINONE DEHYDROGENASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 21 | U | 75 | Total | C | N | O | 0 | 0 |
| | | | 375 | 225 | 75 | 75 | | |

- Molecule 22 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 22 | V | 71 | Total | C | N | O | 0 | 0 |
| | | | 355 | 213 | 71 | 71 | | |

- Molecule 23 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 23 | W | 72 | Total | C | N | O | 0 | 0 |
| | | | 360 | 216 | 72 | 72 | | |

- Molecule 24 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 24 | X | 79 | Total | C | N | O | 0 | 0 |
| | | | 395 | 237 | 79 | 79 | | |

- Molecule 25 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 25 | Y | 106 | Total | C | N | O | 0 | 0 |
| | | | 530 | 318 | 106 | 106 | | |

- Molecule 26 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 26 | Z | 65 | Total | C | N | O | 0 | 0 |
| | | | 325 | 195 | 65 | 65 | | |

- Molecule 27 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 27 | a | 29 | Total | C | N | O | 0 | 0 |
| | | | 145 | 87 | 29 | 29 | | |

- Molecule 28 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28 | b | 42 | Total | C | N | O | 0 | 0 |
| | | | 210 | 126 | 42 | 42 | | |

- Molecule 29 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 29 | c | 27 | Total | C | N | O | 0 | 0 |
| | | | 135 | 81 | 27 | 27 | | |
| 29 | w | 27 | Total | C | N | O | 0 | 0 |
| | | | 135 | 81 | 27 | 27 | | |

- Molecule 30 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 30 | d | 39 | Total | C | N | O | 0 | 0 |
| | | | 195 | 117 | 39 | 39 | | |

- Molecule 31 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 31 | e | 20 | Total | C | N | O | 0 | 0 |
| | | | 100 | 60 | 20 | 20 | | |

- Molecule 32 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 32 | f | 30 | Total | C | N | O | 0 | 0 |
| | | | 150 | 90 | 30 | 30 | | |
| 32 | h | 30 | Total | C | N | O | 0 | 0 |
| | | | 150 | 90 | 30 | 30 | | |
| 32 | i | 30 | Total | C | N | O | 0 | 0 |
| | | | 150 | 90 | 30 | 30 | | |

- Molecule 33 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 33 | g | 22 | Total | C | N | O | 0 | 0 |
| | | | 110 | 66 | 22 | 22 | | |

- Molecule 34 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 34 | j | 24 | Total | C | N | O | 0 | 0 |
| | | | 120 | 72 | 24 | 24 | | |
| 34 | l | 24 | Total | C | N | O | 0 | 0 |
| | | | 120 | 72 | 24 | 24 | | |

- Molecule 35 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 35 | k | 28 | Total | C | N | O | 0 | 0 |
| | | | 140 | 84 | 28 | 28 | | |
| 35 | p | 28 | Total | C | N | O | 0 | 0 |
| | | | 140 | 84 | 28 | 28 | | |
| 35 | s | 28 | Total | C | N | O | 0 | 0 |
| | | | 140 | 84 | 28 | 28 | | |

- Molecule 36 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 36 | m | 34 | Total | C | N | O | 0 | 0 |
| | | | 170 | 102 | 34 | 34 | | |

- Molecule 37 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 37 | n | 59 | Total | C | N | O | 0 | 0 |
| | | | 295 | 177 | 59 | 59 | | |

- Molecule 38 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 38 | o | 21 | Total | C | N | O | 0 | 0 |
| | | | 105 | 63 | 21 | 21 | | |

- Molecule 39 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 39 | q | 25 | Total | C | N | O | 0 | 0 |
| | | | 125 | 75 | 25 | 25 | | |

- Molecule 40 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 40 | r | 26 | Total | C | N | O | 0 | 0 |
| | | | 130 | 78 | 26 | 26 | | |

- Molecule 41 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 41 | t | 57 | Total | C | N | O | 0 | 0 |
| | | | 285 | 171 | 57 | 57 | | |

- Molecule 42 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 42 | u | 15 | Total | C | N | O | 0 | 0 |
| | | | 75 | 45 | 15 | 15 | | |

- Molecule 43 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

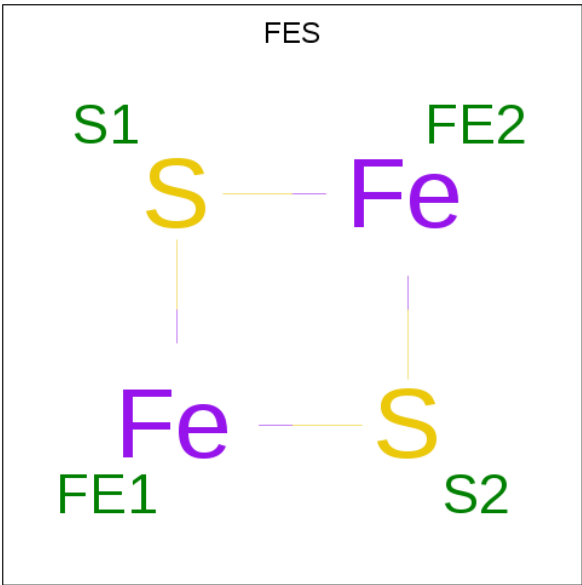
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 43 | v | 32 | Total | C | N | O | 0 | 0 |
| | | | 160 | 96 | 32 | 32 | | |

- Molecule 44 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 44 | B | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 44 | F | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 44 | G | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 44 | G | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 44 | I | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 44 | I | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

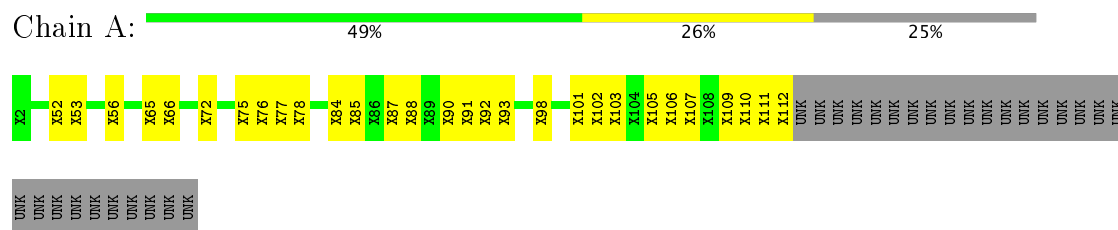


| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45 | E | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 45 | G | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

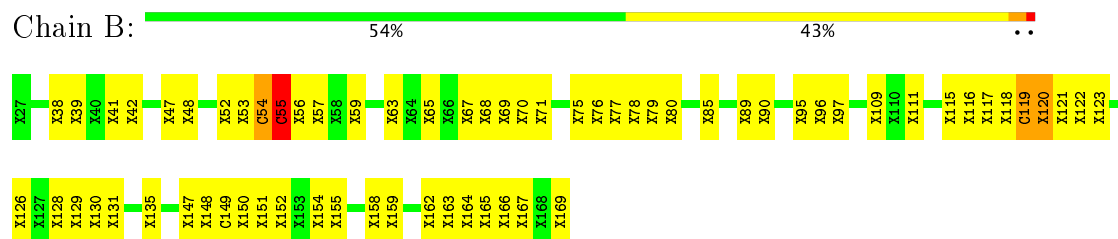
3 Residue-property plots

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.

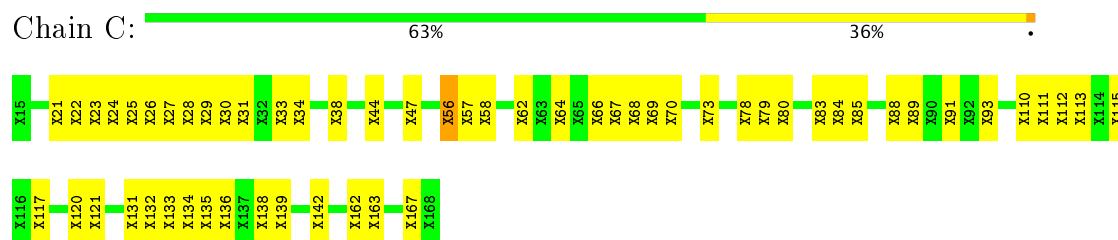
• Molecule 1: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 3



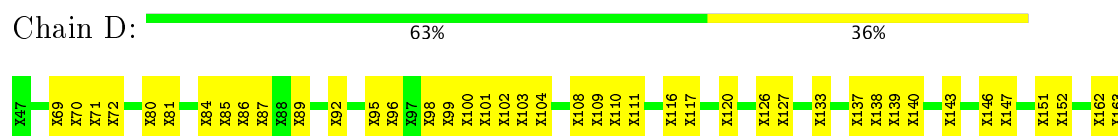
• Molecule 2: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL

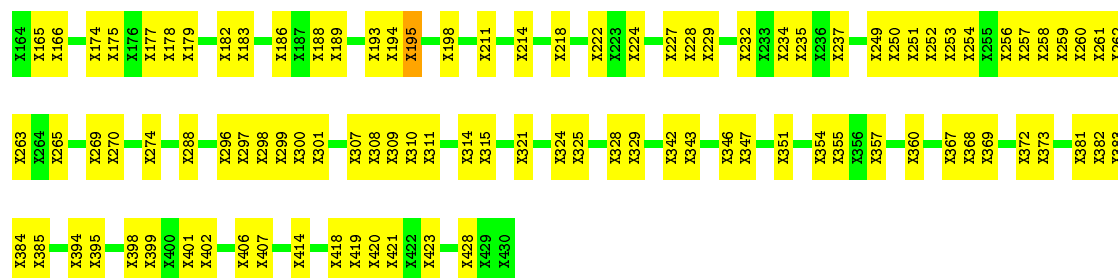


• Molecule 3: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL



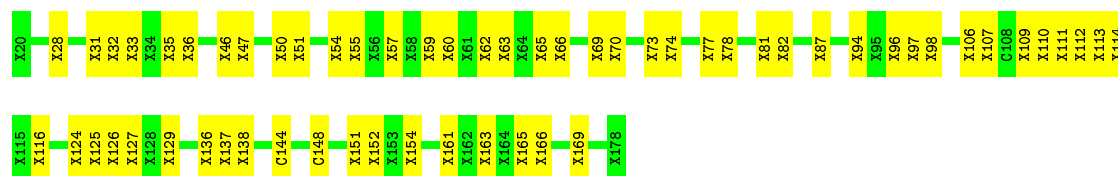
• Molecule 4: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 2, MITOCHONDRIAL





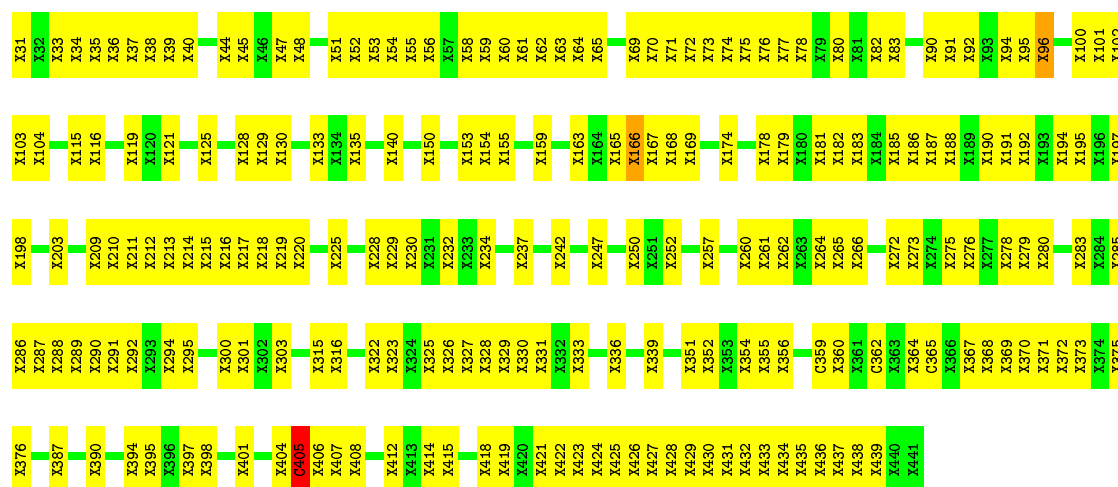
- Molecule 5: NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 2, MITOCHONDRIAL

Chain E: 63% 37%



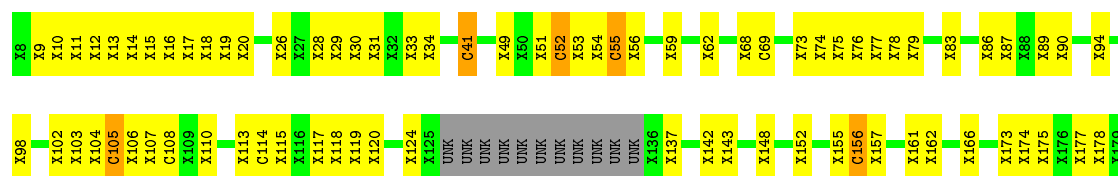
- Molecule 6: NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 1, MITOCHONDRIAL

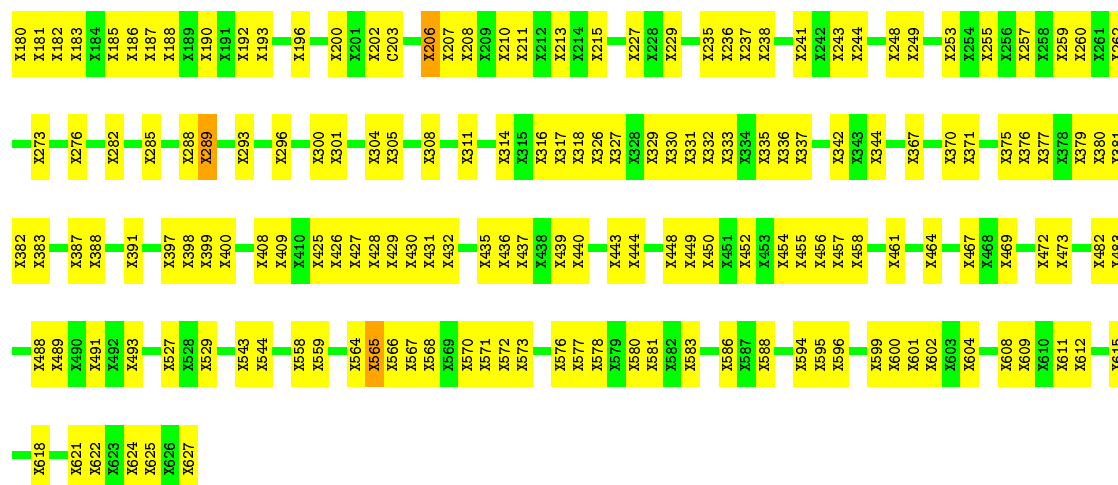
Chain F: 49% 51%



- Molecule 7: NADH-UBIQUINONE OXIDOREDUCTASE 75 KDA SUBUNIT, MITOCHONDRIAL

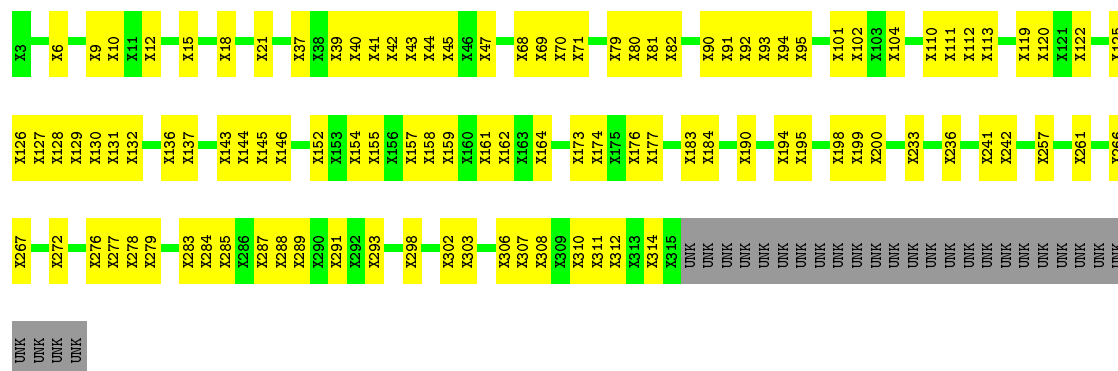
Chain G: 53% 44%





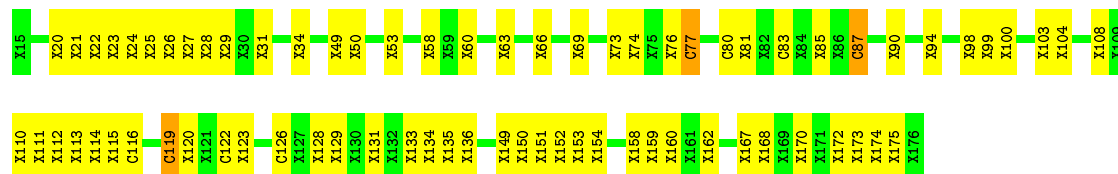
• Molecule 8: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1

Chain H: 57% 34% 9%



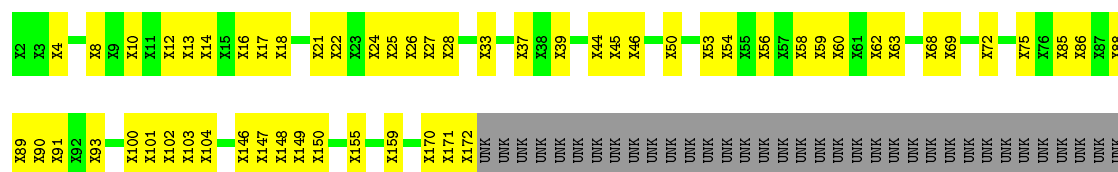
• Molecule 9: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL

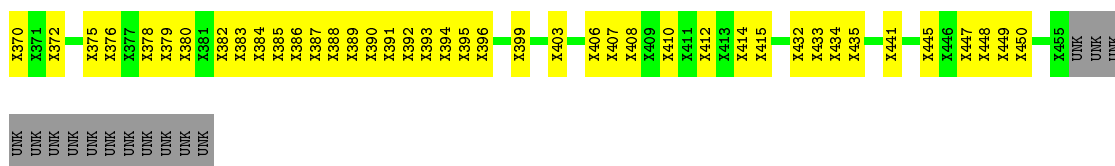
Chain I: 55% 43% 2%



• Molecule 10: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 6

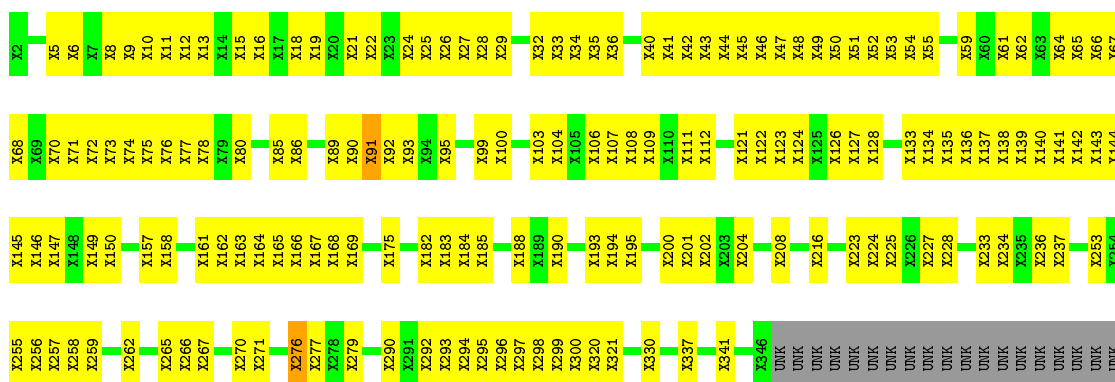
Chain J: 43% 33% 23%





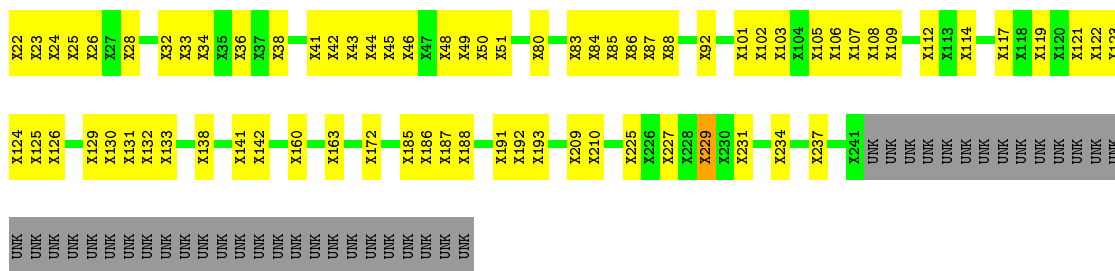
• Molecule 14: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 2

Chain N: 46% 48% 6%



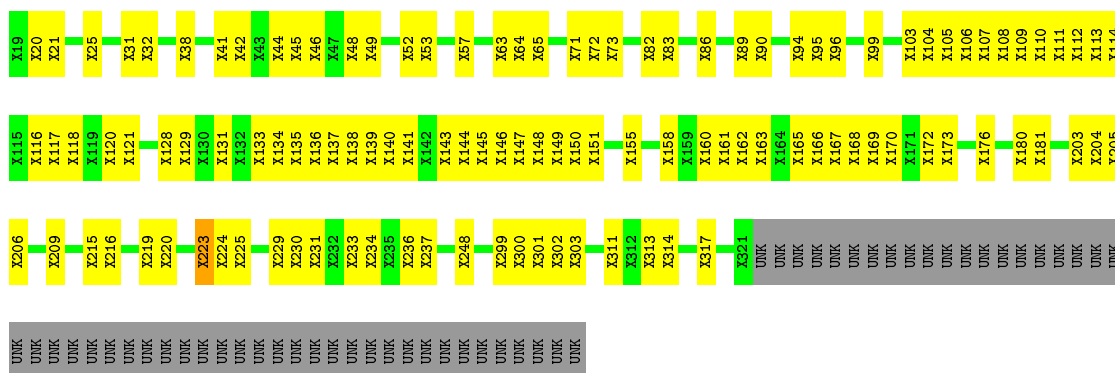
• Molecule 15: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 10

Chain O: 49% 33% 18%



• Molecule 16: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 9, MITOCHONDRIAL

Chain P: 45% 38% 17%



- Molecule 17: NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 4

Chain Q: 



- Molecule 18: NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 6

Chain R: 



- Molecule 19: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 2

Chain S: 



- Molecule 20: ACYL CARRIER PROTEIN, MITOCHONDRIAL

Chain T: 



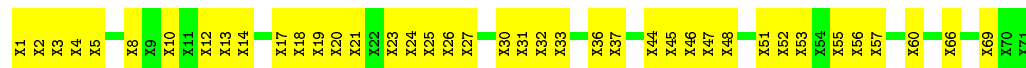
- Molecule 21: NADH UBIQUINONE DEHYDROGENASE

Chain U: 



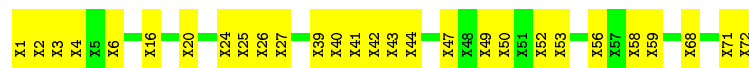
- Molecule 22: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 5

Chain V: 



- Molecule 23: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 6

Chain W: 



- Molecule 24: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 8

Chain X:  66% 34%



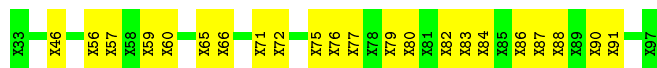
- Molecule 25: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT; 11

Chain Y:  67% 33%



- Molecule 26: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 13

Chain Z:  66% 34%



- Molecule 27: NADH UBIQUINONE OXIDOREDUCTASE

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: NADH UBIQUINONE OXIDOREDUCTASE

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: NADH UBIQUINONE OXIDOREDUCTASE

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: NADH UBIQUINONE OXIDOREDUCTASE

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: NADH UBIQUINONE OXIDOREDUCTASE

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: NADH UBIQUINONE OXIDOREDUCTASE

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: NADH UBIQUINONE OXIDOREDUCTASE

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: NADH UBIQUINONE OXIDOREDUCTASE

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: NADH UBIQUINONE OXIDOREDUCTASE

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: NADH UBIQUINONE OXIDOREDUCTASE

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: NADH UBIQUINONE OXIDOREDUCTASE

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: NADH UBIQUINONE OXIDOREDUCTASE

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: NADH UBIQUINONE OXIDOREDUCTASE

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: NADH UBIQUINONE OXIDOREDUCTASE

Chain r:  100%

There are no outlier residues recorded for this chain.

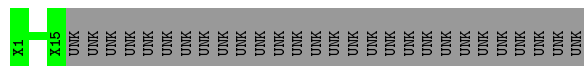
- Molecule 41: NADH UBIQUINONE OXIDOREDUCTASE

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: NADH UBIQUINONE OXIDOREDUCTASE

Chain u:  35% 65%



- Molecule 43: NADH UBIQUINONE OXIDOREDUCTASE

Chain v:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 25492 | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | EACH PARTICLE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 64 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 5000 | Depositor |
| Magnification | 81495 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES

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 | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 2 | B | 1.57 | 1/21 (4.8%) | 2.68 | 2/23 (8.7%) |
| 21 | U | 0.08 | 0/4 | 0.20 | 0/4 |
| 5 | E | 0.77 | 0/20 | 1.59 | 0/20 |
| 6 | F | 2.57 | 1/20 (5.0%) | 2.24 | 0/20 |
| 7 | G | 1.04 | 0/65 | 1.60 | 0/67 |
| 9 | I | 2.32 | 2/40 (5.0%) | 1.47 | 0/40 |
| All | All | 1.68 | 4/170 (2.4%) | 1.82 | 2/174 (1.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 12 | L | 0 | 4 |
| 14 | N | 0 | 2 |
| 15 | O | 0 | 2 |
| 16 | P | 0 | 3 |
| 17 | Q | 0 | 1 |
| 19 | S | 0 | 1 |
| 2 | B | 0 | 2 |
| 23 | W | 0 | 1 |
| 24 | X | 0 | 1 |
| 3 | C | 0 | 1 |
| 4 | D | 0 | 1 |
| 6 | F | 0 | 2 |
| 7 | G | 0 | 6 |
| 9 | I | 0 | 1 |
| All | All | 0 | 28 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6 | F | 405 | CYS | CA-CB | -8.99 | 1.34 | 1.53 |
| 9 | I | 87 | CYS | CA-CB | 7.91 | 1.71 | 1.53 |
| 9 | I | 77 | CYS | CA-CB | 6.99 | 1.69 | 1.53 |
| 2 | B | 55 | CYS | CA-CB | 5.36 | 1.65 | 1.53 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 55 | CYS | CA-CB-SG | -9.60 | 96.72 | 114.00 |
| 2 | B | 55 | CYS | CB-CA-C | -5.16 | 100.09 | 110.40 |

There are no chirality outliers.

All (28) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | B | 120 | UNK | Peptide |
| 2 | B | 130 | UNK | Peptide |
| 3 | C | 56 | UNK | Peptide |
| 4 | D | 195 | UNK | Peptide |
| 6 | F | 166 | UNK | Mainchain |
| 6 | F | 96 | UNK | Peptide |
| 7 | G | 177 | UNK | Peptide |
| 7 | G | 178 | UNK | Mainchain |
| 7 | G | 206 | UNK | Peptide |
| 7 | G | 289 | UNK | Peptide |
| 7 | G | 399 | UNK | Mainchain |
| 7 | G | 565 | UNK | Mainchain |
| 9 | I | 160 | UNK | Mainchain |
| 12 | L | 133 | UNK | Peptide |
| 12 | L | 366 | UNK | Peptide |
| 12 | L | 446 | UNK | Peptide |
| 12 | L | 546 | UNK | Mainchain |
| 14 | N | 276 | UNK | Peptide |
| 14 | N | 91 | UNK | Peptide |
| 15 | O | 229 | UNK | Peptide |
| 15 | O | 92 | UNK | Peptide |
| 16 | P | 223 | UNK | Peptide |
| 16 | P | 225 | UNK | Peptide |
| 16 | P | 42 | UNK | Peptide |
| 17 | Q | 40 | UNK | Peptide |
| 19 | S | 75 | UNK | Mainchain |
| 23 | W | 40 | UNK | Peptide |
| 24 | X | 56 | UNK | Peptide |

5.2 Too-close contacts ⓘ

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 | 415 | 0 | 88 | 26 | 0 |
| 2 | B | 719 | 0 | 161 | 89 | 0 |
| 3 | C | 770 | 0 | 163 | 66 | 0 |
| 4 | D | 1920 | 0 | 402 | 128 | 0 |
| 5 | E | 799 | 0 | 176 | 55 | 0 |
| 6 | F | 2059 | 0 | 444 | 258 | 0 |
| 7 | G | 2651 | 0 | 606 | 230 | 0 |
| 8 | H | 1425 | 0 | 295 | 105 | 0 |
| 9 | I | 818 | 0 | 195 | 77 | 0 |
| 10 | J | 655 | 0 | 138 | 51 | 0 |
| 11 | K | 420 | 0 | 89 | 18 | 0 |
| 12 | L | 2790 | 0 | 583 | 260 | 0 |
| 13 | M | 2195 | 0 | 455 | 212 | 0 |
| 14 | N | 1630 | 0 | 340 | 171 | 0 |
| 15 | O | 905 | 0 | 197 | 68 | 0 |
| 16 | P | 1260 | 0 | 271 | 142 | 0 |
| 17 | Q | 345 | 0 | 80 | 13 | 0 |
| 18 | R | 235 | 0 | 54 | 21 | 0 |
| 19 | S | 400 | 0 | 86 | 51 | 0 |
| 20 | T | 355 | 0 | 76 | 26 | 0 |
| 21 | U | 375 | 0 | 84 | 17 | 0 |
| 22 | V | 355 | 0 | 77 | 35 | 0 |
| 23 | W | 360 | 0 | 75 | 21 | 0 |
| 24 | X | 395 | 0 | 83 | 19 | 0 |
| 25 | Y | 530 | 0 | 111 | 29 | 0 |
| 26 | Z | 325 | 0 | 67 | 24 | 0 |
| 27 | a | 145 | 0 | 31 | 0 | 0 |
| 28 | b | 210 | 0 | 44 | 0 | 0 |
| 29 | c | 135 | 0 | 30 | 0 | 0 |
| 29 | w | 135 | 0 | 29 | 0 | 0 |
| 30 | d | 195 | 0 | 41 | 0 | 0 |
| 31 | e | 100 | 0 | 22 | 0 | 0 |
| 32 | f | 150 | 0 | 33 | 0 | 0 |
| 32 | h | 150 | 0 | 32 | 0 | 0 |
| 32 | i | 150 | 0 | 33 | 0 | 0 |
| 33 | g | 110 | 0 | 24 | 0 | 0 |
| 34 | j | 120 | 0 | 27 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34 | l | 120 | 0 | 26 | 0 | 0 |
| 35 | k | 140 | 0 | 30 | 0 | 0 |
| 35 | p | 140 | 0 | 30 | 0 | 0 |
| 35 | s | 140 | 0 | 31 | 0 | 0 |
| 36 | m | 170 | 0 | 36 | 0 | 0 |
| 37 | n | 295 | 0 | 61 | 0 | 0 |
| 38 | o | 105 | 0 | 23 | 0 | 0 |
| 39 | q | 125 | 0 | 27 | 0 | 0 |
| 40 | r | 130 | 0 | 28 | 0 | 0 |
| 41 | t | 285 | 0 | 61 | 0 | 0 |
| 42 | u | 75 | 0 | 17 | 0 | 0 |
| 43 | v | 160 | 0 | 34 | 0 | 0 |
| 44 | B | 8 | 0 | 0 | 4 | 0 |
| 44 | F | 8 | 0 | 0 | 1 | 0 |
| 44 | G | 16 | 0 | 0 | 0 | 0 |
| 44 | I | 16 | 0 | 0 | 5 | 0 |
| 45 | E | 4 | 0 | 0 | 0 | 0 |
| 45 | G | 4 | 0 | 0 | 2 | 0 |
| All | All | 28647 | 0 | 6146 | 2173 | 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 64.

All (2173) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:148:UNK:CB | 2:B:151:UNK:CA | 1.77 | 1.57 |
| 6:F:405:CYS:CB | 6:F:406:UNK:CB | 1.78 | 1.54 |
| 6:F:405:CYS:HB2 | 6:F:406:UNK:CB | 1.04 | 1.50 |
| 12:L:321:UNK:CB | 12:L:324:UNK:CB | 1.92 | 1.46 |
| 5:E:148:CYS:SG | 6:F:103:UNK:CB | 2.04 | 1.44 |
| 2:B:119:CYS:N | 2:B:122:UNK:CB | 1.81 | 1.44 |
| 7:G:55:CYS:HB2 | 7:G:68:UNK:CB | 1.49 | 1.42 |
| 12:L:247:UNK:HA | 12:L:251:UNK:CB | 1.52 | 1.37 |
| 5:E:148:CYS:CB | 6:F:103:UNK:CB | 2.06 | 1.33 |
| 5:E:148:CYS:HB2 | 6:F:103:UNK:CB | 1.59 | 1.31 |
| 6:F:405:CYS:CA | 6:F:406:UNK:CB | 2.07 | 1.29 |
| 5:E:148:CYS:SG | 6:F:102:UNK:O | 1.91 | 1.29 |
| 6:F:100:UNK:O | 6:F:102:UNK:N | 1.67 | 1.26 |
| 19:S:25:UNK:CA | 19:S:57:UNK:CB | 2.13 | 1.25 |
| 7:G:376:UNK:N | 7:G:449:UNK:N | 1.83 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 12:L:65:UNK:CB | 12:L:67:UNK:N | 1.98 | 1.24 |
| 12:L:161:UNK:HA | 12:L:162:UNK:C | 1.65 | 1.24 |
| 7:G:10:UNK:O | 7:G:76:UNK:HA | 1.33 | 1.24 |
| 2:B:119:CYS:CA | 2:B:122:UNK:CB | 2.18 | 1.22 |
| 16:P:170:UNK:CB | 16:P:204:UNK:HA | 1.70 | 1.21 |
| 7:G:55:CYS:CB | 7:G:68:UNK:CB | 2.19 | 1.21 |
| 6:F:408:UNK:CB | 44:F:508:SF4:S4 | 2.29 | 1.21 |
| 9:I:151:UNK:O | 9:I:154:UNK:N | 1.75 | 1.20 |
| 19:S:25:UNK:N | 19:S:57:UNK:CB | 2.06 | 1.18 |
| 12:L:161:UNK:HA | 12:L:163:UNK:N | 1.59 | 1.18 |
| 8:H:158:UNK:CB | 8:H:314:UNK:O | 1.93 | 1.17 |
| 12:L:225:UNK:HA | 12:L:229:UNK:CB | 1.73 | 1.17 |
| 7:G:152:UNK:CB | 7:G:206:UNK:CB | 2.23 | 1.16 |
| 6:F:405:CYS:HA | 6:F:406:UNK:CB | 1.70 | 1.15 |
| 13:M:58:UNK:HA | 13:M:59:UNK:CB | 1.71 | 1.13 |
| 13:M:347:UNK:O | 13:M:351:UNK:N | 1.81 | 1.13 |
| 14:N:103:UNK:O | 14:N:107:UNK:N | 1.83 | 1.12 |
| 8:H:40:UNK:C | 8:H:47:UNK:CB | 2.28 | 1.11 |
| 7:G:41:CYS:N | 45:G:804:FES:S2 | 2.23 | 1.10 |
| 16:P:103:UNK:O | 16:P:107:UNK:N | 1.84 | 1.10 |
| 24:X:77:UNK:O | 24:X:79:UNK:N | 1.84 | 1.10 |
| 7:G:10:UNK:O | 7:G:76:UNK:CA | 1.99 | 1.10 |
| 7:G:377:UNK:H | 7:G:449:UNK:HA | 1.00 | 1.10 |
| 2:B:119:CYS:HA | 2:B:122:UNK:CB | 1.80 | 1.10 |
| 16:P:203:UNK:HA | 16:P:234:UNK:HA | 1.33 | 1.09 |
| 25:Y:102:UNK:O | 25:Y:105:UNK:CB | 2.01 | 1.08 |
| 8:H:143:UNK:O | 8:H:146:UNK:N | 1.86 | 1.08 |
| 10:J:101:UNK:O | 10:J:104:UNK:N | 1.86 | 1.08 |
| 2:B:118:UNK:O | 2:B:122:UNK:N | 1.85 | 1.07 |
| 25:Y:11:UNK:HA | 25:Y:48:UNK:CB | 1.84 | 1.07 |
| 6:F:423:UNK:O | 6:F:427:UNK:N | 1.87 | 1.07 |
| 10:J:68:UNK:O | 10:J:72:UNK:N | 1.87 | 1.07 |
| 16:P:105:UNK:O | 16:P:109:UNK:N | 1.87 | 1.07 |
| 12:L:32:UNK:O | 12:L:36:UNK:N | 1.87 | 1.07 |
| 3:C:34:UNK:O | 3:C:38:UNK:N | 1.88 | 1.07 |
| 15:O:229:UNK:CB | 15:O:231:UNK:CA | 2.32 | 1.07 |
| 16:P:21:UNK:N | 16:P:44:UNK:O | 1.88 | 1.07 |
| 12:L:209:UNK:O | 12:L:212:UNK:N | 1.88 | 1.07 |
| 16:P:106:UNK:O | 16:P:110:UNK:N | 1.87 | 1.07 |
| 8:H:6:UNK:O | 8:H:10:UNK:CB | 4.00 | 1.06 |
| 12:L:29:UNK:O | 12:L:33:UNK:N | 1.88 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 7:G:175:UNK:N | 7:G:182:UNK:O | 1.87 | 1.06 |
| 12:L:4:UNK:O | 12:L:8:UNK:N | 3.34 | 1.06 |
| 7:G:227:UNK:O | 7:G:238:UNK:O | 1.72 | 1.05 |
| 15:O:229:UNK:CB | 15:O:231:UNK:N | 2.19 | 1.05 |
| 5:E:70:UNK:O | 5:E:74:UNK:N | 1.89 | 1.05 |
| 19:S:40:UNK:O | 19:S:44:UNK:N | 1.88 | 1.05 |
| 12:L:33:UNK:O | 12:L:37:UNK:N | 1.90 | 1.04 |
| 7:G:241:UNK:O | 7:G:248:UNK:N | 1.88 | 1.04 |
| 5:E:148:CYS:SG | 6:F:102:UNK:C | 2.45 | 1.04 |
| 6:F:262:UNK:CB | 6:F:286:UNK:N | 2.21 | 1.04 |
| 7:G:435:UNK:C | 7:G:437:UNK:HA | 1.86 | 1.04 |
| 8:H:177:UNK:HA | 26:Z:46:UNK:CB | 1.86 | 1.04 |
| 19:S:25:UNK:CB | 19:S:57:UNK:CB | 2.36 | 1.03 |
| 16:P:133:UNK:N | 16:P:166:UNK:O | 1.91 | 1.03 |
| 25:Y:103:UNK:O | 25:Y:106:UNK:N | 1.92 | 1.02 |
| 12:L:28:UNK:O | 12:L:32:UNK:N | 1.92 | 1.02 |
| 6:F:369:UNK:O | 6:F:370:UNK:O | 1.78 | 1.02 |
| 6:F:422:UNK:O | 6:F:426:UNK:N | 1.92 | 1.02 |
| 6:F:261:UNK:O | 6:F:286:UNK:O | 1.75 | 1.02 |
| 7:G:142:UNK:O | 7:G:190:UNK:HA | 1.59 | 1.02 |
| 16:P:300:UNK:HA | 16:P:302:UNK:CB | 1.90 | 1.01 |
| 16:P:172:UNK:N | 16:P:205:UNK:O | 1.93 | 1.01 |
| 4:D:133:UNK:CB | 4:D:321:UNK:CB | 2.39 | 1.01 |
| 12:L:181:UNK:O | 12:L:184:UNK:N | 1.92 | 1.01 |
| 18:R:77:UNK:O | 18:R:78:UNK:C | 2.09 | 1.01 |
| 7:G:604:UNK:CB | 7:G:609:UNK:O | 2.08 | 1.01 |
| 6:F:294:UNK:N | 6:F:339:UNK:CB | 2.23 | 1.01 |
| 6:F:51:UNK:HA | 6:F:52:UNK:CB | 1.90 | 1.01 |
| 6:F:74:UNK:CB | 6:F:77:UNK:CB | 2.38 | 1.01 |
| 17:Q:99:UNK:HA | 17:Q:100:UNK:CB | 1.90 | 1.00 |
| 2:B:118:UNK:C | 2:B:122:UNK:CB | 2.39 | 1.00 |
| 25:Y:55:UNK:O | 25:Y:58:UNK:CB | 2.08 | 1.00 |
| 7:G:435:UNK:CB | 7:G:440:UNK:CB | 2.38 | 1.00 |
| 16:P:170:UNK:O | 16:P:205:UNK:N | 1.94 | 1.00 |
| 16:P:108:UNK:O | 16:P:112:UNK:N | 1.94 | 1.00 |
| 2:B:148:UNK:CB | 2:B:151:UNK:C | 2.38 | 0.99 |
| 7:G:380:UNK:CB | 7:G:408:UNK:CB | 2.39 | 0.99 |
| 7:G:55:CYS:SG | 7:G:68:UNK:CB | 2.50 | 0.99 |
| 12:L:247:UNK:O | 12:L:252:UNK:N | 1.95 | 0.99 |
| 24:X:93:UNK:CB | 24:X:94:UNK:CB | 2.39 | 0.99 |
| 10:J:147:UNK:O | 10:J:149:UNK:N | 1.95 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:F:289:UNK:HA | 6:F:290:UNK:C | 1.93 | 0.99 |
| 4:D:101:UNK:O | 4:D:102:UNK:C | 2.09 | 0.99 |
| 6:F:423:UNK:HA | 6:F:426:UNK:CB | 1.92 | 0.99 |
| 6:F:288:UNK:CB | 6:F:291:UNK:CB | 2.40 | 0.99 |
| 12:L:239:UNK:O | 12:L:240:UNK:C | 2.07 | 0.99 |
| 5:E:87:UNK:CB | 6:F:181:UNK:CB | 2.40 | 0.98 |
| 19:S:63:UNK:C | 19:S:78:UNK:CB | 2.40 | 0.98 |
| 12:L:131:UNK:HA | 12:L:143:UNK:CB | 1.92 | 0.98 |
| 13:M:387:UNK:C | 13:M:389:UNK:HA | 1.93 | 0.98 |
| 14:N:293:UNK:O | 14:N:294:UNK:C | 2.09 | 0.97 |
| 2:B:118:UNK:O | 2:B:121:UNK:N | 1.97 | 0.97 |
| 12:L:82:UNK:O | 12:L:87:UNK:N | 1.96 | 0.97 |
| 5:E:144:CYS:SG | 6:F:102:UNK:HA | 2.03 | 0.97 |
| 7:G:52:CYS:O | 7:G:53:UNK:C | 2.13 | 0.97 |
| 3:C:64:UNK:O | 3:C:70:UNK:CB | 2.13 | 0.97 |
| 8:H:40:UNK:O | 8:H:47:UNK:CA | 2.12 | 0.97 |
| 12:L:189:UNK:O | 12:L:194:UNK:N | 1.98 | 0.96 |
| 14:N:276:UNK:O | 14:N:279:UNK:N | 1.98 | 0.96 |
| 12:L:246:UNK:O | 12:L:251:UNK:N | 1.96 | 0.96 |
| 4:D:162:UNK:HA | 8:H:279:UNK:CB | 1.95 | 0.96 |
| 8:H:9:UNK:O | 8:H:12:UNK:CB | 4.04 | 0.96 |
| 7:G:435:UNK:HA | 7:G:440:UNK:CB | 1.96 | 0.96 |
| 22:V:55:UNK:O | 22:V:57:UNK:N | 1.98 | 0.96 |
| 7:G:377:UNK:N | 7:G:449:UNK:HA | 1.80 | 0.96 |
| 6:F:166:UNK:O | 6:F:169:UNK:N | 1.99 | 0.96 |
| 15:O:129:UNK:O | 15:O:132:UNK:CB | 2.14 | 0.96 |
| 7:G:14:UNK:N | 7:G:79:UNK:O | 1.99 | 0.95 |
| 7:G:376:UNK:N | 7:G:448:UNK:C | 2.17 | 0.95 |
| 8:H:40:UNK:O | 8:H:47:UNK:CB | 2.12 | 0.95 |
| 19:S:25:UNK:HA | 19:S:57:UNK:CB | 1.93 | 0.95 |
| 19:S:26:UNK:O | 19:S:28:UNK:O | 5.29 | 0.95 |
| 13:M:388:UNK:N | 13:M:389:UNK:HA | 1.79 | 0.95 |
| 14:N:100:UNK:O | 14:N:104:UNK:N | 2.00 | 0.95 |
| 15:O:188:UNK:O | 15:O:192:UNK:N | 1.99 | 0.95 |
| 7:G:483:UNK:HA | 7:G:576:UNK:CB | 1.96 | 0.95 |
| 12:L:319:UNK:O | 12:L:320:UNK:CB | 2.13 | 0.95 |
| 6:F:190:UNK:CB | 6:F:203:UNK:HA | 1.96 | 0.95 |
| 2:B:48:UNK:CB | 2:B:80:UNK:HA | 1.96 | 0.95 |
| 12:L:83:UNK:HA | 12:L:87:UNK:CB | 1.97 | 0.94 |
| 15:O:87:UNK:CB | 15:O:88:UNK:HA | 1.96 | 0.94 |
| 6:F:155:UNK:O | 6:F:159:UNK:N | 2.00 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:F:51:UNK:CA | 6:F:52:UNK:CB | 2.45 | 0.94 |
| 7:G:142:UNK:O | 7:G:190:UNK:CB | 2.14 | 0.94 |
| 13:M:58:UNK:CA | 13:M:59:UNK:CB | 2.42 | 0.94 |
| 24:X:90:UNK:O | 24:X:92:UNK:N | 2.00 | 0.94 |
| 2:B:52:UNK:CB | 2:B:89:UNK:O | 2.15 | 0.93 |
| 13:M:51:UNK:CB | 13:M:58:UNK:CB | 2.46 | 0.93 |
| 6:F:34:UNK:O | 6:F:38:UNK:N | 2.02 | 0.93 |
| 6:F:121:UNK:CB | 6:F:229:UNK:HA | 1.99 | 0.93 |
| 6:F:60:UNK:O | 6:F:64:UNK:N | 2.02 | 0.93 |
| 13:M:103:UNK:O | 13:M:107:UNK:N | 2.02 | 0.93 |
| 10:J:58:UNK:O | 10:J:62:UNK:N | 2.00 | 0.93 |
| 3:C:83:UNK:O | 3:C:85:UNK:N | 2.02 | 0.92 |
| 18:R:63:UNK:O | 18:R:64:UNK:C | 2.14 | 0.92 |
| 15:O:49:UNK:HA | 15:O:50:UNK:CB | 1.98 | 0.92 |
| 6:F:426:UNK:HA | 6:F:429:UNK:CB | 2.00 | 0.92 |
| 7:G:237:UNK:O | 7:G:253:UNK:N | 2.02 | 0.92 |
| 14:N:43:UNK:O | 14:N:46:UNK:N | 2.71 | 0.92 |
| 16:P:109:UNK:O | 16:P:113:UNK:N | 2.03 | 0.92 |
| 23:W:49:UNK:HA | 23:W:52:UNK:CB | 1.99 | 0.92 |
| 6:F:372:UNK:O | 6:F:376:UNK:N | 2.03 | 0.92 |
| 25:Y:102:UNK:O | 25:Y:105:UNK:N | 2.03 | 0.92 |
| 7:G:377:UNK:H | 7:G:449:UNK:CA | 1.83 | 0.92 |
| 12:L:210:UNK:O | 12:L:214:UNK:N | 2.01 | 0.92 |
| 13:M:189:UNK:N | 13:M:191:UNK:O | 2.03 | 0.92 |
| 3:C:83:UNK:O | 3:C:84:UNK:C | 2.16 | 0.92 |
| 12:L:321:UNK:O | 12:L:324:UNK:CB | 2.18 | 0.92 |
| 22:V:45:UNK:O | 22:V:48:UNK:N | 2.02 | 0.92 |
| 14:N:142:UNK:O | 14:N:145:UNK:CB | 2.18 | 0.91 |
| 16:P:52:UNK:HA | 16:P:72:UNK:CB | 2.00 | 0.91 |
| 2:B:148:UNK:CB | 2:B:151:UNK:CB | 2.48 | 0.91 |
| 22:V:44:UNK:O | 22:V:47:UNK:CB | 2.19 | 0.91 |
| 12:L:247:UNK:CA | 12:L:251:UNK:CB | 2.47 | 0.91 |
| 12:L:55:UNK:N | 12:L:56:UNK:O | 2.02 | 0.91 |
| 20:T:55:UNK:CB | 20:T:60:UNK:O | 2.19 | 0.91 |
| 3:C:21:UNK:O | 3:C:24:UNK:N | 2.02 | 0.91 |
| 6:F:287:UNK:O | 6:F:291:UNK:O | 1.87 | 0.91 |
| 7:G:142:UNK:O | 7:G:190:UNK:CA | 2.18 | 0.91 |
| 7:G:436:UNK:N | 7:G:437:UNK:HA | 1.82 | 0.91 |
| 7:G:604:UNK:O | 7:G:608:UNK:N | 2.04 | 0.91 |
| 3:C:133:UNK:HA | 3:C:136:UNK:CB | 2.01 | 0.91 |
| 3:C:25:UNK:O | 3:C:26:UNK:O | 3.07 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:F:33:UNK:O | 6:F:37:UNK:N | 2.04 | 0.91 |
| 9:I:113:UNK:O | 9:I:115:UNK:O | 1.89 | 0.90 |
| 18:R:77:UNK:O | 18:R:78:UNK:O | 1.89 | 0.90 |
| 3:C:131:UNK:O | 3:C:132:UNK:C | 2.18 | 0.90 |
| 7:G:193:UNK:HA | 7:G:196:UNK:CB | 2.01 | 0.90 |
| 12:L:263:UNK:O | 12:L:265:UNK:N | 2.05 | 0.90 |
| 23:W:39:UNK:C | 23:W:41:UNK:CB | 2.49 | 0.90 |
| 6:F:52:UNK:O | 6:F:56:UNK:N | 2.05 | 0.90 |
| 4:D:96:UNK:N | 4:D:385:UNK:CB | 2.35 | 0.90 |
| 13:M:347:UNK:O | 13:M:351:UNK:CB | 2.20 | 0.89 |
| 12:L:161:UNK:CA | 12:L:162:UNK:C | 2.41 | 0.89 |
| 15:O:234:UNK:O | 15:O:237:UNK:CB | 2.20 | 0.89 |
| 12:L:29:UNK:HA | 12:L:32:UNK:CB | 2.03 | 0.89 |
| 13:M:348:UNK:HA | 13:M:351:UNK:CB | 2.03 | 0.88 |
| 14:N:33:UNK:O | 14:N:36:UNK:N | 2.06 | 0.88 |
| 14:N:5:UNK:O | 14:N:8:UNK:N | 3.27 | 0.88 |
| 13:M:68:UNK:O | 13:M:69:UNK:C | 2.19 | 0.88 |
| 3:C:89:UNK:N | 3:C:112:UNK:O | 2.07 | 0.88 |
| 4:D:395:UNK:O | 4:D:399:UNK:N | 2.07 | 0.88 |
| 12:L:151:UNK:O | 12:L:155:UNK:CB | 2.21 | 0.88 |
| 2:B:121:UNK:HA | 2:B:135:UNK:CB | 2.03 | 0.87 |
| 6:F:369:UNK:O | 6:F:370:UNK:C | 2.21 | 0.87 |
| 21:U:23:UNK:CB | 21:U:24:UNK:HA | 2.03 | 0.87 |
| 6:F:212:UNK:HA | 6:F:220:UNK:O | 1.74 | 0.87 |
| 6:F:294:UNK:CA | 6:F:339:UNK:CB | 2.52 | 0.87 |
| 6:F:359:CYS:O | 6:F:360:UNK:CB | 2.22 | 0.87 |
| 7:G:318:UNK:O | 7:G:529:UNK:N | 2.07 | 0.87 |
| 16:P:106:UNK:HA | 16:P:109:UNK:CB | 2.05 | 0.87 |
| 16:P:71:UNK:O | 16:P:72:UNK:C | 2.18 | 0.87 |
| 6:F:323:UNK:O | 6:F:326:UNK:N | 2.08 | 0.87 |
| 9:I:111:UNK:O | 9:I:113:UNK:N | 2.06 | 0.87 |
| 7:G:435:UNK:CA | 7:G:440:UNK:CB | 2.53 | 0.87 |
| 12:L:321:UNK:O | 12:L:324:UNK:N | 2.08 | 0.87 |
| 13:M:49:UNK:HA | 13:M:50:UNK:CB | 2.05 | 0.87 |
| 16:P:21:UNK:O | 16:P:46:UNK:N | 2.08 | 0.87 |
| 6:F:419:UNK:HA | 6:F:423:UNK:CB | 2.05 | 0.86 |
| 7:G:380:UNK:O | 7:G:409:UNK:N | 2.08 | 0.86 |
| 9:I:123:UNK:CB | 9:I:131:UNK:O | 2.23 | 0.86 |
| 14:N:146:UNK:N | 14:N:147:UNK:HA | 1.89 | 0.86 |
| 6:F:60:UNK:O | 6:F:63:UNK:CB | 2.24 | 0.86 |
| 7:G:192:UNK:HA | 7:G:193:UNK:CB | 2.06 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 26:Z:77:UNK:O | 26:Z:80:UNK:N | 2.08 | 0.86 |
| 13:M:281:UNK:O | 13:M:284:UNK:CB | 2.24 | 0.86 |
| 16:P:99:UNK:CB | 16:P:103:UNK:CB | 2.54 | 0.86 |
| 16:P:21:UNK:CB | 16:P:45:UNK:HA | 2.04 | 0.86 |
| 7:G:52:CYS:O | 7:G:54:UNK:N | 2.08 | 0.86 |
| 8:H:120:UNK:CB | 8:H:132:UNK:CB | 2.54 | 0.86 |
| 12:L:316:UNK:O | 12:L:319:UNK:N | 2.09 | 0.86 |
| 13:M:146:UNK:O | 13:M:149:UNK:N | 2.09 | 0.85 |
| 23:W:47:UNK:CB | 23:W:50:UNK:CB | 2.54 | 0.85 |
| 12:L:67:UNK:CB | 12:L:76:UNK:HA | 2.05 | 0.85 |
| 14:N:72:UNK:O | 14:N:75:UNK:CB | 2.24 | 0.85 |
| 1:A:103:UNK:HA | 1:A:106:UNK:CB | 2.07 | 0.85 |
| 16:P:301:UNK:HA | 16:P:302:UNK:CB | 2.06 | 0.85 |
| 15:O:229:UNK:CB | 15:O:231:UNK:HA | 2.04 | 0.85 |
| 7:G:174:UNK:HA | 7:G:183:UNK:HA | 1.55 | 0.85 |
| 7:G:187:UNK:N | 7:G:188:UNK:HA | 1.88 | 0.85 |
| 12:L:46:UNK:O | 12:L:49:UNK:CB | 2.25 | 0.84 |
| 16:P:63:UNK:C | 16:P:65:UNK:CB | 2.55 | 0.84 |
| 12:L:288:UNK:CB | 12:L:308:UNK:CB | 2.55 | 0.84 |
| 14:N:89:UNK:C | 14:N:91:UNK:HA | 2.07 | 0.84 |
| 6:F:300:UNK:CB | 6:F:329:UNK:HA | 2.06 | 0.84 |
| 1:A:102:UNK:O | 1:A:106:UNK:N | 2.10 | 0.84 |
| 14:N:128:UNK:CB | 14:N:216:UNK:CB | 2.55 | 0.84 |
| 19:S:27:UNK:O | 19:S:28:UNK:CB | 2.24 | 0.84 |
| 20:T:33:UNK:O | 20:T:36:UNK:CB | 8.74 | 0.84 |
| 2:B:148:UNK:CB | 2:B:152:UNK:N | 2.41 | 0.84 |
| 6:F:56:UNK:O | 6:F:59:UNK:CB | 2.26 | 0.84 |
| 19:S:43:UNK:O | 19:S:47:UNK:N | 2.10 | 0.84 |
| 19:S:63:UNK:O | 19:S:78:UNK:HA | 1.78 | 0.84 |
| 3:C:23:UNK:HA | 3:C:26:UNK:CB | 2.08 | 0.84 |
| 12:L:34:UNK:O | 12:L:38:UNK:N | 2.10 | 0.84 |
| 13:M:176:UNK:N | 13:M:177:UNK:HA | 1.89 | 0.84 |
| 18:R:67:UNK:C | 18:R:69:UNK:N | 2.33 | 0.84 |
| 8:H:43:UNK:N | 8:H:44:UNK:HA | 1.91 | 0.83 |
| 12:L:297:UNK:HA | 12:L:356:UNK:N | 1.92 | 0.83 |
| 14:N:233:UNK:O | 14:N:236:UNK:CB | 2.25 | 0.83 |
| 6:F:303:UNK:O | 6:F:414:UNK:CB | 2.26 | 0.83 |
| 12:L:197:UNK:O | 12:L:201:UNK:N | 2.11 | 0.83 |
| 6:F:365:CYS:HA | 6:F:368:UNK:CB | 2.08 | 0.83 |
| 10:J:12:UNK:HA | 11:K:7:UNK:CB | 10.90 | 0.83 |
| 20:T:55:UNK:O | 20:T:59:UNK:N | 2.11 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 15:O:229:UNK:CB | 15:O:231:UNK:CB | 2.57 | 0.83 |
| 3:C:131:UNK:O | 3:C:134:UNK:N | 2.12 | 0.83 |
| 12:L:321:UNK:O | 12:L:325:UNK:N | 2.12 | 0.83 |
| 7:G:594:UNK:HA | 7:G:595:UNK:CB | 2.06 | 0.82 |
| 20:T:34:UNK:O | 20:T:37:UNK:N | 6.53 | 0.82 |
| 4:D:258:UNK:O | 4:D:262:UNK:N | 2.12 | 0.82 |
| 7:G:104:UNK:O | 7:G:107:UNK:N | 2.12 | 0.82 |
| 13:M:281:UNK:O | 13:M:285:UNK:N | 2.13 | 0.82 |
| 9:I:22:UNK:O | 9:I:25:UNK:N | 2.68 | 0.82 |
| 2:B:78:UNK:N | 2:B:79:UNK:HA | 1.94 | 0.82 |
| 19:S:24:UNK:CB | 19:S:59:UNK:O | 2.27 | 0.82 |
| 6:F:294:UNK:C | 6:F:339:UNK:CB | 2.52 | 0.82 |
| 6:F:426:UNK:O | 6:F:429:UNK:N | 2.12 | 0.82 |
| 7:G:595:UNK:O | 7:G:599:UNK:N | 2.12 | 0.82 |
| 17:Q:109:UNK:HA | 17:Q:110:UNK:CB | 2.09 | 0.82 |
| 4:D:250:UNK:O | 4:D:253:UNK:N | 2.12 | 0.82 |
| 16:P:172:UNK:O | 16:P:206:UNK:HA | 1.80 | 0.82 |
| 7:G:41:CYS:HB2 | 45:G:804:FES:S2 | 2.20 | 0.82 |
| 5:E:98:UNK:O | 5:E:137:UNK:HA | 1.80 | 0.81 |
| 6:F:405:CYS:SG | 6:F:407:UNK:N | 2.53 | 0.81 |
| 16:P:223:UNK:HA | 16:P:224:UNK:CB | 2.10 | 0.81 |
| 6:F:44:UNK:O | 6:F:47:UNK:N | 2.13 | 0.81 |
| 12:L:77:UNK:HA | 12:L:78:UNK:CB | 2.09 | 0.81 |
| 16:P:64:UNK:N | 16:P:65:UNK:CB | 2.43 | 0.81 |
| 9:I:98:UNK:O | 9:I:103:UNK:O | 1.98 | 0.81 |
| 8:H:68:UNK:O | 8:H:69:UNK:C | 2.24 | 0.81 |
| 13:M:210:UNK:HA | 13:M:268:UNK:CB | 2.10 | 0.81 |
| 6:F:265:UNK:O | 6:F:266:UNK:CB | 2.29 | 0.81 |
| 14:N:10:UNK:O | 14:N:13:UNK:N | 2.61 | 0.81 |
| 16:P:131:UNK:O | 16:P:165:UNK:HA | 1.80 | 0.81 |
| 13:M:118:UNK:O | 13:M:122:UNK:N | 2.14 | 0.81 |
| 16:P:103:UNK:O | 16:P:106:UNK:N | 2.13 | 0.81 |
| 2:B:121:UNK:C | 2:B:135:UNK:HA | 2.12 | 0.80 |
| 6:F:264:UNK:CB | 6:F:283:UNK:O | 2.29 | 0.80 |
| 12:L:225:UNK:CA | 12:L:229:UNK:CB | 2.58 | 0.80 |
| 16:P:203:UNK:HA | 16:P:234:UNK:CA | 2.11 | 0.80 |
| 19:S:26:UNK:O | 19:S:27:UNK:C | 3.97 | 0.80 |
| 2:B:154:UNK:O | 2:B:158:UNK:N | 2.15 | 0.80 |
| 7:G:428:UNK:O | 7:G:432:UNK:N | 2.14 | 0.80 |
| 12:L:578:UNK:O | 12:L:579:UNK:C | 2.28 | 0.80 |
| 16:P:139:UNK:HA | 16:P:140:UNK:CB | 2.12 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 5:E:165:UNK:O | 5:E:169:UNK:N | 2.14 | 0.80 |
| 16:P:146:UNK:O | 16:P:149:UNK:N | 2.15 | 0.80 |
| 12:L:321:UNK:O | 12:L:324:UNK:CA | 2.29 | 0.80 |
| 13:M:108:UNK:HA | 13:M:111:UNK:CB | 2.12 | 0.80 |
| 16:P:145:UNK:O | 16:P:148:UNK:CB | 2.30 | 0.80 |
| 20:T:62:UNK:CB | 20:T:66:UNK:CB | 2.60 | 0.80 |
| 9:I:94:UNK:HA | 9:I:108:UNK:O | 1.82 | 0.80 |
| 16:P:170:UNK:CB | 16:P:204:UNK:CA | 2.57 | 0.80 |
| 16:P:53:UNK:CB | 16:P:57:UNK:CB | 2.60 | 0.80 |
| 19:S:41:UNK:HA | 19:S:44:UNK:CB | 2.11 | 0.80 |
| 19:S:83:UNK:O | 19:S:87:UNK:N | 2.15 | 0.80 |
| 6:F:212:UNK:O | 6:F:220:UNK:N | 2.15 | 0.80 |
| 6:F:133:UNK:CB | 6:F:174:UNK:CB | 2.60 | 0.79 |
| 13:M:241:UNK:O | 13:M:244:UNK:N | 2.15 | 0.79 |
| 7:G:381:UNK:HA | 7:G:409:UNK:O | 1.82 | 0.79 |
| 9:I:128:UNK:O | 9:I:129:UNK:C | 2.29 | 0.79 |
| 19:S:84:UNK:O | 19:S:88:UNK:N | 2.14 | 0.79 |
| 16:P:311:UNK:O | 16:P:314:UNK:N | 2.16 | 0.79 |
| 12:L:580:UNK:N | 12:L:581:UNK:HA | 1.98 | 0.79 |
| 18:R:87:UNK:O | 18:R:89:UNK:N | 2.15 | 0.79 |
| 4:D:174:UNK:O | 4:D:177:UNK:N | 2.15 | 0.79 |
| 7:G:120:UNK:O | 7:G:124:UNK:O | 2.01 | 0.79 |
| 26:Z:82:UNK:O | 26:Z:86:UNK:N | 2.14 | 0.79 |
| 7:G:10:UNK:O | 7:G:76:UNK:N | 2.14 | 0.79 |
| 10:J:24:UNK:O | 10:J:25:UNK:CB | 2.31 | 0.79 |
| 13:M:207:UNK:O | 13:M:208:UNK:CB | 2.30 | 0.79 |
| 23:W:49:UNK:O | 23:W:53:UNK:N | 2.15 | 0.79 |
| 14:N:163:UNK:O | 14:N:166:UNK:N | 2.15 | 0.79 |
| 21:U:35:UNK:CB | 21:U:38:UNK:CB | 2.60 | 0.79 |
| 16:P:136:UNK:HA | 16:P:137:UNK:CB | 2.11 | 0.79 |
| 6:F:262:UNK:CB | 6:F:285:UNK:HA | 2.13 | 0.79 |
| 7:G:11:UNK:CB | 7:G:77:UNK:O | 2.32 | 0.78 |
| 16:P:135:UNK:HA | 16:P:168:UNK:N | 1.98 | 0.78 |
| 16:P:203:UNK:HA | 16:P:233:UNK:CB | 2.13 | 0.78 |
| 2:B:116:UNK:O | 2:B:117:UNK:CB | 2.31 | 0.78 |
| 7:G:577:UNK:O | 7:G:578:UNK:CB | 2.25 | 0.78 |
| 7:G:311:UNK:CB | 7:G:314:UNK:CB | 2.62 | 0.78 |
| 22:V:1:UNK:O | 22:V:2:UNK:C | 2.30 | 0.78 |
| 4:D:163:UNK:CA | 8:H:278:UNK:HA | 2.14 | 0.78 |
| 2:B:95:UNK:O | 2:B:97:UNK:N | 2.16 | 0.78 |
| 8:H:101:UNK:N | 8:H:161:UNK:HA | 1.99 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 18:R:81:UNK:CB | 18:R:91:UNK:O | 2.31 | 0.78 |
| 6:F:65:UNK:O | 6:F:75:UNK:N | 2.16 | 0.78 |
| 10:J:13:UNK:O | 10:J:16:UNK:N | 2.76 | 0.78 |
| 6:F:61:UNK:O | 6:F:64:UNK:N | 2.16 | 0.78 |
| 14:N:165:UNK:CB | 14:N:185:UNK:CB | 2.62 | 0.77 |
| 12:L:181:UNK:O | 12:L:182:UNK:C | 2.32 | 0.77 |
| 12:L:14:UNK:O | 12:L:17:UNK:CB | 3.29 | 0.77 |
| 12:L:67:UNK:CB | 12:L:76:UNK:CB | 2.63 | 0.77 |
| 12:L:142:UNK:HA | 13:M:370:UNK:CB | 2.14 | 0.77 |
| 2:B:147:UNK:O | 2:B:148:UNK:CB | 2.33 | 0.77 |
| 13:M:113:UNK:HA | 13:M:114:UNK:CB | 2.14 | 0.77 |
| 26:Z:71:UNK:O | 26:Z:75:UNK:CB | 2.33 | 0.77 |
| 14:N:175:UNK:CB | 14:N:225:UNK:O | 2.33 | 0.77 |
| 12:L:223:UNK:CB | 12:L:256:UNK:CB | 2.62 | 0.77 |
| 13:M:258:UNK:O | 13:M:262:UNK:N | 2.17 | 0.77 |
| 6:F:426:UNK:O | 6:F:430:UNK:N | 2.18 | 0.77 |
| 8:H:194:UNK:O | 8:H:195:UNK:CB | 2.33 | 0.77 |
| 13:M:25:UNK:O | 13:M:28:UNK:N | 2.18 | 0.77 |
| 14:N:257:UNK:O | 14:N:259:UNK:N | 2.18 | 0.77 |
| 7:G:16:UNK:O | 7:G:19:UNK:N | 7.49 | 0.76 |
| 17:Q:95:UNK:O | 17:Q:99:UNK:N | 2.17 | 0.76 |
| 4:D:234:UNK:O | 4:D:237:UNK:N | 2.18 | 0.76 |
| 4:D:193:UNK:O | 4:D:194:UNK:CB | 2.34 | 0.76 |
| 13:M:191:UNK:CB | 13:M:192:UNK:HA | 2.14 | 0.76 |
| 23:W:41:UNK:O | 23:W:42:UNK:CB | 2.33 | 0.76 |
| 6:F:352:UNK:O | 6:F:355:UNK:N | 2.19 | 0.76 |
| 7:G:227:UNK:O | 7:G:238:UNK:C | 2.33 | 0.76 |
| 13:M:62:UNK:N | 13:M:63:UNK:HA | 2.00 | 0.76 |
| 14:N:204:UNK:O | 14:N:208:UNK:N | 2.18 | 0.76 |
| 16:P:223:UNK:CA | 16:P:224:UNK:CB | 2.63 | 0.76 |
| 7:G:148:UNK:CB | 7:G:207:UNK:O | 2.34 | 0.76 |
| 8:H:195:UNK:O | 8:H:198:UNK:CB | 2.34 | 0.76 |
| 13:M:347:UNK:O | 13:M:351:UNK:CA | 2.34 | 0.76 |
| 12:L:11:UNK:O | 12:L:14:UNK:N | 3.26 | 0.76 |
| 12:L:453:UNK:O | 12:L:456:UNK:N | 2.18 | 0.76 |
| 16:P:203:UNK:CA | 16:P:234:UNK:HA | 2.14 | 0.76 |
| 3:C:111:UNK:CB | 3:C:113:UNK:CB | 2.64 | 0.76 |
| 3:C:62:UNK:O | 3:C:66:UNK:N | 2.18 | 0.76 |
| 6:F:61:UNK:O | 6:F:64:UNK:CA | 2.33 | 0.76 |
| 6:F:82:UNK:O | 6:F:83:UNK:C | 2.34 | 0.76 |
| 2:B:119:CYS:H | 2:B:122:UNK:CB | 1.94 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 12:L:503:UNK:O | 12:L:507:UNK:N | 2.19 | 0.75 |
| 6:F:352:UNK:O | 6:F:355:UNK:CB | 2.35 | 0.75 |
| 7:G:185:UNK:O | 7:G:188:UNK:CB | 2.35 | 0.75 |
| 7:G:316:UNK:HA | 7:G:342:UNK:O | 1.85 | 0.75 |
| 7:G:382:UNK:CB | 7:G:454:UNK:HA | 2.15 | 0.75 |
| 12:L:190:UNK:HA | 12:L:194:UNK:HA | 1.68 | 0.75 |
| 3:C:21:UNK:O | 3:C:24:UNK:CB | 2.33 | 0.75 |
| 7:G:210:UNK:O | 7:G:213:UNK:N | 2.20 | 0.75 |
| 15:O:130:UNK:O | 15:O:131:UNK:C | 2.35 | 0.75 |
| 2:B:155:UNK:O | 2:B:159:UNK:N | 2.19 | 0.75 |
| 13:M:372:UNK:O | 13:M:376:UNK:N | 2.20 | 0.75 |
| 16:P:53:UNK:CA | 16:P:57:UNK:CB | 2.64 | 0.75 |
| 4:D:139:UNK:O | 4:D:143:UNK:N | 2.20 | 0.75 |
| 18:R:60:UNK:O | 18:R:61:UNK:C | 2.35 | 0.75 |
| 5:E:28:UNK:O | 5:E:32:UNK:N | 2.20 | 0.75 |
| 1:A:84:UNK:O | 1:A:85:UNK:C | 2.32 | 0.75 |
| 4:D:218:UNK:O | 4:D:222:UNK:CB | 2.34 | 0.75 |
| 6:F:300:UNK:CA | 6:F:329:UNK:HA | 2.18 | 0.74 |
| 7:G:12:UNK:O | 7:G:78:UNK:HA | 1.87 | 0.74 |
| 13:M:241:UNK:O | 13:M:242:UNK:C | 2.35 | 0.74 |
| 6:F:322:UNK:O | 6:F:327:UNK:N | 2.19 | 0.74 |
| 13:M:23:UNK:O | 13:M:25:UNK:N | 2.20 | 0.74 |
| 13:M:447:UNK:O | 13:M:450:UNK:O | 2.04 | 0.74 |
| 17:Q:40:UNK:CB | 17:Q:41:UNK:HA | 2.17 | 0.74 |
| 6:F:421:UNK:O | 6:F:425:UNK:N | 2.20 | 0.74 |
| 16:P:38:UNK:O | 16:P:41:UNK:O | 2.05 | 0.74 |
| 7:G:317:UNK:HA | 7:G:527:UNK:O | 1.87 | 0.74 |
| 5:E:106:UNK:O | 5:E:110:UNK:N | 2.20 | 0.74 |
| 9:I:73:UNK:O | 9:I:74:UNK:CB | 2.34 | 0.74 |
| 12:L:224:UNK:N | 12:L:256:UNK:CB | 2.51 | 0.74 |
| 13:M:275:UNK:O | 13:M:278:UNK:CB | 2.35 | 0.74 |
| 12:L:207:UNK:HA | 12:L:208:UNK:CB | 2.18 | 0.74 |
| 16:P:236:UNK:O | 16:P:237:UNK:CB | 2.36 | 0.74 |
| 12:L:165:UNK:O | 12:L:169:UNK:N | 2.20 | 0.73 |
| 22:V:66:UNK:O | 22:V:69:UNK:CB | 2.36 | 0.73 |
| 6:F:140:UNK:CB | 6:F:182:UNK:HA | 2.18 | 0.73 |
| 19:S:63:UNK:CB | 19:S:78:UNK:CB | 2.66 | 0.73 |
| 6:F:61:UNK:C | 6:F:64:UNK:N | 2.51 | 0.73 |
| 25:Y:103:UNK:O | 25:Y:104:UNK:C | 2.36 | 0.73 |
| 6:F:405:CYS:SG | 6:F:408:UNK:N | 2.60 | 0.73 |
| 18:R:78:UNK:O | 18:R:79:UNK:C | 2.36 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:103:UNK:O | 1:A:107:UNK:N | 2.21 | 0.73 |
| 2:B:128:UNK:O | 2:B:131:UNK:CB | 2.36 | 0.73 |
| 22:V:45:UNK:C | 22:V:47:UNK:N | 2.50 | 0.73 |
| 25:Y:35:UNK:O | 25:Y:39:UNK:N | 2.21 | 0.73 |
| 8:H:40:UNK:O | 8:H:47:UNK:HA | 1.88 | 0.73 |
| 13:M:27:UNK:O | 13:M:30:UNK:N | 2.21 | 0.73 |
| 19:S:84:UNK:O | 19:S:87:UNK:N | 2.22 | 0.73 |
| 23:W:68:UNK:O | 23:W:72:UNK:CB | 2.37 | 0.73 |
| 7:G:565:UNK:O | 7:G:568:UNK:N | 2.22 | 0.73 |
| 13:M:87:UNK:CB | 13:M:88:UNK:HA | 2.17 | 0.73 |
| 2:B:121:UNK:HA | 2:B:135:UNK:CA | 2.18 | 0.72 |
| 5:E:152:UNK:O | 5:E:163:UNK:N | 2.20 | 0.72 |
| 7:G:469:UNK:O | 7:G:473:UNK:N | 2.21 | 0.72 |
| 12:L:530:UNK:O | 12:L:534:UNK:N | 2.21 | 0.72 |
| 3:C:111:UNK:C | 3:C:113:UNK:CB | 2.67 | 0.72 |
| 6:F:163:UNK:O | 6:F:165:UNK:O | 2.06 | 0.72 |
| 12:L:161:UNK:CA | 12:L:163:UNK:N | 2.46 | 0.72 |
| 12:L:209:UNK:O | 12:L:212:UNK:CB | 2.37 | 0.72 |
| 10:J:58:UNK:O | 10:J:62:UNK:CB | 2.37 | 0.72 |
| 16:P:137:UNK:CB | 16:P:138:UNK:HA | 2.19 | 0.72 |
| 26:Z:88:UNK:O | 26:Z:91:UNK:N | 2.22 | 0.72 |
| 9:I:149:UNK:HA | 9:I:150:UNK:CB | 2.19 | 0.72 |
| 12:L:239:UNK:O | 12:L:240:UNK:O | 2.06 | 0.72 |
| 12:L:580:UNK:N | 12:L:581:UNK:CA | 2.51 | 0.72 |
| 14:N:223:UNK:HA | 14:N:224:UNK:C | 2.19 | 0.72 |
| 14:N:33:UNK:O | 14:N:34:UNK:C | 2.38 | 0.72 |
| 10:J:22:UNK:CB | 10:J:24:UNK:O | 2.37 | 0.72 |
| 19:S:23:UNK:O | 19:S:56:UNK:O | 2.07 | 0.72 |
| 3:C:113:UNK:O | 3:C:115:UNK:N | 2.22 | 0.72 |
| 12:L:223:UNK:C | 12:L:256:UNK:CB | 2.66 | 0.72 |
| 14:N:90:UNK:N | 14:N:91:UNK:HA | 2.01 | 0.72 |
| 19:S:41:UNK:O | 19:S:45:UNK:N | 2.23 | 0.72 |
| 4:D:360:UNK:CB | 4:D:381:UNK:HA | 2.19 | 0.72 |
| 14:N:123:UNK:HA | 14:N:124:UNK:CB | 2.18 | 0.72 |
| 8:H:177:UNK:CA | 26:Z:46:UNK:CB | 2.67 | 0.72 |
| 12:L:67:UNK:CB | 12:L:76:UNK:CA | 2.68 | 0.72 |
| 16:P:104:UNK:O | 16:P:108:UNK:N | 2.22 | 0.72 |
| 14:N:61:UNK:O | 14:N:64:UNK:N | 2.23 | 0.72 |
| 20:T:53:UNK:O | 20:T:56:UNK:O | 4.88 | 0.72 |
| 12:L:530:UNK:O | 12:L:533:UNK:N | 2.23 | 0.71 |
| 5:E:98:UNK:N | 5:E:136:UNK:O | 2.23 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:F:214:UNK:HA | 6:F:218:UNK:O | 1.90 | 0.71 |
| 7:G:52:CYS:C | 7:G:54:UNK:N | 2.41 | 0.71 |
| 12:L:180:UNK:O | 12:L:181:UNK:C | 2.37 | 0.71 |
| 12:L:182:UNK:O | 12:L:186:UNK:N | 2.24 | 0.71 |
| 14:N:258:UNK:CB | 14:N:330:UNK:O | 2.39 | 0.71 |
| 6:F:362:CYS:SG | 6:F:404:UNK:CB | 2.78 | 0.71 |
| 16:P:52:UNK:CA | 16:P:72:UNK:CB | 2.68 | 0.71 |
| 6:F:370:UNK:O | 6:F:372:UNK:N | 2.24 | 0.71 |
| 6:F:398:UNK:O | 6:F:401:UNK:CB | 2.39 | 0.71 |
| 9:I:100:UNK:N | 9:I:103:UNK:O | 2.24 | 0.71 |
| 9:I:113:UNK:O | 9:I:114:UNK:C | 2.37 | 0.71 |
| 7:G:332:UNK:O | 7:G:336:UNK:N | 2.23 | 0.71 |
| 9:I:151:UNK:O | 9:I:154:UNK:CB | 2.38 | 0.71 |
| 14:N:158:UNK:O | 14:N:161:UNK:CB | 2.39 | 0.71 |
| 7:G:16:UNK:O | 7:G:17:UNK:C | 3.70 | 0.71 |
| 16:P:146:UNK:O | 16:P:150:UNK:N | 2.24 | 0.71 |
| 19:S:44:UNK:O | 19:S:48:UNK:N | 2.24 | 0.71 |
| 22:V:44:UNK:O | 22:V:47:UNK:N | 2.24 | 0.71 |
| 12:L:71:UNK:O | 12:L:72:UNK:CB | 2.36 | 0.71 |
| 15:O:24:UNK:HA | 15:O:122:UNK:O | 1.90 | 0.71 |
| 2:B:122:UNK:HA | 2:B:123:UNK:CB | 2.21 | 0.71 |
| 6:F:289:UNK:CA | 6:F:290:UNK:C | 2.66 | 0.71 |
| 6:F:74:UNK:O | 6:F:78:UNK:N | 2.22 | 0.71 |
| 13:M:32:UNK:O | 13:M:35:UNK:N | 2.23 | 0.71 |
| 10:J:13:UNK:O | 10:J:14:UNK:C | 2.94 | 0.71 |
| 13:M:13:UNK:O | 13:M:16:UNK:CB | 3.40 | 0.71 |
| 14:N:142:UNK:O | 14:N:145:UNK:N | 2.24 | 0.70 |
| 14:N:158:UNK:O | 14:N:162:UNK:N | 2.24 | 0.70 |
| 2:B:166:UNK:HA | 2:B:169:UNK:O | 1.90 | 0.70 |
| 6:F:351:UNK:O | 6:F:354:UNK:N | 2.23 | 0.70 |
| 15:O:50:UNK:CB | 15:O:123:UNK:O | 2.39 | 0.70 |
| 15:O:130:UNK:O | 15:O:133:UNK:N | 2.24 | 0.70 |
| 1:A:109:UNK:O | 1:A:110:UNK:CB | 2.38 | 0.70 |
| 22:V:27:UNK:O | 22:V:31:UNK:N | 2.23 | 0.70 |
| 26:Z:77:UNK:O | 26:Z:80:UNK:CB | 2.40 | 0.70 |
| 7:G:367:UNK:O | 7:G:370:UNK:CB | 2.40 | 0.70 |
| 7:G:288:UNK:HA | 7:G:289:UNK:C | 2.20 | 0.70 |
| 11:K:32:UNK:O | 11:K:35:UNK:CB | 2.39 | 0.70 |
| 16:P:64:UNK:N | 16:P:65:UNK:CA | 2.54 | 0.70 |
| 6:F:323:UNK:HA | 6:F:327:UNK:O | 1.92 | 0.70 |
| 7:G:12:UNK:O | 7:G:79:UNK:N | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 12:L:34:UNK:HA | 12:L:37:UNK:CB | 2.22 | 0.70 |
| 25:Y:102:UNK:O | 25:Y:105:UNK:CA | 2.39 | 0.70 |
| 3:C:131:UNK:C | 3:C:133:UNK:N | 2.54 | 0.70 |
| 6:F:70:UNK:CB | 6:F:330:UNK:CB | 2.69 | 0.70 |
| 7:G:59:UNK:CB | 7:G:62:UNK:CB | 2.69 | 0.70 |
| 4:D:182:UNK:O | 4:D:186:UNK:N | 2.25 | 0.70 |
| 7:G:73:UNK:O | 7:G:74:UNK:CB | 2.39 | 0.70 |
| 13:M:279:UNK:CB | 13:M:280:UNK:HA | 2.20 | 0.70 |
| 7:G:367:UNK:O | 7:G:370:UNK:N | 2.24 | 0.70 |
| 18:R:81:UNK:CB | 18:R:92:UNK:HA | 2.22 | 0.70 |
| 12:L:321:UNK:CA | 12:L:324:UNK:CB | 2.70 | 0.69 |
| 6:F:34:UNK:O | 6:F:38:UNK:CB | 2.40 | 0.69 |
| 22:V:45:UNK:O | 22:V:46:UNK:C | 2.38 | 0.69 |
| 12:L:35:UNK:O | 12:L:39:UNK:N | 2.25 | 0.69 |
| 13:M:274:UNK:O | 13:M:278:UNK:CB | 2.40 | 0.69 |
| 22:V:3:UNK:C | 22:V:5:UNK:N | 3.21 | 0.69 |
| 10:J:58:UNK:O | 10:J:62:UNK:CA | 2.40 | 0.69 |
| 14:N:190:UNK:CB | 14:N:204:UNK:CB | 2.69 | 0.69 |
| 3:C:132:UNK:O | 3:C:136:UNK:N | 2.25 | 0.69 |
| 24:X:93:UNK:CA | 24:X:94:UNK:CB | 2.71 | 0.69 |
| 12:L:314:UNK:O | 12:L:317:UNK:CB | 2.41 | 0.69 |
| 26:Z:56:UNK:O | 26:Z:59:UNK:CB | 2.41 | 0.69 |
| 6:F:150:UNK:O | 6:F:154:UNK:N | 2.25 | 0.69 |
| 7:G:367:UNK:O | 7:G:371:UNK:N | 2.25 | 0.69 |
| 10:J:85:UNK:O | 10:J:88:UNK:N | 2.25 | 0.69 |
| 7:G:94:UNK:O | 7:G:98:UNK:N | 2.25 | 0.69 |
| 8:H:127:UNK:O | 8:H:131:UNK:CB | 2.41 | 0.69 |
| 2:B:121:UNK:CA | 2:B:135:UNK:HA | 2.22 | 0.69 |
| 8:H:285:UNK:O | 8:H:289:UNK:N | 2.26 | 0.69 |
| 14:N:108:UNK:O | 14:N:112:UNK:N | 2.26 | 0.69 |
| 14:N:204:UNK:O | 14:N:208:UNK:CB | 2.41 | 0.69 |
| 12:L:369:UNK:O | 12:L:373:UNK:N | 2.26 | 0.68 |
| 16:P:160:UNK:N | 16:P:162:UNK:N | 2.42 | 0.68 |
| 7:G:229:UNK:N | 7:G:238:UNK:CB | 2.56 | 0.68 |
| 13:M:60:UNK:C | 13:M:63:UNK:N | 2.57 | 0.68 |
| 14:N:77:UNK:O | 14:N:80:UNK:O | 2.12 | 0.68 |
| 6:F:92:UNK:O | 6:F:220:UNK:HA | 1.92 | 0.68 |
| 13:M:60:UNK:C | 13:M:62:UNK:C | 2.72 | 0.68 |
| 14:N:158:UNK:O | 14:N:161:UNK:N | 2.26 | 0.68 |
| 14:N:52:UNK:O | 14:N:55:UNK:N | 2.27 | 0.68 |
| 21:U:43:UNK:O | 21:U:47:UNK:N | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:F:294:UNK:CB | 6:F:339:UNK:CB | 2.72 | 0.68 |
| 16:P:134:UNK:O | 16:P:167:UNK:HA | 1.93 | 0.68 |
| 1:A:76:UNK:O | 1:A:77:UNK:C | 2.38 | 0.68 |
| 2:B:95:UNK:C | 2:B:97:UNK:N | 2.55 | 0.68 |
| 16:P:311:UNK:O | 16:P:314:UNK:CB | 2.42 | 0.68 |
| 5:E:96:UNK:O | 5:E:98:UNK:O | 2.11 | 0.68 |
| 6:F:51:UNK:CB | 6:F:52:UNK:CB | 2.72 | 0.68 |
| 7:G:375:UNK:CB | 7:G:376:UNK:HA | 2.18 | 0.68 |
| 13:M:167:UNK:O | 13:M:171:UNK:N | 2.26 | 0.68 |
| 12:L:151:UNK:O | 12:L:155:UNK:N | 2.26 | 0.68 |
| 12:L:419:UNK:O | 12:L:422:UNK:CB | 2.42 | 0.68 |
| 9:I:26:UNK:O | 9:I:28:UNK:O | 5.64 | 0.68 |
| 14:N:224:UNK:N | 14:N:225:UNK:HA | 2.08 | 0.68 |
| 14:N:43:UNK:O | 14:N:44:UNK:C | 2.72 | 0.68 |
| 2:B:148:UNK:CA | 2:B:151:UNK:CA | 2.58 | 0.68 |
| 3:C:131:UNK:O | 3:C:133:UNK:N | 2.27 | 0.68 |
| 3:C:25:UNK:C | 3:C:26:UNK:O | 3.62 | 0.67 |
| 15:O:28:UNK:O | 15:O:172:UNK:CB | 2.42 | 0.67 |
| 2:B:117:UNK:O | 2:B:120:UNK:N | 2.27 | 0.67 |
| 12:L:281:UNK:CB | 12:L:315:UNK:HA | 2.25 | 0.67 |
| 16:P:112:UNK:O | 16:P:116:UNK:N | 2.26 | 0.67 |
| 15:O:41:UNK:O | 15:O:44:UNK:CB | 2.42 | 0.67 |
| 4:D:357:UNK:HA | 4:D:384:UNK:CB | 2.25 | 0.67 |
| 9:I:173:UNK:HA | 9:I:174:UNK:C | 2.23 | 0.67 |
| 13:M:21:UNK:O | 13:M:22:UNK:C | 2.41 | 0.67 |
| 14:N:293:UNK:O | 14:N:296:UNK:N | 2.27 | 0.67 |
| 4:D:296:UNK:O | 4:D:299:UNK:N | 2.28 | 0.67 |
| 10:J:50:UNK:O | 10:J:54:UNK:N | 2.27 | 0.67 |
| 4:D:234:UNK:O | 4:D:237:UNK:CB | 2.43 | 0.67 |
| 23:W:47:UNK:O | 23:W:50:UNK:CB | 2.43 | 0.67 |
| 12:L:178:UNK:CB | 12:L:222:UNK:CB | 2.73 | 0.67 |
| 12:L:321:UNK:C | 12:L:324:UNK:CB | 2.73 | 0.67 |
| 13:M:24:UNK:O | 13:M:27:UNK:CB | 2.42 | 0.67 |
| 6:F:194:UNK:O | 6:F:197:UNK:CB | 2.42 | 0.67 |
| 7:G:155:UNK:C | 7:G:156:CYS:O | 2.41 | 0.67 |
| 13:M:102:UNK:O | 13:M:106:UNK:CB | 2.43 | 0.67 |
| 25:Y:103:UNK:C | 25:Y:105:UNK:N | 2.56 | 0.67 |
| 2:B:65:UNK:HA | 2:B:68:UNK:CB | 2.25 | 0.66 |
| 20:T:34:UNK:O | 20:T:35:UNK:C | 3.19 | 0.66 |
| 7:G:380:UNK:O | 7:G:409:UNK:O | 2.13 | 0.66 |
| 8:H:143:UNK:O | 8:H:144:UNK:C | 2.42 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 12:L:226:UNK:HA | 12:L:284:UNK:CB | 2.25 | 0.66 |
| 16:P:134:UNK:O | 16:P:167:UNK:CB | 2.43 | 0.66 |
| 2:B:48:UNK:HA | 2:B:78:UNK:CB | 2.26 | 0.66 |
| 14:N:135:UNK:O | 14:N:136:UNK:C | 2.43 | 0.66 |
| 4:D:218:UNK:O | 4:D:222:UNK:N | 2.28 | 0.66 |
| 6:F:101:UNK:O | 6:F:102:UNK:CB | 2.43 | 0.66 |
| 7:G:11:UNK:O | 7:G:12:UNK:C | 3.59 | 0.66 |
| 12:L:207:UNK:CB | 12:L:209:UNK:HA | 2.25 | 0.66 |
| 12:L:46:UNK:O | 12:L:49:UNK:N | 2.27 | 0.66 |
| 13:M:32:UNK:O | 13:M:33:UNK:C | 2.42 | 0.66 |
| 18:R:51:UNK:HA | 18:R:92:UNK:O | 1.95 | 0.66 |
| 26:Z:87:UNK:O | 26:Z:90:UNK:N | 2.28 | 0.66 |
| 7:G:388:UNK:CB | 7:G:391:UNK:CB | 2.74 | 0.66 |
| 8:H:152:UNK:O | 8:H:155:UNK:N | 2.29 | 0.66 |
| 12:L:297:UNK:HA | 12:L:355:UNK:HA | 1.77 | 0.66 |
| 14:N:24:UNK:O | 14:N:28:UNK:N | 2.28 | 0.66 |
| 14:N:44:UNK:O | 14:N:48:UNK:N | 5.16 | 0.66 |
| 4:D:383:UNK:CB | 4:D:385:UNK:O | 2.44 | 0.66 |
| 14:N:108:UNK:O | 14:N:109:UNK:C | 2.41 | 0.66 |
| 6:F:262:UNK:CB | 6:F:285:UNK:CA | 2.73 | 0.66 |
| 9:I:172:UNK:O | 9:I:175:UNK:HA | 1.95 | 0.66 |
| 9:I:21:UNK:O | 9:I:25:UNK:N | 2.29 | 0.66 |
| 14:N:227:UNK:O | 14:N:228:UNK:C | 2.39 | 0.66 |
| 15:O:87:UNK:CB | 15:O:88:UNK:CA | 2.73 | 0.66 |
| 10:J:101:UNK:O | 10:J:102:UNK:C | 2.44 | 0.66 |
| 12:L:375:UNK:O | 12:L:376:UNK:C | 2.43 | 0.66 |
| 6:F:121:UNK:HA | 6:F:232:UNK:CB | 2.26 | 0.66 |
| 7:G:426:UNK:O | 7:G:430:UNK:N | 2.29 | 0.66 |
| 7:G:375:UNK:C | 7:G:449:UNK:N | 2.58 | 0.65 |
| 12:L:579:UNK:CB | 12:L:581:UNK:CB | 2.74 | 0.65 |
| 14:N:124:UNK:O | 14:N:127:UNK:N | 2.29 | 0.65 |
| 14:N:142:UNK:O | 14:N:145:UNK:CA | 2.43 | 0.65 |
| 22:V:3:UNK:O | 22:V:4:UNK:C | 2.89 | 0.65 |
| 7:G:12:UNK:HA | 7:G:17:UNK:HA | 1.77 | 0.65 |
| 7:G:311:UNK:O | 7:G:314:UNK:CB | 2.43 | 0.65 |
| 7:G:26:UNK:O | 7:G:29:UNK:CB | 2.45 | 0.65 |
| 13:M:281:UNK:O | 13:M:284:UNK:N | 2.29 | 0.65 |
| 1:A:111:UNK:O | 1:A:112:UNK:CB | 2.43 | 0.65 |
| 3:C:31:UNK:O | 3:C:33:UNK:N | 2.30 | 0.65 |
| 6:F:289:UNK:HA | 6:F:291:UNK:N | 2.11 | 0.65 |
| 13:M:180:UNK:O | 13:M:181:UNK:C | 2.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 13:M:278:UNK:O | 13:M:279:UNK:CB | 2.43 | 0.65 |
| 16:P:147:UNK:O | 16:P:151:UNK:N | 2.29 | 0.65 |
| 3:C:133:UNK:O | 3:C:136:UNK:N | 2.30 | 0.65 |
| 4:D:126:UNK:O | 4:D:127:UNK:CB | 2.45 | 0.65 |
| 6:F:291:UNK:O | 6:F:292:UNK:C | 2.43 | 0.65 |
| 12:L:326:UNK:O | 12:L:330:UNK:N | 2.29 | 0.65 |
| 7:G:241:UNK:O | 7:G:248:UNK:CB | 2.44 | 0.65 |
| 15:O:130:UNK:C | 15:O:132:UNK:N | 2.59 | 0.65 |
| 6:F:429:UNK:O | 6:F:432:UNK:CB | 2.44 | 0.65 |
| 12:L:61:UNK:HA | 12:L:80:UNK:CB | 2.26 | 0.65 |
| 19:S:84:UNK:HA | 19:S:87:UNK:CB | 2.27 | 0.65 |
| 4:D:229:UNK:O | 4:D:232:UNK:N | 2.29 | 0.65 |
| 9:I:26:UNK:O | 9:I:28:UNK:N | 2.29 | 0.65 |
| 6:F:166:UNK:O | 6:F:167:UNK:C | 2.45 | 0.65 |
| 6:F:370:UNK:O | 6:F:371:UNK:C | 2.45 | 0.65 |
| 7:G:11:UNK:O | 7:G:14:UNK:N | 7.26 | 0.65 |
| 9:I:99:UNK:HA | 9:I:104:UNK:HA | 1.79 | 0.65 |
| 14:N:99:UNK:O | 14:N:103:UNK:N | 2.30 | 0.65 |
| 10:J:4:UNK:O | 10:J:8:UNK:N | 2.30 | 0.64 |
| 13:M:271:UNK:O | 13:M:272:UNK:C | 2.45 | 0.64 |
| 6:F:288:UNK:O | 6:F:289:UNK:CB | 2.45 | 0.64 |
| 7:G:26:UNK:O | 7:G:29:UNK:N | 2.30 | 0.64 |
| 7:G:55:CYS:O | 7:G:56:UNK:C | 2.45 | 0.64 |
| 14:N:43:UNK:C | 14:N:45:UNK:N | 2.90 | 0.64 |
| 13:M:271:UNK:O | 13:M:274:UNK:N | 2.30 | 0.64 |
| 13:M:432:UNK:O | 13:M:435:UNK:CB | 2.45 | 0.64 |
| 14:N:73:UNK:O | 14:N:74:UNK:C | 2.39 | 0.64 |
| 3:C:112:UNK:N | 3:C:113:UNK:CB | 2.61 | 0.64 |
| 4:D:163:UNK:N | 8:H:278:UNK:HA | 2.12 | 0.64 |
| 6:F:325:UNK:O | 6:F:326:UNK:CB | 2.45 | 0.64 |
| 8:H:40:UNK:O | 8:H:47:UNK:N | 2.31 | 0.64 |
| 14:N:77:UNK:O | 14:N:78:UNK:C | 2.44 | 0.64 |
| 17:Q:42:UNK:O | 17:Q:45:UNK:N | 2.30 | 0.64 |
| 20:T:21:UNK:O | 20:T:23:UNK:N | 3.42 | 0.64 |
| 6:F:39:UNK:O | 6:F:40:UNK:CB | 2.45 | 0.64 |
| 7:G:615:UNK:O | 7:G:618:UNK:N | 2.30 | 0.64 |
| 14:N:25:UNK:O | 14:N:26:UNK:C | 4.17 | 0.64 |
| 6:F:103:UNK:CB | 6:F:104:UNK:HA | 2.27 | 0.64 |
| 25:Y:11:UNK:CA | 25:Y:48:UNK:CB | 2.69 | 0.64 |
| 4:D:347:UNK:O | 4:D:351:UNK:N | 2.31 | 0.64 |
| 12:L:209:UNK:O | 12:L:212:UNK:CA | 2.46 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 5:E:124:UNK:O | 5:E:125:UNK:CB | 2.46 | 0.64 |
| 6:F:188:UNK:O | 6:F:192:UNK:N | 2.31 | 0.64 |
| 13:M:375:UNK:O | 13:M:379:UNK:N | 2.30 | 0.64 |
| 13:M:60:UNK:O | 13:M:62:UNK:O | 2.15 | 0.64 |
| 5:E:151:UNK:HA | 5:E:152:UNK:C | 2.28 | 0.64 |
| 7:G:543:UNK:O | 7:G:558:UNK:O | 2.15 | 0.64 |
| 13:M:123:UNK:O | 13:M:126:UNK:N | 2.31 | 0.64 |
| 15:O:229:UNK:C | 15:O:231:UNK:N | 2.55 | 0.64 |
| 2:B:56:UNK:O | 2:B:59:UNK:N | 2.31 | 0.63 |
| 4:D:382:UNK:C | 4:D:384:UNK:HA | 2.28 | 0.63 |
| 7:G:114:CYS:O | 7:G:118:UNK:N | 2.30 | 0.63 |
| 7:G:332:UNK:O | 7:G:336:UNK:CB | 2.46 | 0.63 |
| 26:Z:57:UNK:O | 26:Z:60:UNK:N | 2.30 | 0.63 |
| 13:M:382:UNK:O | 13:M:385:UNK:N | 2.31 | 0.63 |
| 10:J:85:UNK:O | 10:J:88:UNK:CB | 2.46 | 0.63 |
| 12:L:210:UNK:O | 12:L:211:UNK:C | 2.45 | 0.63 |
| 13:M:10:UNK:O | 13:M:14:UNK:N | 3.27 | 0.63 |
| 13:M:32:UNK:O | 13:M:34:UNK:N | 2.31 | 0.63 |
| 7:G:624:UNK:O | 7:G:627:UNK:N | 2.32 | 0.63 |
| 1:A:52:UNK:O | 1:A:56:UNK:N | 2.31 | 0.63 |
| 3:C:112:UNK:N | 3:C:113:UNK:CA | 2.62 | 0.63 |
| 16:P:53:UNK:HA | 16:P:57:UNK:CB | 2.28 | 0.63 |
| 23:W:1:UNK:O | 23:W:2:UNK:CB | 2.46 | 0.63 |
| 3:C:68:UNK:O | 3:C:69:UNK:CB | 2.45 | 0.63 |
| 6:F:434:UNK:O | 6:F:438:UNK:N | 2.32 | 0.63 |
| 11:K:14:UNK:CB | 11:K:36:UNK:CB | 2.76 | 0.63 |
| 12:L:420:UNK:O | 12:L:424:UNK:N | 2.31 | 0.63 |
| 16:P:134:UNK:C | 16:P:136:UNK:H2 | 2.11 | 0.63 |
| 9:I:151:UNK:O | 9:I:154:UNK:CA | 2.47 | 0.63 |
| 12:L:571:UNK:O | 12:L:574:UNK:N | 2.31 | 0.63 |
| 19:S:84:UNK:O | 19:S:87:UNK:CB | 2.47 | 0.63 |
| 14:N:262:UNK:O | 14:N:265:UNK:N | 2.32 | 0.63 |
| 16:P:167:UNK:O | 16:P:230:UNK:N | 2.31 | 0.63 |
| 6:F:370:UNK:O | 6:F:373:UNK:N | 2.32 | 0.63 |
| 21:U:62:UNK:CB | 21:U:66:UNK:CB | 2.77 | 0.63 |
| 6:F:116:UNK:O | 6:F:119:UNK:N | 2.31 | 0.62 |
| 7:G:330:UNK:CB | 7:G:600:UNK:CB | 2.77 | 0.62 |
| 15:O:87:UNK:N | 15:O:88:UNK:CB | 2.62 | 0.62 |
| 2:B:71:UNK:C | 8:H:37:UNK:CB | 2.77 | 0.62 |
| 14:N:157:UNK:O | 14:N:161:UNK:CB | 2.46 | 0.62 |
| 16:P:167:UNK:CB | 16:P:229:UNK:HA | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 13:M:281:UNK:O | 13:M:284:UNK:CA | 2.46 | 0.62 |
| 16:P:103:UNK:HA | 16:P:106:UNK:CB | 2.30 | 0.62 |
| 8:H:9:UNK:O | 8:H:12:UNK:N | 3.30 | 0.62 |
| 2:B:89:UNK:O | 2:B:90:UNK:CB | 2.47 | 0.62 |
| 3:C:44:UNK:O | 3:C:47:UNK:N | 2.33 | 0.62 |
| 9:I:126:CYS:HA | 44:I:223:SF4:S3 | 2.39 | 0.62 |
| 13:M:31:UNK:O | 13:M:32:UNK:C | 2.37 | 0.62 |
| 14:N:45:UNK:O | 14:N:46:UNK:C | 2.44 | 0.62 |
| 25:Y:92:UNK:O | 25:Y:95:UNK:CB | 2.48 | 0.62 |
| 2:B:163:UNK:O | 2:B:164:UNK:C | 2.47 | 0.62 |
| 16:P:113:UNK:O | 16:P:117:UNK:N | 2.33 | 0.62 |
| 1:A:103:UNK:O | 1:A:106:UNK:N | 2.33 | 0.62 |
| 6:F:428:UNK:O | 6:F:431:UNK:CB | 2.47 | 0.62 |
| 12:L:376:UNK:O | 12:L:377:UNK:C | 2.46 | 0.62 |
| 12:L:383:UNK:O | 12:L:389:UNK:CB | 2.48 | 0.62 |
| 14:N:21:UNK:O | 14:N:22:UNK:CB | 4.17 | 0.62 |
| 16:P:64:UNK:N | 16:P:65:UNK:HA | 2.15 | 0.62 |
| 4:D:360:UNK:CB | 4:D:381:UNK:CA | 2.77 | 0.62 |
| 4:D:99:UNK:O | 4:D:100:UNK:C | 2.44 | 0.62 |
| 7:G:104:UNK:O | 7:G:106:UNK:N | 2.33 | 0.62 |
| 7:G:367:UNK:O | 7:G:370:UNK:CA | 2.47 | 0.62 |
| 26:Z:56:UNK:O | 26:Z:59:UNK:N | 2.31 | 0.62 |
| 4:D:360:UNK:HA | 4:D:381:UNK:HA | 1.81 | 0.62 |
| 6:F:428:UNK:O | 6:F:431:UNK:N | 2.33 | 0.62 |
| 6:F:434:UNK:O | 6:F:437:UNK:N | 2.32 | 0.62 |
| 8:H:154:UNK:O | 8:H:157:UNK:O | 2.18 | 0.62 |
| 13:M:68:UNK:O | 13:M:70:UNK:N | 2.32 | 0.62 |
| 6:F:103:UNK:HA | 6:F:104:UNK:C | 2.30 | 0.62 |
| 7:G:296:UNK:O | 7:G:300:UNK:CB | 2.48 | 0.62 |
| 12:L:376:UNK:O | 12:L:378:UNK:N | 2.33 | 0.62 |
| 15:O:160:UNK:O | 15:O:163:UNK:N | 2.32 | 0.62 |
| 2:B:118:UNK:CB | 44:B:201:SF4:S3 | 2.88 | 0.61 |
| 3:C:23:UNK:O | 3:C:26:UNK:N | 2.33 | 0.61 |
| 6:F:44:UNK:O | 6:F:47:UNK:CB | 2.47 | 0.61 |
| 9:I:87:CYS:SG | 9:I:90:UNK:N | 2.73 | 0.61 |
| 13:M:441:UNK:O | 13:M:445:UNK:N | 2.32 | 0.61 |
| 4:D:70:UNK:O | 4:D:71:UNK:C | 2.48 | 0.61 |
| 6:F:294:UNK:CB | 6:F:295:UNK:HA | 2.30 | 0.61 |
| 3:C:79:UNK:O | 3:C:93:UNK:N | 2.33 | 0.61 |
| 7:G:331:UNK:O | 7:G:335:UNK:N | 2.33 | 0.61 |
| 16:P:155:UNK:O | 16:P:158:UNK:CB | 2.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 23:W:3:UNK:O | 23:W:6:UNK:N | 4.40 | 0.61 |
| 6:F:129:UNK:O | 6:F:130:UNK:CB | 2.48 | 0.61 |
| 6:F:166:UNK:O | 6:F:168:UNK:N | 2.33 | 0.61 |
| 14:N:100:UNK:HA | 14:N:103:UNK:CB | 2.30 | 0.61 |
| 3:C:27:UNK:O | 3:C:30:UNK:N | 2.34 | 0.61 |
| 6:F:262:UNK:HA | 6:F:286:UNK:CB | 2.31 | 0.61 |
| 3:C:83:UNK:C | 3:C:85:UNK:N | 2.64 | 0.61 |
| 7:G:425:UNK:O | 7:G:428:UNK:CB | 2.49 | 0.61 |
| 13:M:342:UNK:O | 13:M:343:UNK:CB | 2.45 | 0.61 |
| 6:F:44:UNK:O | 6:F:48:UNK:N | 2.34 | 0.61 |
| 6:F:60:UNK:O | 6:F:63:UNK:CA | 2.48 | 0.61 |
| 7:G:464:UNK:O | 7:G:467:UNK:N | 2.33 | 0.61 |
| 14:N:144:UNK:O | 14:N:145:UNK:C | 2.46 | 0.61 |
| 19:S:63:UNK:O | 19:S:78:UNK:CA | 2.49 | 0.61 |
| 5:E:60:UNK:CB | 5:E:94:UNK:HA | 2.30 | 0.60 |
| 12:L:321:UNK:C | 12:L:324:UNK:N | 2.64 | 0.60 |
| 13:M:68:UNK:O | 13:M:71:UNK:N | 2.34 | 0.60 |
| 4:D:383:UNK:CB | 4:D:385:UNK:C | 2.79 | 0.60 |
| 4:D:80:UNK:O | 4:D:81:UNK:CB | 2.47 | 0.60 |
| 12:L:19:UNK:O | 12:L:22:UNK:O | 6.59 | 0.60 |
| 19:S:23:UNK:O | 19:S:26:UNK:CB | 8.20 | 0.60 |
| 8:H:128:UNK:O | 8:H:132:UNK:N | 2.34 | 0.60 |
| 12:L:546:UNK:O | 12:L:549:UNK:N | 2.34 | 0.60 |
| 16:P:135:UNK:O | 16:P:136:UNK:C | 2.48 | 0.60 |
| 12:L:116:UNK:O | 12:L:117:UNK:C | 2.45 | 0.60 |
| 15:O:225:UNK:C | 15:O:227:UNK:O | 2.49 | 0.60 |
| 7:G:333:UNK:O | 7:G:337:UNK:N | 2.33 | 0.60 |
| 22:V:20:UNK:O | 22:V:24:UNK:N | 9.33 | 0.60 |
| 24:X:77:UNK:C | 24:X:79:UNK:N | 2.56 | 0.60 |
| 4:D:211:UNK:O | 4:D:214:UNK:N | 2.34 | 0.60 |
| 13:M:168:UNK:CB | 13:M:174:UNK:HA | 2.30 | 0.60 |
| 13:M:94:UNK:O | 13:M:95:UNK:C | 2.48 | 0.60 |
| 18:R:77:UNK:C | 18:R:78:UNK:O | 2.45 | 0.60 |
| 3:C:80:UNK:HA | 3:C:91:UNK:O | 2.01 | 0.60 |
| 7:G:119:UNK:O | 7:G:120:UNK:C | 2.48 | 0.60 |
| 7:G:565:UNK:O | 7:G:566:UNK:C | 2.48 | 0.60 |
| 12:L:502:UNK:O | 12:L:506:UNK:N | 2.35 | 0.60 |
| 14:N:9:UNK:O | 14:N:12:UNK:N | 3.07 | 0.60 |
| 2:B:166:UNK:O | 2:B:169:UNK:O | 2.19 | 0.60 |
| 6:F:272:UNK:O | 6:F:273:UNK:CB | 2.49 | 0.60 |
| 13:M:137:UNK:O | 13:M:138:UNK:CB | 2.50 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 13:M:356:UNK:O | 13:M:360:UNK:N | 2.35 | 0.60 |
| 14:N:45:UNK:O | 14:N:47:UNK:N | 2.35 | 0.60 |
| 20:T:20:UNK:O | 20:T:21:UNK:CB | 4.25 | 0.60 |
| 7:G:383:UNK:O | 7:G:387:UNK:CB | 2.49 | 0.60 |
| 9:I:99:UNK:O | 9:I:104:UNK:CB | 2.50 | 0.60 |
| 15:O:25:UNK:O | 15:O:123:UNK:HA | 2.02 | 0.60 |
| 17:Q:32:UNK:CB | 17:Q:59:UNK:C | 2.80 | 0.60 |
| 19:S:83:UNK:O | 19:S:86:UNK:CB | 2.50 | 0.60 |
| 3:C:138:UNK:O | 3:C:139:UNK:CB | 2.50 | 0.60 |
| 4:D:165:UNK:O | 4:D:166:UNK:CB | 2.49 | 0.60 |
| 3:C:56:UNK:O | 3:C:57:UNK:C | 2.49 | 0.59 |
| 13:M:324:UNK:O | 13:M:328:UNK:CB | 2.50 | 0.59 |
| 13:M:26:UNK:O | 13:M:27:UNK:C | 2.47 | 0.59 |
| 2:B:67:UNK:N | 2:B:68:UNK:HA | 2.17 | 0.59 |
| 7:G:180:UNK:O | 7:G:181:UNK:C | 2.47 | 0.59 |
| 8:H:79:UNK:O | 8:H:81:UNK:N | 2.36 | 0.59 |
| 13:M:108:UNK:CA | 13:M:111:UNK:CB | 2.80 | 0.59 |
| 8:H:136:UNK:O | 8:H:137:UNK:C | 2.50 | 0.59 |
| 13:M:113:UNK:HA | 13:M:114:UNK:C | 2.31 | 0.59 |
| 6:F:212:UNK:C | 6:F:220:UNK:H | 2.16 | 0.59 |
| 9:I:23:UNK:O | 9:I:26:UNK:CB | 3.64 | 0.59 |
| 12:L:316:UNK:O | 12:L:319:UNK:CB | 2.51 | 0.59 |
| 12:L:576:UNK:CB | 14:N:167:UNK:CB | 2.80 | 0.59 |
| 24:X:108:UNK:O | 24:X:111:UNK:CB | 2.49 | 0.59 |
| 6:F:163:UNK:H | 6:F:166:UNK:CB | 2.16 | 0.59 |
| 12:L:128:UNK:O | 12:L:131:UNK:N | 2.35 | 0.59 |
| 2:B:122:UNK:CA | 2:B:123:UNK:CB | 2.80 | 0.59 |
| 7:G:102:UNK:O | 7:G:103:UNK:CB | 2.43 | 0.59 |
| 7:G:186:UNK:HA | 7:G:187:UNK:C | 2.31 | 0.59 |
| 12:L:457:UNK:O | 12:L:458:UNK:C | 2.51 | 0.59 |
| 12:L:547:UNK:O | 12:L:550:UNK:N | 2.36 | 0.59 |
| 14:N:298:UNK:O | 14:N:300:UNK:N | 2.35 | 0.59 |
| 19:S:84:UNK:O | 19:S:87:UNK:CA | 2.50 | 0.59 |
| 14:N:5:UNK:O | 14:N:6:UNK:C | 2.98 | 0.59 |
| 15:O:26:UNK:HA | 15:O:124:UNK:O | 2.03 | 0.59 |
| 6:F:435:UNK:O | 6:F:439:UNK:N | 2.36 | 0.59 |
| 16:P:103:UNK:O | 16:P:106:UNK:CA | 2.51 | 0.59 |
| 2:B:121:UNK:HA | 2:B:135:UNK:HA | 1.82 | 0.58 |
| 6:F:212:UNK:HA | 6:F:220:UNK:C | 2.33 | 0.58 |
| 6:F:352:UNK:HA | 6:F:355:UNK:CB | 2.33 | 0.58 |
| 14:N:85:UNK:O | 14:N:86:UNK:CB | 2.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 18:R:64:UNK:O | 18:R:65:UNK:C | 2.51 | 0.58 |
| 21:U:9:UNK:O | 21:U:12:UNK:CB | 2.51 | 0.58 |
| 13:M:42:UNK:O | 13:M:44:UNK:N | 2.36 | 0.58 |
| 6:F:183:UNK:O | 6:F:186:UNK:N | 2.37 | 0.58 |
| 10:J:14:UNK:O | 10:J:17:UNK:CB | 3.14 | 0.58 |
| 12:L:211:UNK:O | 12:L:214:UNK:CB | 2.50 | 0.58 |
| 14:N:276:UNK:O | 14:N:279:UNK:CB | 2.51 | 0.58 |
| 14:N:32:UNK:O | 14:N:35:UNK:CB | 2.51 | 0.58 |
| 16:P:136:UNK:HA | 16:P:137:UNK:C | 2.33 | 0.58 |
| 21:U:22:UNK:O | 21:U:23:UNK:CB | 2.51 | 0.58 |
| 2:B:77:UNK:CB | 2:B:78:UNK:C | 2.82 | 0.58 |
| 3:C:23:UNK:CA | 3:C:26:UNK:CB | 2.81 | 0.58 |
| 26:Z:72:UNK:O | 26:Z:76:UNK:CB | 2.51 | 0.58 |
| 11:K:13:UNK:O | 11:K:16:UNK:CB | 2.52 | 0.58 |
| 12:L:419:UNK:O | 12:L:422:UNK:N | 2.37 | 0.58 |
| 6:F:352:UNK:O | 6:F:355:UNK:CA | 2.51 | 0.58 |
| 6:F:387:UNK:O | 6:F:390:UNK:N | 2.37 | 0.58 |
| 7:G:318:UNK:HA | 7:G:344:UNK:O | 2.03 | 0.58 |
| 7:G:439:UNK:O | 7:G:443:UNK:N | 2.37 | 0.58 |
| 7:G:377:UNK:N | 7:G:449:UNK:CA | 2.53 | 0.58 |
| 13:M:75:UNK:O | 13:M:78:UNK:N | 2.37 | 0.58 |
| 14:N:143:UNK:O | 14:N:145:UNK:O | 2.21 | 0.58 |
| 7:G:33:UNK:O | 7:G:34:UNK:CB | 2.50 | 0.58 |
| 7:G:11:UNK:CB | 7:G:77:UNK:N | 2.67 | 0.58 |
| 9:I:113:UNK:C | 9:I:115:UNK:N | 2.65 | 0.58 |
| 13:M:80:UNK:O | 13:M:81:UNK:C | 2.48 | 0.58 |
| 20:T:9:UNK:O | 20:T:12:UNK:N | 5.79 | 0.58 |
| 5:E:97:UNK:N | 5:E:136:UNK:O | 2.37 | 0.58 |
| 7:G:114:CYS:O | 7:G:118:UNK:CB | 2.52 | 0.58 |
| 9:I:159:UNK:O | 9:I:162:UNK:CB | 2.52 | 0.58 |
| 10:J:101:UNK:O | 10:J:104:UNK:CA | 2.51 | 0.58 |
| 11:K:23:UNK:O | 11:K:26:UNK:CB | 6.51 | 0.58 |
| 16:P:147:UNK:O | 16:P:150:UNK:CB | 2.52 | 0.58 |
| 5:E:96:UNK:C | 5:E:98:UNK:O | 2.52 | 0.58 |
| 7:G:379:UNK:O | 7:G:452:UNK:N | 2.37 | 0.58 |
| 12:L:382:UNK:CB | 12:L:389:UNK:HA | 2.34 | 0.58 |
| 13:M:340:UNK:O | 13:M:342:UNK:N | 2.37 | 0.58 |
| 14:N:91:UNK:H | 14:N:92:UNK:C | 2.16 | 0.58 |
| 16:P:25:UNK:CB | 16:P:95:UNK:CB | 2.82 | 0.58 |
| 2:B:54:CYS:O | 2:B:57:UNK:N | 2.37 | 0.58 |
| 7:G:594:UNK:CB | 7:G:595:UNK:C | 2.82 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 9:I:24:UNK:O | 9:I:27:UNK:CB | 7.23 | 0.58 |
| 14:N:59:UNK:O | 14:N:62:UNK:N | 2.36 | 0.58 |
| 2:B:166:UNK:O | 2:B:169:UNK:C | 2.51 | 0.57 |
| 7:G:604:UNK:O | 7:G:608:UNK:CA | 2.51 | 0.57 |
| 14:N:9:UNK:O | 14:N:12:UNK:CB | 3.14 | 0.57 |
| 25:Y:56:UNK:C | 25:Y:58:UNK:N | 2.66 | 0.57 |
| 4:D:163:UNK:HA | 8:H:278:UNK:HA | 1.87 | 0.57 |
| 8:H:176:UNK:O | 26:Z:46:UNK:CB | 2.53 | 0.57 |
| 4:D:269:UNK:CB | 4:D:368:UNK:CB | 2.82 | 0.57 |
| 9:I:81:UNK:N | 44:I:223:SF4:S1 | 2.77 | 0.57 |
| 12:L:38:UNK:O | 12:L:41:UNK:N | 2.37 | 0.57 |
| 12:L:21:UNK:O | 12:L:22:UNK:C | 2.52 | 0.57 |
| 15:O:119:UNK:C | 15:O:121:UNK:H | 2.16 | 0.57 |
| 20:T:55:UNK:CA | 20:T:60:UNK:O | 2.51 | 0.57 |
| 1:A:65:UNK:O | 1:A:66:UNK:C | 2.52 | 0.57 |
| 6:F:69:UNK:O | 6:F:70:UNK:CB | 2.53 | 0.57 |
| 12:L:604:UNK:CB | 14:N:93:UNK:N | 2.67 | 0.57 |
| 16:P:103:UNK:O | 16:P:104:UNK:C | 2.52 | 0.57 |
| 16:P:133:UNK:CA | 16:P:166:UNK:O | 2.52 | 0.57 |
| 19:S:66:UNK:HA | 19:S:75:UNK:O | 2.04 | 0.57 |
| 8:H:41:UNK:CB | 8:H:44:UNK:CB | 2.82 | 0.57 |
| 12:L:137:UNK:O | 12:L:140:UNK:N | 2.38 | 0.57 |
| 6:F:315:UNK:HA | 6:F:316:UNK:CB | 2.34 | 0.57 |
| 7:G:456:UNK:CB | 7:G:457:UNK:CA | 2.83 | 0.57 |
| 9:I:69:UNK:CB | 9:I:74:UNK:O | 2.53 | 0.57 |
| 16:P:103:UNK:O | 16:P:106:UNK:C | 2.53 | 0.57 |
| 18:R:75:UNK:O | 18:R:76:UNK:CB | 2.53 | 0.57 |
| 22:V:30:UNK:O | 22:V:33:UNK:N | 2.38 | 0.57 |
| 6:F:150:UNK:O | 6:F:153:UNK:CB | 2.52 | 0.57 |
| 6:F:315:UNK:HA | 6:F:316:UNK:O | 2.04 | 0.57 |
| 8:H:93:UNK:N | 8:H:94:UNK:HA | 2.20 | 0.57 |
| 13:M:293:UNK:O | 13:M:294:UNK:C | 2.52 | 0.57 |
| 15:O:43:UNK:O | 15:O:46:UNK:N | 2.38 | 0.57 |
| 16:P:170:UNK:CB | 16:P:203:UNK:O | 2.52 | 0.57 |
| 6:F:209:UNK:CA | 6:F:210:UNK:C | 2.82 | 0.57 |
| 6:F:275:UNK:CB | 6:F:278:UNK:CB | 2.83 | 0.57 |
| 10:J:59:UNK:O | 10:J:63:UNK:CB | 2.52 | 0.57 |
| 14:N:50:UNK:O | 14:N:51:UNK:C | 2.86 | 0.57 |
| 16:P:143:UNK:C | 16:P:145:UNK:N | 2.65 | 0.57 |
| 22:V:52:UNK:O | 22:V:53:UNK:CB | 2.50 | 0.57 |
| 2:B:71:UNK:CB | 8:H:37:UNK:CB | 2.82 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:K:9:UNK:O | 11:K:12:UNK:N | 2.38 | 0.57 |
| 4:D:188:UNK:O | 4:D:189:UNK:CB | 2.52 | 0.56 |
| 6:F:60:UNK:O | 6:F:63:UNK:C | 2.52 | 0.56 |
| 7:G:425:UNK:O | 7:G:428:UNK:N | 2.38 | 0.56 |
| 13:M:91:UNK:O | 13:M:94:UNK:N | 2.38 | 0.56 |
| 24:X:72:UNK:O | 24:X:73:UNK:CB | 2.53 | 0.56 |
| 6:F:212:UNK:O | 6:F:219:UNK:HA | 2.05 | 0.56 |
| 8:H:79:UNK:O | 8:H:82:UNK:N | 2.38 | 0.56 |
| 11:K:17:UNK:O | 11:K:21:UNK:N | 5.63 | 0.56 |
| 25:Y:25:UNK:O | 25:Y:28:UNK:O | 2.23 | 0.56 |
| 4:D:383:UNK:N | 4:D:384:UNK:HA | 2.21 | 0.56 |
| 4:D:402:UNK:O | 4:D:406:UNK:N | 2.38 | 0.56 |
| 11:K:50:UNK:O | 11:K:51:UNK:C | 2.52 | 0.56 |
| 12:L:65:UNK:CB | 12:L:66:UNK:CA | 2.83 | 0.56 |
| 13:M:410:UNK:O | 13:M:414:UNK:N | 2.38 | 0.56 |
| 14:N:45:UNK:O | 14:N:49:UNK:N | 5.02 | 0.56 |
| 16:P:111:UNK:HA | 16:P:151:UNK:CB | 2.35 | 0.56 |
| 8:H:183:UNK:O | 8:H:184:UNK:C | 2.51 | 0.56 |
| 12:L:117:UNK:O | 12:L:118:UNK:C | 2.53 | 0.56 |
| 12:L:368:UNK:O | 12:L:372:UNK:N | 2.37 | 0.56 |
| 13:M:121:UNK:O | 13:M:124:UNK:CB | 2.53 | 0.56 |
| 15:O:109:UNK:O | 15:O:112:UNK:N | 2.38 | 0.56 |
| 16:P:169:UNK:CB | 16:P:231:UNK:CB | 2.84 | 0.56 |
| 6:F:303:UNK:HA | 6:F:414:UNK:CB | 2.36 | 0.56 |
| 8:H:6:UNK:O | 8:H:10:UNK:N | 3.17 | 0.56 |
| 9:I:149:UNK:CA | 9:I:150:UNK:CB | 2.84 | 0.56 |
| 12:L:351:UNK:O | 12:L:352:UNK:CB | 2.53 | 0.56 |
| 14:N:107:UNK:CB | 14:N:108:UNK:HA | 2.35 | 0.56 |
| 16:P:140:UNK:N | 16:P:141:UNK:HA | 2.20 | 0.56 |
| 4:D:394:UNK:O | 4:D:398:UNK:N | 2.38 | 0.56 |
| 6:F:209:UNK:HA | 6:F:210:UNK:C | 2.36 | 0.56 |
| 6:F:214:UNK:HA | 6:F:218:UNK:C | 2.36 | 0.56 |
| 6:F:371:UNK:O | 6:F:375:UNK:CB | 2.52 | 0.56 |
| 7:G:333:UNK:O | 7:G:337:UNK:CB | 2.53 | 0.56 |
| 10:J:170:UNK:O | 10:J:171:UNK:C | 2.53 | 0.56 |
| 12:L:366:UNK:O | 12:L:369:UNK:N | 2.39 | 0.56 |
| 12:L:383:UNK:C | 12:L:389:UNK:CB | 2.84 | 0.56 |
| 12:L:546:UNK:O | 12:L:547:UNK:C | 2.53 | 0.56 |
| 14:N:158:UNK:O | 14:N:161:UNK:CA | 2.53 | 0.56 |
| 16:P:137:UNK:CB | 16:P:138:UNK:CA | 2.84 | 0.56 |
| 19:S:28:UNK:C | 19:S:30:UNK:N | 2.62 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 21:U:10:UNK:O | 21:U:13:UNK:CB | 2.54 | 0.56 |
| 4:D:117:UNK:CB | 4:D:367:UNK:CB | 2.83 | 0.56 |
| 4:D:259:UNK:O | 4:D:261:UNK:N | 2.39 | 0.56 |
| 4:D:369:UNK:N | 4:D:372:UNK:O | 2.38 | 0.56 |
| 5:E:154:UNK:N | 5:E:161:UNK:O | 2.39 | 0.56 |
| 2:B:118:UNK:C | 2:B:120:UNK:N | 2.69 | 0.56 |
| 4:D:163:UNK:CB | 8:H:278:UNK:CB | 2.83 | 0.56 |
| 4:D:224:UNK:O | 4:D:227:UNK:N | 2.38 | 0.56 |
| 4:D:234:UNK:HA | 4:D:237:UNK:CB | 2.35 | 0.56 |
| 12:L:207:UNK:CA | 12:L:208:UNK:C | 2.82 | 0.56 |
| 18:R:63:UNK:O | 18:R:64:UNK:O | 2.22 | 0.56 |
| 19:S:62:UNK:O | 19:S:78:UNK:CB | 2.54 | 0.56 |
| 22:V:1:UNK:C | 22:V:3:UNK:N | 2.67 | 0.56 |
| 22:V:45:UNK:O | 22:V:47:UNK:N | 2.39 | 0.56 |
| 9:I:150:UNK:CB | 9:I:154:UNK:CB | 2.83 | 0.56 |
| 10:J:10:UNK:O | 10:J:13:UNK:N | 3.22 | 0.56 |
| 13:M:31:UNK:O | 13:M:32:UNK:O | 2.23 | 0.56 |
| 21:U:49:UNK:O | 21:U:53:UNK:N | 2.39 | 0.56 |
| 4:D:137:UNK:O | 4:D:140:UNK:N | 2.39 | 0.56 |
| 7:G:210:UNK:O | 7:G:211:UNK:C | 2.52 | 0.56 |
| 9:I:63:UNK:CB | 9:I:133:UNK:CB | 2.84 | 0.56 |
| 12:L:156:UNK:O | 12:L:157:UNK:CB | 2.54 | 0.56 |
| 12:L:207:UNK:CB | 12:L:208:UNK:C | 2.84 | 0.56 |
| 14:N:108:UNK:O | 14:N:111:UNK:N | 2.39 | 0.56 |
| 16:P:94:UNK:O | 16:P:95:UNK:CB | 2.54 | 0.56 |
| 9:I:66:UNK:HA | 9:I:158:UNK:CB | 2.36 | 0.56 |
| 12:L:512:UNK:O | 12:L:513:UNK:C | 2.53 | 0.56 |
| 12:L:579:UNK:C | 12:L:581:UNK:CB | 2.83 | 0.56 |
| 13:M:42:UNK:O | 13:M:43:UNK:C | 2.53 | 0.56 |
| 18:R:68:UNK:CB | 18:R:86:UNK:CB | 2.84 | 0.56 |
| 2:B:123:UNK:N | 2:B:126:UNK:O | 2.40 | 0.55 |
| 6:F:300:UNK:O | 6:F:333:UNK:N | 2.39 | 0.55 |
| 6:F:44:UNK:O | 6:F:47:UNK:CA | 2.54 | 0.55 |
| 12:L:242:UNK:O | 12:L:245:UNK:N | 2.39 | 0.55 |
| 12:L:510:UNK:O | 12:L:513:UNK:CB | 2.54 | 0.55 |
| 14:N:253:UNK:HA | 14:N:259:UNK:CB | 2.36 | 0.55 |
| 3:C:135:UNK:O | 3:C:139:UNK:HA | 2.06 | 0.55 |
| 6:F:52:UNK:O | 6:F:55:UNK:CB | 2.54 | 0.55 |
| 10:J:101:UNK:O | 10:J:104:UNK:CB | 2.54 | 0.55 |
| 12:L:188:UNK:CB | 12:L:211:UNK:CB | 2.84 | 0.55 |
| 13:M:328:UNK:O | 13:M:329:UNK:C | 2.52 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 16:P:82:UNK:O | 16:P:86:UNK:N | 2.39 | 0.55 |
| 6:F:433:UNK:O | 6:F:436:UNK:N | 2.40 | 0.55 |
| 12:L:181:UNK:O | 12:L:183:UNK:N | 2.39 | 0.55 |
| 15:O:32:UNK:C | 15:O:34:UNK:N | 2.67 | 0.55 |
| 4:D:395:UNK:CB | 4:D:428:UNK:CB | 2.85 | 0.55 |
| 6:F:100:UNK:C | 6:F:102:UNK:N | 2.57 | 0.55 |
| 6:F:294:UNK:CB | 6:F:295:UNK:CA | 2.85 | 0.55 |
| 6:F:322:UNK:CB | 6:F:327:UNK:CB | 2.85 | 0.55 |
| 14:N:32:UNK:O | 14:N:35:UNK:N | 2.40 | 0.55 |
| 6:F:209:UNK:CB | 6:F:210:UNK:C | 2.85 | 0.55 |
| 7:G:215:UNK:CB | 9:I:99:UNK:CB | 2.85 | 0.55 |
| 13:M:227:UNK:CA | 13:M:228:UNK:CB | 2.85 | 0.55 |
| 14:N:122:UNK:O | 14:N:124:UNK:HA | 2.05 | 0.55 |
| 1:A:72:UNK:O | 1:A:75:UNK:N | 2.40 | 0.55 |
| 5:E:96:UNK:N | 5:E:138:UNK:CB | 2.70 | 0.55 |
| 7:G:11:UNK:C | 7:G:13:UNK:N | 4.01 | 0.55 |
| 7:G:200:UNK:CB | 7:G:208:UNK:CB | 2.85 | 0.55 |
| 7:G:273:UNK:O | 7:G:276:UNK:N | 2.39 | 0.55 |
| 7:G:527:UNK:HA | 7:G:544:UNK:O | 2.05 | 0.55 |
| 12:L:201:UNK:O | 12:L:202:UNK:C | 2.54 | 0.55 |
| 12:L:38:UNK:O | 12:L:39:UNK:C | 2.55 | 0.55 |
| 13:M:241:UNK:O | 13:M:243:UNK:N | 2.40 | 0.55 |
| 13:M:94:UNK:O | 13:M:97:UNK:N | 2.40 | 0.55 |
| 19:S:64:UNK:HA | 19:S:78:UNK:CA | 2.37 | 0.55 |
| 21:U:30:UNK:CB | 21:U:34:UNK:CB | 2.85 | 0.55 |
| 12:L:531:UNK:O | 12:L:532:UNK:C | 2.53 | 0.55 |
| 12:L:61:UNK:CB | 12:L:80:UNK:CB | 2.85 | 0.55 |
| 15:O:234:UNK:O | 15:O:237:UNK:N | 2.39 | 0.55 |
| 5:E:60:UNK:CB | 5:E:94:UNK:CA | 2.85 | 0.55 |
| 8:H:159:UNK:CB | 8:H:164:UNK:CB | 2.85 | 0.55 |
| 4:D:186:UNK:CB | 9:I:60:UNK:C | 2.85 | 0.55 |
| 13:M:176:UNK:CB | 13:M:179:UNK:N | 2.69 | 0.55 |
| 6:F:301:UNK:CB | 6:F:331:UNK:CB | 2.85 | 0.55 |
| 6:F:31:UNK:H | 6:F:35:UNK:CB | 2.20 | 0.55 |
| 12:L:111:UNK:CB | 12:L:114:UNK:CB | 2.85 | 0.55 |
| 14:N:70:UNK:O | 14:N:71:UNK:C | 2.52 | 0.55 |
| 16:P:215:UNK:O | 16:P:219:UNK:N | 2.40 | 0.55 |
| 3:C:133:UNK:CA | 3:C:136:UNK:CB | 2.82 | 0.55 |
| 3:C:73:UNK:O | 4:D:252:UNK:HA | 2.07 | 0.55 |
| 6:F:195:UNK:O | 6:F:198:UNK:N | 2.40 | 0.55 |
| 6:F:367:UNK:O | 6:F:371:UNK:N | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 7:G:375:UNK:CB | 7:G:376:UNK:CA | 2.85 | 0.55 |
| 9:I:80:CYS:N | 44:I:223:SF4:S1 | 2.79 | 0.55 |
| 14:N:107:UNK:CB | 14:N:108:UNK:CA | 2.85 | 0.55 |
| 15:O:188:UNK:CB | 15:O:191:UNK:CB | 2.85 | 0.55 |
| 19:S:48:UNK:CB | 19:S:51:UNK:CB | 2.85 | 0.55 |
| 2:B:47:UNK:CB | 2:B:85:UNK:CB | 2.85 | 0.54 |
| 4:D:357:UNK:CA | 4:D:384:UNK:CB | 2.84 | 0.54 |
| 6:F:351:UNK:O | 6:F:352:UNK:C | 2.54 | 0.54 |
| 12:L:197:UNK:CB | 12:L:200:UNK:CB | 2.85 | 0.54 |
| 13:M:113:UNK:CA | 13:M:114:UNK:C | 2.85 | 0.54 |
| 13:M:188:UNK:CB | 13:M:189:UNK:CB | 2.84 | 0.54 |
| 14:N:24:UNK:C | 14:N:28:UNK:CB | 2.85 | 0.54 |
| 14:N:91:UNK:CB | 14:N:92:UNK:CB | 2.85 | 0.54 |
| 16:P:203:UNK:CA | 16:P:234:UNK:C | 2.85 | 0.54 |
| 3:C:34:UNK:CB | 3:C:38:UNK:CB | 2.85 | 0.54 |
| 4:D:96:UNK:O | 4:D:99:UNK:CB | 2.55 | 0.54 |
| 6:F:140:UNK:CB | 6:F:182:UNK:CA | 2.86 | 0.54 |
| 6:F:260:UNK:CB | 6:F:336:UNK:CB | 2.84 | 0.54 |
| 7:G:202:UNK:O | 7:G:203:CYS:C | 2.43 | 0.54 |
| 7:G:456:UNK:CB | 7:G:457:UNK:HA | 2.37 | 0.54 |
| 13:M:25:UNK:O | 13:M:26:UNK:C | 2.55 | 0.54 |
| 14:N:55:UNK:CB | 14:N:121:UNK:CB | 2.84 | 0.54 |
| 16:P:233:UNK:CB | 16:P:234:UNK:HA | 2.37 | 0.54 |
| 17:Q:50:UNK:CB | 17:Q:51:UNK:C | 2.85 | 0.54 |
| 7:G:137:UNK:CB | 18:R:75:UNK:O | 2.55 | 0.54 |
| 7:G:570:UNK:HA | 7:G:583:UNK:O | 2.07 | 0.54 |
| 8:H:143:UNK:C | 8:H:145:UNK:N | 2.66 | 0.54 |
| 12:L:210:UNK:O | 12:L:213:UNK:N | 2.41 | 0.54 |
| 13:M:209:UNK:O | 13:M:211:UNK:O | 2.25 | 0.54 |
| 15:O:102:UNK:O | 15:O:106:UNK:CB | 2.55 | 0.54 |
| 2:B:78:UNK:CB | 2:B:79:UNK:C | 2.86 | 0.54 |
| 4:D:360:UNK:CB | 4:D:381:UNK:CB | 2.85 | 0.54 |
| 6:F:183:UNK:CB | 6:F:186:UNK:CB | 2.86 | 0.54 |
| 6:F:31:UNK:N | 6:F:35:UNK:CB | 2.70 | 0.54 |
| 8:H:101:UNK:O | 8:H:104:UNK:N | 2.40 | 0.54 |
| 8:H:307:UNK:O | 8:H:310:UNK:CB | 2.56 | 0.54 |
| 12:L:310:UNK:O | 12:L:313:UNK:CB | 2.55 | 0.54 |
| 12:L:55:UNK:CB | 12:L:56:UNK:CB | 2.86 | 0.54 |
| 13:M:372:UNK:CB | 13:M:375:UNK:CB | 2.85 | 0.54 |
| 14:N:26:UNK:CB | 14:N:27:UNK:CB | 2.84 | 0.54 |
| 16:P:160:UNK:N | 16:P:161:UNK:C | 2.70 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 13:M:176:UNK:O | 19:S:18:UNK:CB | 157.81 | 0.54 |
| 8:H:42:UNK:C | 8:H:44:UNK:HA | 2.37 | 0.54 |
| 9:I:22:UNK:O | 9:I:23:UNK:C | 2.87 | 0.54 |
| 13:M:61:UNK:CA | 13:M:62:UNK:C | 2.85 | 0.54 |
| 14:N:10:UNK:C | 14:N:12:UNK:N | 2.95 | 0.54 |
| 14:N:292:UNK:O | 14:N:295:UNK:CB | 2.55 | 0.54 |
| 20:T:55:UNK:HA | 20:T:60:UNK:O | 2.07 | 0.54 |
| 2:B:65:UNK:C | 2:B:68:UNK:CB | 2.85 | 0.54 |
| 6:F:397:UNK:O | 6:F:401:UNK:N | 2.41 | 0.54 |
| 8:H:173:UNK:O | 8:H:174:UNK:C | 2.54 | 0.54 |
| 8:H:92:UNK:C | 8:H:94:UNK:CB | 2.85 | 0.54 |
| 8:H:93:UNK:CA | 8:H:94:UNK:CB | 2.86 | 0.54 |
| 14:N:24:UNK:CB | 14:N:28:UNK:CB | 2.86 | 0.54 |
| 14:N:293:UNK:C | 14:N:295:UNK:N | 2.63 | 0.54 |
| 15:O:84:UNK:O | 15:O:85:UNK:C | 2.53 | 0.54 |
| 4:D:178:UNK:O | 4:D:182:UNK:N | 2.41 | 0.54 |
| 6:F:214:UNK:CB | 6:F:218:UNK:HA | 2.36 | 0.54 |
| 6:F:433:UNK:O | 6:F:434:UNK:C | 2.55 | 0.54 |
| 7:G:440:UNK:O | 7:G:444:UNK:N | 2.41 | 0.54 |
| 12:L:448:UNK:CB | 12:L:451:UNK:CB | 2.85 | 0.54 |
| 12:L:47:UNK:O | 12:L:48:UNK:C | 2.53 | 0.54 |
| 14:N:25:UNK:C | 14:N:27:UNK:C | 2.85 | 0.54 |
| 19:S:36:UNK:CB | 19:S:84:UNK:CB | 2.85 | 0.54 |
| 2:B:77:UNK:N | 2:B:78:UNK:HA | 2.23 | 0.54 |
| 7:G:108:CYS:SG | 7:G:110:UNK:CB | 2.96 | 0.54 |
| 12:L:593:UNK:O | 12:L:594:UNK:C | 2.52 | 0.54 |
| 14:N:135:UNK:O | 14:N:138:UNK:N | 2.41 | 0.54 |
| 16:P:49:UNK:N | 16:P:73:UNK:CB | 2.71 | 0.54 |
| 16:P:20:UNK:CB | 16:P:89:UNK:CB | 2.85 | 0.54 |
| 20:T:34:UNK:C | 20:T:36:UNK:N | 4.12 | 0.54 |
| 26:Z:83:UNK:O | 26:Z:84:UNK:C | 2.54 | 0.54 |
| 6:F:103:UNK:CB | 6:F:104:UNK:CA | 2.85 | 0.54 |
| 7:G:9:UNK:N | 7:G:20:UNK:O | 2.40 | 0.54 |
| 4:D:163:UNK:CB | 8:H:278:UNK:CA | 2.85 | 0.54 |
| 9:I:63:UNK:CB | 9:I:134:UNK:N | 2.71 | 0.54 |
| 9:I:151:UNK:C | 9:I:153:UNK:N | 2.68 | 0.54 |
| 12:L:28:UNK:CB | 12:L:31:UNK:CB | 2.86 | 0.54 |
| 12:L:77:UNK:CA | 12:L:78:UNK:CB | 2.84 | 0.54 |
| 20:T:43:UNK:CB | 20:T:46:UNK:CB | 2.86 | 0.54 |
| 21:U:43:UNK:CB | 21:U:46:UNK:CB | 2.85 | 0.54 |
| 6:F:242:UNK:O | 6:F:252:UNK:HA | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 10:J:86:UNK:O | 10:J:89:UNK:N | 2.41 | 0.54 |
| 13:M:325:UNK:O | 13:M:329:UNK:N | 2.41 | 0.54 |
| 14:N:134:UNK:O | 14:N:137:UNK:CB | 2.55 | 0.54 |
| 14:N:44:UNK:O | 14:N:45:UNK:C | 2.93 | 0.54 |
| 14:N:72:UNK:O | 14:N:76:UNK:N | 2.41 | 0.54 |
| 25:Y:59:UNK:O | 25:Y:60:UNK:C | 2.56 | 0.54 |
| 6:F:53:UNK:O | 6:F:54:UNK:C | 2.55 | 0.53 |
| 7:G:210:UNK:CB | 7:G:213:UNK:CB | 2.85 | 0.53 |
| 7:G:235:UNK:O | 7:G:236:UNK:CB | 2.56 | 0.53 |
| 7:G:464:UNK:O | 7:G:467:UNK:CB | 2.56 | 0.53 |
| 8:H:40:UNK:CB | 8:H:47:UNK:CB | 2.85 | 0.53 |
| 13:M:133:UNK:CA | 13:M:224:UNK:CB | 2.85 | 0.53 |
| 13:M:362:UNK:O | 13:M:365:UNK:N | 2.42 | 0.53 |
| 13:M:391:UNK:O | 13:M:392:UNK:CB | 2.56 | 0.53 |
| 16:P:138:UNK:CB | 16:P:149:UNK:CB | 2.85 | 0.53 |
| 25:Y:98:UNK:O | 25:Y:101:UNK:N | 2.41 | 0.53 |
| 2:B:78:UNK:N | 2:B:79:UNK:CA | 2.70 | 0.53 |
| 5:E:96:UNK:O | 5:E:98:UNK:C | 2.56 | 0.53 |
| 12:L:127:UNK:O | 12:L:131:UNK:N | 2.41 | 0.53 |
| 12:L:488:UNK:O | 12:L:489:UNK:C | 2.50 | 0.53 |
| 12:L:587:UNK:O | 12:L:591:UNK:N | 2.41 | 0.53 |
| 20:T:70:UNK:HA | 20:T:75:UNK:CB | 2.39 | 0.53 |
| 6:F:322:UNK:CA | 6:F:327:UNK:CB | 2.87 | 0.53 |
| 6:F:398:UNK:O | 6:F:401:UNK:N | 2.40 | 0.53 |
| 7:G:285:UNK:CB | 7:G:288:UNK:CB | 2.86 | 0.53 |
| 9:I:135:UNK:O | 9:I:136:UNK:C | 2.56 | 0.53 |
| 14:N:253:UNK:CB | 14:N:259:UNK:CB | 2.85 | 0.53 |
| 15:O:103:UNK:O | 15:O:107:UNK:CB | 2.56 | 0.53 |
| 23:W:56:UNK:O | 23:W:59:UNK:CB | 2.56 | 0.53 |
| 5:E:126:UNK:O | 5:E:127:UNK:C | 2.55 | 0.53 |
| 5:E:46:UNK:O | 5:E:47:UNK:C | 2.55 | 0.53 |
| 6:F:125:UNK:O | 6:F:128:UNK:N | 2.40 | 0.53 |
| 7:G:16:UNK:C | 7:G:18:UNK:N | 4.10 | 0.53 |
| 10:J:147:UNK:C | 10:J:149:UNK:N | 2.71 | 0.53 |
| 13:M:279:UNK:CB | 13:M:280:UNK:CA | 2.85 | 0.53 |
| 22:V:8:UNK:O | 22:V:12:UNK:N | 2.42 | 0.53 |
| 3:C:21:UNK:O | 3:C:24:UNK:CA | 2.56 | 0.53 |
| 4:D:163:UNK:N | 8:H:278:UNK:CB | 2.72 | 0.53 |
| 6:F:426:UNK:C | 6:F:429:UNK:N | 2.72 | 0.53 |
| 6:F:60:UNK:O | 6:F:63:UNK:N | 2.41 | 0.53 |
| 7:G:110:UNK:O | 7:G:113:UNK:O | 2.26 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 9:I:111:UNK:C | 9:I:113:UNK:N | 2.71 | 0.53 |
| 12:L:176:UNK:O | 12:L:179:UNK:CB | 2.56 | 0.53 |
| 16:P:134:UNK:O | 16:P:167:UNK:CA | 2.57 | 0.53 |
| 17:Q:113:UNK:O | 17:Q:114:UNK:CB | 2.55 | 0.53 |
| 19:S:83:UNK:O | 19:S:86:UNK:N | 2.41 | 0.53 |
| 26:Z:87:UNK:O | 26:Z:90:UNK:CB | 2.56 | 0.53 |
| 3:C:113:UNK:C | 3:C:115:UNK:N | 2.66 | 0.53 |
| 6:F:215:UNK:C | 6:F:217:UNK:N | 2.63 | 0.53 |
| 15:O:102:UNK:O | 15:O:106:UNK:N | 2.41 | 0.53 |
| 16:P:301:UNK:CB | 16:P:303:UNK:CB | 2.85 | 0.53 |
| 23:W:26:UNK:O | 23:W:27:UNK:C | 2.89 | 0.53 |
| 7:G:436:UNK:N | 7:G:437:UNK:CA | 2.62 | 0.53 |
| 14:N:33:UNK:C | 14:N:35:UNK:N | 2.67 | 0.53 |
| 16:P:203:UNK:HA | 16:P:234:UNK:C | 2.39 | 0.53 |
| 4:D:259:UNK:C | 4:D:261:UNK:N | 2.71 | 0.53 |
| 5:E:154:UNK:O | 5:E:161:UNK:N | 2.42 | 0.53 |
| 7:G:114:CYS:SG | 7:G:117:UNK:CB | 2.97 | 0.53 |
| 12:L:11:UNK:O | 12:L:14:UNK:CB | 3.44 | 0.53 |
| 13:M:114:UNK:N | 13:M:177:UNK:CB | 2.72 | 0.53 |
| 14:N:26:UNK:CA | 14:N:27:UNK:CB | 2.87 | 0.53 |
| 16:P:143:UNK:O | 16:P:145:UNK:N | 2.42 | 0.53 |
| 23:W:49:UNK:CA | 23:W:52:UNK:CB | 2.81 | 0.53 |
| 8:H:190:UNK:O | 8:H:194:UNK:CB | 2.57 | 0.53 |
| 10:J:13:UNK:CB | 10:J:39:UNK:CB | 2.87 | 0.53 |
| 12:L:31:UNK:O | 12:L:35:UNK:N | 2.41 | 0.53 |
| 12:L:94:UNK:O | 12:L:95:UNK:C | 2.56 | 0.53 |
| 26:Z:79:UNK:O | 26:Z:80:UNK:C | 2.56 | 0.53 |
| 3:C:88:UNK:HA | 3:C:112:UNK:HA | 1.91 | 0.53 |
| 7:G:31:UNK:O | 7:G:34:UNK:N | 2.42 | 0.52 |
| 12:L:207:UNK:CB | 12:L:209:UNK:N | 2.72 | 0.52 |
| 12:L:383:UNK:N | 12:L:389:UNK:CB | 2.72 | 0.52 |
| 12:L:602:UNK:C | 12:L:604:UNK:N | 2.72 | 0.52 |
| 12:L:67:UNK:CB | 12:L:75:UNK:O | 2.57 | 0.52 |
| 13:M:139:UNK:HA | 13:M:140:UNK:CB | 2.39 | 0.52 |
| 13:M:180:UNK:C | 13:M:182:UNK:N | 2.65 | 0.52 |
| 13:M:364:UNK:O | 13:M:367:UNK:CB | 2.56 | 0.52 |
| 13:M:68:UNK:C | 13:M:70:UNK:N | 2.66 | 0.52 |
| 14:N:25:UNK:C | 14:N:28:UNK:N | 2.72 | 0.52 |
| 14:N:25:UNK:O | 14:N:28:UNK:N | 2.48 | 0.52 |
| 16:P:203:UNK:N | 16:P:234:UNK:O | 2.41 | 0.52 |
| 21:U:37:UNK:HA | 21:U:42:UNK:CB | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:F:209:UNK:CB | 6:F:211:UNK:HA | 2.39 | 0.52 |
| 7:G:282:UNK:O | 7:G:293:UNK:HA | 2.09 | 0.52 |
| 8:H:101:UNK:N | 8:H:161:UNK:CB | 2.72 | 0.52 |
| 12:L:69:UNK:CB | 12:L:74:UNK:HA | 2.39 | 0.52 |
| 13:M:227:UNK:N | 13:M:228:UNK:CB | 2.72 | 0.52 |
| 13:M:3:UNK:H | 13:M:6:UNK:CB | 2.22 | 0.52 |
| 16:P:140:UNK:N | 16:P:141:UNK:CA | 2.72 | 0.52 |
| 16:P:216:UNK:O | 16:P:220:UNK:N | 2.42 | 0.52 |
| 1:A:90:UNK:O | 1:A:93:UNK:CB | 2.58 | 0.52 |
| 4:D:383:UNK:N | 4:D:384:UNK:CA | 2.72 | 0.52 |
| 12:L:524:UNK:HA | 12:L:527:UNK:CB | 2.40 | 0.52 |
| 12:L:82:UNK:N | 12:L:86:UNK:CB | 2.73 | 0.52 |
| 13:M:190:UNK:N | 13:M:191:UNK:C | 2.73 | 0.52 |
| 14:N:26:UNK:N | 14:N:27:UNK:CB | 2.73 | 0.52 |
| 16:P:114:UNK:O | 16:P:118:UNK:N | 2.43 | 0.52 |
| 22:V:23:UNK:O | 22:V:24:UNK:CB | 2.58 | 0.52 |
| 4:D:211:UNK:O | 4:D:214:UNK:CB | 2.58 | 0.52 |
| 4:D:258:UNK:N | 4:D:261:UNK:CB | 2.72 | 0.52 |
| 6:F:102:UNK:O | 6:F:103:UNK:CB | 2.58 | 0.52 |
| 6:F:257:UNK:O | 6:F:333:UNK:HA | 2.09 | 0.52 |
| 6:F:300:UNK:N | 6:F:329:UNK:HA | 2.25 | 0.52 |
| 6:F:421:UNK:N | 6:F:424:UNK:CB | 2.73 | 0.52 |
| 7:G:282:UNK:N | 7:G:293:UNK:CB | 2.73 | 0.52 |
| 7:G:565:UNK:O | 7:G:567:UNK:N | 2.43 | 0.52 |
| 10:J:59:UNK:HA | 10:J:63:UNK:CB | 2.39 | 0.52 |
| 12:L:161:UNK:CB | 12:L:162:UNK:HA | 2.40 | 0.52 |
| 13:M:61:UNK:N | 13:M:62:UNK:C | 2.73 | 0.52 |
| 14:N:224:UNK:N | 14:N:225:UNK:CA | 2.73 | 0.52 |
| 14:N:234:UNK:O | 14:N:237:UNK:O | 2.28 | 0.52 |
| 19:S:34:UNK:O | 19:S:38:UNK:N | 2.42 | 0.52 |
| 20:T:63:UNK:O | 20:T:66:UNK:N | 2.42 | 0.52 |
| 8:H:93:UNK:N | 8:H:94:UNK:CA | 2.73 | 0.52 |
| 9:I:119:CYS:O | 9:I:120:UNK:CB | 2.58 | 0.52 |
| 10:J:21:UNK:O | 10:J:22:UNK:C | 2.55 | 0.52 |
| 14:N:66:UNK:O | 14:N:67:UNK:C | 2.55 | 0.52 |
| 16:P:203:UNK:N | 16:P:234:UNK:C | 2.73 | 0.52 |
| 16:P:223:UNK:N | 16:P:224:UNK:CB | 2.73 | 0.52 |
| 2:B:54:CYS:C | 2:B:56:UNK:N | 2.61 | 0.52 |
| 4:D:307:UNK:O | 4:D:308:UNK:C | 2.57 | 0.52 |
| 5:E:109:UNK:O | 5:E:112:UNK:N | 2.42 | 0.52 |
| 12:L:257:UNK:O | 12:L:261:UNK:N | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 13:M:364:UNK:O | 13:M:367:UNK:N | 2.42 | 0.52 |
| 13:M:393:UNK:O | 13:M:394:UNK:C | 2.57 | 0.52 |
| 22:V:21:UNK:O | 22:V:25:UNK:N | 9.03 | 0.52 |
| 23:W:3:UNK:O | 23:W:4:UNK:C | 2.02 | 0.52 |
| 4:D:163:UNK:N | 8:H:278:UNK:CA | 2.72 | 0.52 |
| 6:F:300:UNK:CB | 6:F:330:UNK:N | 2.73 | 0.52 |
| 7:G:329:UNK:O | 7:G:333:UNK:N | 2.42 | 0.52 |
| 11:K:42:UNK:O | 11:K:45:UNK:CB | 2.58 | 0.52 |
| 12:L:241:UNK:O | 12:L:244:UNK:CB | 2.57 | 0.52 |
| 12:L:279:UNK:O | 12:L:282:UNK:N | 2.43 | 0.52 |
| 14:N:26:UNK:N | 14:N:27:UNK:C | 2.73 | 0.52 |
| 20:T:40:UNK:O | 20:T:41:UNK:CB | 2.58 | 0.52 |
| 5:E:113:UNK:O | 5:E:114:UNK:C | 2.57 | 0.52 |
| 6:F:121:UNK:CB | 6:F:232:UNK:CB | 2.88 | 0.52 |
| 9:I:110:UNK:HA | 9:I:150:UNK:O | 2.10 | 0.52 |
| 9:I:21:UNK:HA | 9:I:24:UNK:CB | 2.40 | 0.52 |
| 9:I:21:UNK:O | 9:I:24:UNK:CB | 2.58 | 0.52 |
| 13:M:115:UNK:N | 13:M:175:UNK:CB | 2.73 | 0.52 |
| 4:D:174:UNK:O | 4:D:175:UNK:C | 2.57 | 0.52 |
| 4:D:95:UNK:N | 4:D:98:UNK:CB | 2.72 | 0.52 |
| 6:F:262:UNK:CB | 6:F:285:UNK:C | 2.87 | 0.52 |
| 6:F:300:UNK:CB | 6:F:329:UNK:CA | 2.84 | 0.52 |
| 6:F:290:UNK:O | 6:F:291:UNK:CB | 2.57 | 0.52 |
| 7:G:448:UNK:O | 7:G:449:UNK:CB | 2.58 | 0.52 |
| 8:H:93:UNK:HA | 8:H:94:UNK:CB | 2.40 | 0.52 |
| 13:M:309:UNK:O | 13:M:312:UNK:N | 2.43 | 0.52 |
| 14:N:293:UNK:O | 14:N:295:UNK:N | 2.41 | 0.52 |
| 16:P:203:UNK:C | 16:P:233:UNK:CB | 2.88 | 0.52 |
| 16:P:95:UNK:O | 16:P:96:UNK:CB | 2.57 | 0.52 |
| 5:E:112:UNK:O | 5:E:113:UNK:C | 2.57 | 0.51 |
| 12:L:376:UNK:C | 12:L:378:UNK:N | 2.68 | 0.51 |
| 12:L:580:UNK:N | 12:L:581:UNK:CB | 2.73 | 0.51 |
| 14:N:194:UNK:O | 14:N:195:UNK:C | 2.58 | 0.51 |
| 14:N:91:UNK:N | 14:N:92:UNK:CB | 2.73 | 0.51 |
| 15:O:43:UNK:O | 15:O:45:UNK:N | 2.43 | 0.51 |
| 25:Y:29:UNK:O | 25:Y:30:UNK:CB | 2.58 | 0.51 |
| 25:Y:94:UNK:O | 25:Y:97:UNK:N | 2.43 | 0.51 |
| 13:M:343:UNK:C | 13:M:345:UNK:N | 2.70 | 0.51 |
| 16:P:135:UNK:HA | 16:P:167:UNK:C | 2.41 | 0.51 |
| 16:P:49:UNK:O | 16:P:73:UNK:N | 2.44 | 0.51 |
| 21:U:10:UNK:O | 21:U:13:UNK:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 24:X:88:UNK:O | 24:X:91:UNK:CB | 2.58 | 0.51 |
| 4:D:229:UNK:HA | 4:D:232:UNK:CB | 2.40 | 0.51 |
| 6:F:94:UNK:CB | 6:F:135:UNK:O | 2.57 | 0.51 |
| 12:L:55:UNK:N | 12:L:56:UNK:C | 2.71 | 0.51 |
| 12:L:60:UNK:O | 12:L:81:UNK:N | 2.43 | 0.51 |
| 13:M:341:UNK:O | 13:M:342:UNK:C | 2.56 | 0.51 |
| 13:M:347:UNK:HA | 13:M:415:UNK:HA | 1.92 | 0.51 |
| 22:V:2:UNK:O | 22:V:5:UNK:CB | 3.89 | 0.51 |
| 4:D:360:UNK:CA | 4:D:381:UNK:HA | 2.39 | 0.51 |
| 6:F:276:UNK:O | 6:F:280:UNK:N | 2.43 | 0.51 |
| 12:L:163:UNK:C | 12:L:165:UNK:N | 2.69 | 0.51 |
| 16:P:170:UNK:O | 16:P:172:UNK:N | 2.43 | 0.51 |
| 17:Q:50:UNK:N | 17:Q:51:UNK:HA | 2.25 | 0.51 |
| 9:I:22:UNK:C | 9:I:24:UNK:N | 2.99 | 0.51 |
| 12:L:556:UNK:O | 12:L:560:UNK:N | 2.43 | 0.51 |
| 13:M:241:UNK:C | 13:M:243:UNK:N | 2.71 | 0.51 |
| 13:M:23:UNK:C | 13:M:25:UNK:N | 2.73 | 0.51 |
| 13:M:348:UNK:N | 13:M:415:UNK:CB | 2.74 | 0.51 |
| 14:N:184:UNK:O | 14:N:188:UNK:N | 2.44 | 0.51 |
| 16:P:117:UNK:O | 16:P:120:UNK:N | 2.43 | 0.51 |
| 2:B:129:UNK:O | 2:B:131:UNK:N | 2.43 | 0.51 |
| 2:B:95:UNK:O | 2:B:96:UNK:C | 2.57 | 0.51 |
| 10:J:90:UNK:O | 10:J:93:UNK:N | 2.43 | 0.51 |
| 13:M:378:UNK:C | 13:M:380:UNK:N | 2.72 | 0.51 |
| 13:M:63:UNK:O | 13:M:67:UNK:N | 2.44 | 0.51 |
| 14:N:163:UNK:O | 14:N:166:UNK:CB | 2.58 | 0.51 |
| 16:P:139:UNK:CB | 16:P:140:UNK:C | 2.88 | 0.51 |
| 6:F:426:UNK:C | 6:F:428:UNK:N | 2.70 | 0.51 |
| 23:W:24:UNK:O | 23:W:25:UNK:CB | 2.56 | 0.51 |
| 4:D:270:UNK:O | 4:D:274:UNK:HA | 2.11 | 0.51 |
| 4:D:357:UNK:N | 4:D:384:UNK:CB | 2.74 | 0.51 |
| 13:M:27:UNK:O | 13:M:28:UNK:C | 2.58 | 0.51 |
| 14:N:145:UNK:CB | 14:N:147:UNK:CB | 2.88 | 0.51 |
| 16:P:203:UNK:H2 | 16:P:234:UNK:C | 2.23 | 0.51 |
| 20:T:33:UNK:O | 20:T:36:UNK:N | 6.61 | 0.51 |
| 22:V:14:UNK:O | 22:V:17:UNK:CB | 3.41 | 0.51 |
| 7:G:104:UNK:O | 7:G:105:CYS:C | 2.49 | 0.51 |
| 7:G:10:UNK:C | 7:G:76:UNK:HA | 2.28 | 0.51 |
| 8:H:39:UNK:C | 8:H:41:UNK:N | 2.72 | 0.51 |
| 12:L:246:UNK:O | 12:L:250:UNK:N | 2.44 | 0.51 |
| 12:L:47:UNK:C | 12:L:49:UNK:N | 2.72 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 13:M:62:UNK:CB | 13:M:64:UNK:N | 2.73 | 0.51 |
| 15:O:125:UNK:O | 15:O:126:UNK:CB | 2.59 | 0.51 |
| 16:P:106:UNK:CA | 16:P:109:UNK:CB | 2.86 | 0.51 |
| 16:P:25:UNK:CB | 16:P:95:UNK:CA | 2.89 | 0.51 |
| 7:G:227:UNK:O | 7:G:238:UNK:CB | 2.59 | 0.51 |
| 8:H:110:UNK:O | 8:H:113:UNK:N | 2.44 | 0.51 |
| 10:J:26:UNK:O | 10:J:27:UNK:CB | 2.59 | 0.51 |
| 13:M:287:UNK:O | 13:M:288:UNK:C | 2.57 | 0.51 |
| 14:N:276:UNK:O | 14:N:277:UNK:C | 2.57 | 0.51 |
| 16:P:155:UNK:O | 16:P:158:UNK:N | 2.44 | 0.51 |
| 4:D:162:UNK:CB | 8:H:279:UNK:N | 2.73 | 0.50 |
| 5:E:46:UNK:O | 5:E:50:UNK:N | 2.43 | 0.50 |
| 9:I:100:UNK:CB | 9:I:103:UNK:N | 2.74 | 0.50 |
| 12:L:52:UNK:C | 12:L:54:UNK:N | 2.73 | 0.50 |
| 13:M:30:UNK:C | 13:M:32:UNK:N | 3.07 | 0.50 |
| 15:O:33:UNK:O | 15:O:36:UNK:N | 2.44 | 0.50 |
| 15:O:43:UNK:C | 15:O:45:UNK:N | 2.65 | 0.50 |
| 2:B:129:UNK:CB | 3:C:167:UNK:O | 2.59 | 0.50 |
| 4:D:195:UNK:O | 4:D:198:UNK:O | 2.28 | 0.50 |
| 2:B:71:UNK:O | 8:H:37:UNK:CB | 2.60 | 0.50 |
| 12:L:321:UNK:O | 12:L:324:UNK:C | 2.58 | 0.50 |
| 14:N:5:UNK:O | 14:N:8:UNK:CB | 3.67 | 0.50 |
| 16:P:170:UNK:O | 16:P:205:UNK:CA | 2.59 | 0.50 |
| 22:V:3:UNK:O | 22:V:5:UNK:N | 3.29 | 0.50 |
| 2:B:123:UNK:N | 2:B:126:UNK:C | 2.72 | 0.50 |
| 2:B:150:UNK:HA | 44:B:201:SF4:S1 | 2.51 | 0.50 |
| 4:D:101:UNK:O | 4:D:103:UNK:N | 2.42 | 0.50 |
| 12:L:207:UNK:CB | 12:L:209:UNK:CA | 2.89 | 0.50 |
| 16:P:248:UNK:CB | 16:P:317:UNK:CB | 2.89 | 0.50 |
| 26:Z:65:UNK:O | 26:Z:66:UNK:C | 2.57 | 0.50 |
| 3:C:23:UNK:O | 3:C:27:UNK:N | 2.44 | 0.50 |
| 5:E:62:UNK:O | 5:E:63:UNK:C | 2.58 | 0.50 |
| 6:F:103:UNK:CA | 6:F:104:UNK:C | 2.89 | 0.50 |
| 7:G:236:UNK:CB | 7:G:259:UNK:CB | 2.90 | 0.50 |
| 8:H:79:UNK:C | 8:H:81:UNK:N | 2.73 | 0.50 |
| 9:I:120:UNK:N | 44:I:222:SF4:S4 | 2.85 | 0.50 |
| 9:I:23:UNK:O | 9:I:26:UNK:N | 3.13 | 0.50 |
| 15:O:33:UNK:CB | 15:O:36:UNK:CB | 2.89 | 0.50 |
| 16:P:53:UNK:C | 16:P:57:UNK:CB | 2.90 | 0.50 |
| 24:X:46:UNK:C | 24:X:48:UNK:N | 2.72 | 0.50 |
| 7:G:594:UNK:CA | 7:G:595:UNK:C | 2.87 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 10:J:50:UNK:O | 10:J:54:UNK:CB | 2.60 | 0.50 |
| 12:L:288:UNK:CB | 12:L:308:UNK:CA | 2.89 | 0.50 |
| 12:L:70:UNK:O | 12:L:73:UNK:O | 2.28 | 0.50 |
| 19:S:25:UNK:N | 19:S:57:UNK:CA | 2.73 | 0.50 |
| 8:H:284:UNK:O | 8:H:288:UNK:N | 2.44 | 0.50 |
| 13:M:392:UNK:C | 13:M:394:UNK:N | 2.68 | 0.50 |
| 15:O:129:UNK:O | 15:O:132:UNK:N | 2.44 | 0.50 |
| 15:O:141:UNK:O | 15:O:142:UNK:CB | 2.58 | 0.50 |
| 4:D:257:UNK:O | 4:D:259:UNK:N | 2.45 | 0.50 |
| 6:F:352:UNK:O | 6:F:356:UNK:N | 2.45 | 0.50 |
| 12:L:241:UNK:O | 12:L:244:UNK:N | 2.45 | 0.50 |
| 13:M:256:UNK:O | 13:M:257:UNK:C | 2.56 | 0.50 |
| 13:M:348:UNK:CA | 13:M:351:UNK:CB | 2.85 | 0.50 |
| 19:S:63:UNK:O | 19:S:78:UNK:CB | 2.58 | 0.50 |
| 25:Y:103:UNK:O | 25:Y:106:UNK:CA | 2.60 | 0.50 |
| 6:F:315:UNK:HA | 6:F:316:UNK:C | 2.42 | 0.50 |
| 7:G:227:UNK:O | 7:G:238:UNK:CA | 2.58 | 0.50 |
| 11:K:9:UNK:O | 11:K:12:UNK:CB | 2.60 | 0.50 |
| 12:L:547:UNK:O | 12:L:550:UNK:CB | 2.60 | 0.50 |
| 13:M:396:UNK:O | 13:M:399:UNK:N | 2.45 | 0.50 |
| 22:V:55:UNK:C | 22:V:57:UNK:N | 2.74 | 0.50 |
| 26:Z:87:UNK:O | 26:Z:88:UNK:C | 2.60 | 0.50 |
| 2:B:166:UNK:O | 2:B:167:UNK:C | 2.60 | 0.49 |
| 6:F:194:UNK:O | 6:F:198:UNK:N | 2.45 | 0.49 |
| 4:D:163:UNK:CB | 8:H:278:UNK:HA | 2.41 | 0.49 |
| 12:L:602:UNK:O | 12:L:604:UNK:N | 2.45 | 0.49 |
| 12:L:7:UNK:O | 12:L:8:UNK:C | 2.81 | 0.49 |
| 13:M:106:UNK:O | 13:M:109:UNK:N | 2.44 | 0.49 |
| 14:N:267:UNK:O | 14:N:271:UNK:N | 2.45 | 0.49 |
| 2:B:129:UNK:C | 2:B:131:UNK:N | 2.73 | 0.49 |
| 7:G:573:UNK:O | 7:G:580:UNK:HA | 2.11 | 0.49 |
| 8:H:43:UNK:N | 8:H:44:UNK:CA | 2.70 | 0.49 |
| 13:M:227:UNK:CB | 13:M:228:UNK:CB | 2.90 | 0.49 |
| 14:N:26:UNK:N | 14:N:27:UNK:CA | 2.74 | 0.49 |
| 2:B:121:UNK:CA | 2:B:135:UNK:CB | 2.85 | 0.49 |
| 6:F:234:UNK:O | 6:F:237:UNK:O | 2.29 | 0.49 |
| 6:F:365:CYS:O | 6:F:368:UNK:N | 2.45 | 0.49 |
| 7:G:15:UNK:O | 7:G:18:UNK:CB | 9.57 | 0.49 |
| 12:L:161:UNK:CB | 12:L:162:UNK:CA | 2.90 | 0.49 |
| 12:L:239:UNK:C | 12:L:240:UNK:O | 2.60 | 0.49 |
| 12:L:263:UNK:O | 12:L:264:UNK:C | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 14:N:169:UNK:CB | 14:N:292:UNK:CB | 2.90 | 0.49 |
| 14:N:52:UNK:O | 14:N:55:UNK:CB | 2.70 | 0.49 |
| 16:P:136:UNK:CA | 16:P:137:UNK:CB | 2.85 | 0.49 |
| 19:S:24:UNK:C | 19:S:57:UNK:CB | 2.87 | 0.49 |
| 20:T:62:UNK:C | 20:T:63:UNK:O | 2.56 | 0.49 |
| 2:B:119:CYS:SG | 44:B:201:SF4:S4 | 3.09 | 0.49 |
| 3:C:31:UNK:C | 3:C:33:UNK:N | 2.75 | 0.49 |
| 3:C:67:UNK:O | 3:C:68:UNK:C | 2.59 | 0.49 |
| 4:D:70:UNK:C | 4:D:72:UNK:N | 2.74 | 0.49 |
| 7:G:285:UNK:HA | 7:G:289:UNK:O | 2.13 | 0.49 |
| 7:G:30:UNK:O | 7:G:33:UNK:CB | 2.61 | 0.49 |
| 13:M:384:UNK:C | 13:M:386:UNK:N | 2.72 | 0.49 |
| 14:N:123:UNK:CA | 14:N:124:UNK:CB | 2.90 | 0.49 |
| 14:N:16:UNK:O | 14:N:19:UNK:N | 2.45 | 0.49 |
| 7:G:469:UNK:HA | 7:G:472:UNK:CB | 2.42 | 0.49 |
| 9:I:85:UNK:C | 9:I:87:CYS:H | 2.24 | 0.49 |
| 6:F:431:UNK:O | 6:F:434:UNK:CB | 2.61 | 0.49 |
| 6:F:91:UNK:HA | 6:F:219:UNK:O | 2.12 | 0.49 |
| 7:G:425:UNK:O | 7:G:429:UNK:N | 2.45 | 0.49 |
| 8:H:257:UNK:O | 8:H:261:UNK:N | 2.46 | 0.49 |
| 10:J:147:UNK:O | 10:J:148:UNK:C | 2.57 | 0.49 |
| 12:L:190:UNK:HA | 12:L:194:UNK:CA | 2.40 | 0.49 |
| 13:M:13:UNK:O | 13:M:16:UNK:N | 3.01 | 0.49 |
| 13:M:22:UNK:HA | 13:M:23:UNK:CB | 2.40 | 0.49 |
| 20:T:53:UNK:O | 20:T:54:UNK:C | 2.96 | 0.49 |
| 6:F:100:UNK:O | 6:F:101:UNK:C | 2.48 | 0.49 |
| 6:F:92:UNK:N | 6:F:219:UNK:O | 2.45 | 0.49 |
| 6:F:370:UNK:C | 6:F:372:UNK:N | 2.74 | 0.49 |
| 7:G:173:UNK:O | 7:G:183:UNK:O | 2.30 | 0.49 |
| 7:G:301:UNK:O | 7:G:304:UNK:CB | 2.61 | 0.49 |
| 7:G:75:UNK:C | 7:G:77:UNK:N | 2.73 | 0.49 |
| 11:K:19:UNK:O | 11:K:20:UNK:CB | 2.61 | 0.49 |
| 11:K:40:UNK:O | 11:K:43:UNK:CB | 2.61 | 0.49 |
| 12:L:10:UNK:O | 12:L:11:UNK:C | 2.89 | 0.49 |
| 12:L:48:UNK:O | 12:L:52:UNK:N | 2.46 | 0.49 |
| 15:O:229:UNK:CA | 15:O:231:UNK:N | 2.75 | 0.49 |
| 6:F:426:UNK:CA | 6:F:429:UNK:CB | 2.83 | 0.49 |
| 8:H:143:UNK:O | 8:H:145:UNK:N | 2.46 | 0.49 |
| 9:I:20:UNK:O | 9:I:24:UNK:N | 2.45 | 0.49 |
| 13:M:189:UNK:N | 13:M:191:UNK:C | 2.75 | 0.49 |
| 14:N:297:UNK:C | 14:N:299:UNK:N | 2.72 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 16:P:204:UNK:N | 16:P:233:UNK:CB | 2.75 | 0.49 |
| 17:Q:115:UNK:O | 17:Q:116:UNK:C | 2.61 | 0.49 |
| 24:X:69:UNK:O | 24:X:70:UNK:C | 2.59 | 0.49 |
| 24:X:72:UNK:CB | 24:X:75:UNK:HA | 2.43 | 0.49 |
| 4:D:116:UNK:O | 4:D:120:UNK:N | 2.46 | 0.49 |
| 4:D:250:UNK:C | 4:D:252:UNK:N | 2.73 | 0.49 |
| 6:F:423:UNK:O | 6:F:426:UNK:N | 2.46 | 0.49 |
| 12:L:105:UNK:O | 12:L:109:UNK:N | 2.45 | 0.49 |
| 22:V:14:UNK:O | 22:V:18:UNK:N | 2.86 | 0.49 |
| 3:C:28:UNK:O | 3:C:31:UNK:N | 2.46 | 0.49 |
| 4:D:310:UNK:O | 4:D:314:UNK:N | 2.46 | 0.49 |
| 7:G:570:UNK:O | 7:G:571:UNK:CB | 2.61 | 0.49 |
| 11:K:11:UNK:O | 11:K:12:UNK:C | 2.61 | 0.49 |
| 14:N:53:UNK:O | 14:N:54:UNK:C | 2.76 | 0.49 |
| 19:S:19:UNK:HA | 19:S:66:UNK:O | 2.13 | 0.49 |
| 6:F:191:UNK:O | 6:F:195:UNK:N | 2.46 | 0.48 |
| 24:X:41:UNK:O | 24:X:44:UNK:N | 2.46 | 0.48 |
| 1:A:91:UNK:O | 1:A:92:UNK:C | 2.61 | 0.48 |
| 4:D:108:UNK:O | 4:D:109:UNK:C | 2.58 | 0.48 |
| 4:D:84:UNK:O | 4:D:85:UNK:CB | 2.62 | 0.48 |
| 4:D:86:UNK:O | 4:D:87:UNK:C | 2.58 | 0.48 |
| 5:E:62:UNK:O | 5:E:65:UNK:N | 2.46 | 0.48 |
| 6:F:45:UNK:O | 6:F:48:UNK:CB | 2.61 | 0.48 |
| 12:L:128:UNK:O | 12:L:129:UNK:C | 2.61 | 0.48 |
| 12:L:281:UNK:CB | 12:L:315:UNK:CA | 2.91 | 0.48 |
| 12:L:580:UNK:CB | 12:L:581:UNK:HA | 2.43 | 0.48 |
| 13:M:275:UNK:C | 13:M:278:UNK:CB | 2.91 | 0.48 |
| 14:N:61:UNK:O | 14:N:62:UNK:C | 2.60 | 0.48 |
| 16:P:203:UNK:CA | 16:P:233:UNK:CB | 2.87 | 0.48 |
| 18:R:59:UNK:O | 18:R:70:UNK:HA | 2.13 | 0.48 |
| 3:C:56:UNK:O | 3:C:58:UNK:N | 2.47 | 0.48 |
| 4:D:328:UNK:O | 4:D:329:UNK:C | 2.58 | 0.48 |
| 6:F:405:CYS:SG | 6:F:406:UNK:CB | 2.98 | 0.48 |
| 12:L:137:UNK:O | 12:L:140:UNK:CB | 2.60 | 0.48 |
| 24:X:90:UNK:C | 24:X:92:UNK:N | 2.76 | 0.48 |
| 5:E:109:UNK:C | 5:E:111:UNK:N | 2.73 | 0.48 |
| 7:G:28:UNK:O | 7:G:29:UNK:C | 2.60 | 0.48 |
| 7:G:611:UNK:O | 7:G:612:UNK:CB | 2.60 | 0.48 |
| 14:N:223:UNK:CB | 14:N:224:UNK:HA | 2.43 | 0.48 |
| 16:P:145:UNK:O | 16:P:149:UNK:N | 2.47 | 0.48 |
| 3:C:112:UNK:N | 3:C:113:UNK:HA | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:C:117:UNK:O | 3:C:142:UNK:HA | 2.13 | 0.48 |
| 7:G:488:UNK:O | 7:G:489:UNK:C | 2.61 | 0.48 |
| 9:I:49:UNK:O | 9:I:53:UNK:N | 2.45 | 0.48 |
| 10:J:85:UNK:O | 10:J:86:UNK:C | 2.61 | 0.48 |
| 6:F:322:UNK:HA | 6:F:327:UNK:CB | 2.44 | 0.48 |
| 14:N:201:UNK:O | 14:N:202:UNK:C | 2.57 | 0.48 |
| 15:O:191:UNK:O | 15:O:192:UNK:C | 2.60 | 0.48 |
| 1:A:90:UNK:O | 1:A:93:UNK:N | 2.47 | 0.48 |
| 4:D:234:UNK:O | 4:D:237:UNK:CA | 2.61 | 0.48 |
| 6:F:262:UNK:CA | 6:F:286:UNK:N | 2.76 | 0.48 |
| 6:F:300:UNK:CA | 6:F:329:UNK:CA | 2.90 | 0.48 |
| 4:D:183:UNK:HA | 9:I:58:UNK:CB | 2.43 | 0.48 |
| 12:L:29:UNK:CA | 12:L:32:UNK:CB | 2.85 | 0.48 |
| 12:L:339:UNK:O | 12:L:342:UNK:N | 2.47 | 0.48 |
| 14:N:157:UNK:O | 14:N:158:UNK:C | 2.60 | 0.48 |
| 16:P:135:UNK:CA | 16:P:168:UNK:N | 2.72 | 0.48 |
| 3:C:28:UNK:O | 3:C:31:UNK:CB | 2.61 | 0.48 |
| 8:H:241:UNK:O | 8:H:242:UNK:CB | 2.61 | 0.48 |
| 9:I:98:UNK:C | 9:I:103:UNK:O | 2.60 | 0.48 |
| 15:O:185:UNK:O | 15:O:186:UNK:C | 2.55 | 0.48 |
| 5:E:33:UNK:O | 5:E:36:UNK:N | 2.47 | 0.48 |
| 6:F:364:UNK:O | 6:F:367:UNK:CB | 2.62 | 0.48 |
| 6:F:419:UNK:CA | 6:F:423:UNK:CB | 2.84 | 0.48 |
| 13:M:63:UNK:O | 13:M:66:UNK:N | 2.46 | 0.48 |
| 14:N:134:UNK:O | 14:N:137:UNK:N | 2.47 | 0.48 |
| 14:N:149:UNK:O | 14:N:150:UNK:C | 2.61 | 0.48 |
| 2:B:150:UNK:CA | 44:B:201:SF4:S1 | 3.02 | 0.48 |
| 4:D:101:UNK:C | 4:D:103:UNK:N | 2.75 | 0.48 |
| 6:F:209:UNK:CB | 6:F:211:UNK:N | 2.77 | 0.48 |
| 8:H:101:UNK:N | 8:H:161:UNK:CA | 2.73 | 0.48 |
| 13:M:133:UNK:C | 13:M:224:UNK:CB | 2.92 | 0.48 |
| 23:W:16:UNK:O | 23:W:20:UNK:N | 4.39 | 0.48 |
| 2:B:115:UNK:CB | 2:B:120:UNK:CB | 2.91 | 0.47 |
| 6:F:125:UNK:O | 6:F:128:UNK:CB | 2.62 | 0.47 |
| 6:F:150:UNK:O | 6:F:153:UNK:N | 2.46 | 0.47 |
| 6:F:95:UNK:O | 6:F:96:UNK:C | 2.57 | 0.47 |
| 10:J:22:UNK:C | 10:J:24:UNK:N | 2.77 | 0.47 |
| 14:N:133:UNK:O | 14:N:136:UNK:CB | 2.62 | 0.47 |
| 14:N:137:UNK:O | 14:N:138:UNK:C | 2.56 | 0.47 |
| 16:P:206:UNK:O | 16:P:209:UNK:N | 2.47 | 0.47 |
| 6:F:412:UNK:O | 6:F:415:UNK:CB | 2.61 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 7:G:377:UNK:N | 7:G:449:UNK:CB | 2.77 | 0.47 |
| 10:J:171:UNK:O | 10:J:172:UNK:C | 2.62 | 0.47 |
| 11:K:44:UNK:O | 11:K:45:UNK:C | 2.61 | 0.47 |
| 12:L:65:UNK:CB | 12:L:66:UNK:C | 2.82 | 0.47 |
| 24:X:40:UNK:O | 24:X:44:UNK:N | 2.46 | 0.47 |
| 5:E:111:UNK:C | 5:E:113:UNK:N | 2.72 | 0.47 |
| 6:F:212:UNK:CA | 6:F:220:UNK:H | 2.28 | 0.47 |
| 7:G:305:UNK:O | 7:G:308:UNK:CB | 2.62 | 0.47 |
| 12:L:161:UNK:HA | 12:L:163:UNK:CA | 2.38 | 0.47 |
| 13:M:386:UNK:HA | 13:M:390:UNK:HA | 1.95 | 0.47 |
| 15:O:119:UNK:C | 15:O:121:UNK:N | 2.73 | 0.47 |
| 19:S:21:UNK:O | 19:S:22:UNK:C | 3.54 | 0.47 |
| 7:G:259:UNK:C | 7:G:260:UNK:O | 2.58 | 0.47 |
| 13:M:133:UNK:CB | 13:M:224:UNK:CB | 2.92 | 0.47 |
| 14:N:45:UNK:O | 14:N:48:UNK:N | 2.48 | 0.47 |
| 6:F:163:UNK:N | 6:F:166:UNK:CB | 2.77 | 0.47 |
| 10:J:155:UNK:O | 10:J:159:UNK:N | 2.47 | 0.47 |
| 12:L:544:UNK:O | 12:L:545:UNK:C | 2.61 | 0.47 |
| 25:Y:43:UNK:O | 25:Y:44:UNK:C | 2.57 | 0.47 |
| 12:L:181:UNK:C | 12:L:183:UNK:N | 2.71 | 0.47 |
| 13:M:255:UNK:O | 13:M:258:UNK:CB | 2.63 | 0.47 |
| 13:M:351:UNK:O | 13:M:352:UNK:CB | 2.62 | 0.47 |
| 13:M:42:UNK:C | 13:M:44:UNK:N | 2.76 | 0.47 |
| 15:O:114:UNK:O | 15:O:117:UNK:O | 2.33 | 0.47 |
| 4:D:85:UNK:O | 4:D:86:UNK:C | 2.63 | 0.47 |
| 6:F:212:UNK:C | 6:F:219:UNK:HA | 2.44 | 0.47 |
| 6:F:423:UNK:C | 6:F:425:UNK:N | 2.72 | 0.47 |
| 7:G:601:UNK:O | 7:G:602:UNK:C | 2.63 | 0.47 |
| 4:D:367:UNK:O | 4:D:373:UNK:HA | 2.14 | 0.47 |
| 7:G:87:UNK:O | 7:G:90:UNK:N | 2.48 | 0.47 |
| 12:L:111:UNK:O | 12:L:114:UNK:N | 2.48 | 0.47 |
| 12:L:306:UNK:O | 12:L:307:UNK:C | 2.60 | 0.47 |
| 12:L:604:UNK:CB | 14:N:92:UNK:C | 2.92 | 0.47 |
| 12:L:61:UNK:CA | 12:L:80:UNK:CB | 2.93 | 0.47 |
| 16:P:82:UNK:O | 16:P:83:UNK:C | 2.60 | 0.47 |
| 9:I:119:CYS:N | 44:I:222:SF4:S4 | 2.88 | 0.47 |
| 22:V:26:UNK:O | 22:V:30:UNK:N | 2.48 | 0.47 |
| 1:A:88:UNK:O | 1:A:91:UNK:N | 2.48 | 0.47 |
| 8:H:126:UNK:O | 8:H:130:UNK:CB | 2.63 | 0.47 |
| 12:L:95:UNK:O | 12:L:98:UNK:N | 2.48 | 0.47 |
| 16:P:301:UNK:CB | 16:P:303:UNK:N | 2.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:D:89:UNK:O | 4:D:92:UNK:N | 2.48 | 0.47 |
| 6:F:178:UNK:C | 6:F:179:UNK:O | 2.58 | 0.47 |
| 5:E:77:UNK:O | 5:E:81:UNK:N | 2.48 | 0.46 |
| 6:F:433:UNK:O | 6:F:436:UNK:CB | 2.63 | 0.46 |
| 7:G:11:UNK:O | 7:G:13:UNK:N | 3.83 | 0.46 |
| 14:N:72:UNK:C | 14:N:75:UNK:CB | 2.92 | 0.46 |
| 19:S:64:UNK:HA | 19:S:78:UNK:CB | 2.45 | 0.46 |
| 25:Y:69:UNK:CB | 25:Y:98:UNK:CB | 2.93 | 0.46 |
| 4:D:300:UNK:O | 4:D:301:UNK:C | 2.63 | 0.46 |
| 5:E:28:UNK:HA | 5:E:31:UNK:CB | 2.45 | 0.46 |
| 6:F:286:UNK:HA | 6:F:287:UNK:HA | 1.55 | 0.46 |
| 6:F:351:UNK:O | 6:F:354:UNK:CB | 2.63 | 0.46 |
| 7:G:260:UNK:C | 7:G:262:UNK:N | 2.78 | 0.46 |
| 7:G:49:UNK:C | 7:G:51:UNK:N | 2.76 | 0.46 |
| 9:I:26:UNK:C | 9:I:28:UNK:N | 2.78 | 0.46 |
| 13:M:133:UNK:HA | 13:M:224:UNK:CB | 2.44 | 0.46 |
| 14:N:255:UNK:HA | 14:N:256:UNK:HA | 1.66 | 0.46 |
| 18:R:50:UNK:O | 18:R:91:UNK:HA | 2.15 | 0.46 |
| 20:T:9:UNK:O | 20:T:10:UNK:C | 2.95 | 0.46 |
| 6:F:63:UNK:O | 6:F:64:UNK:C | 2.62 | 0.46 |
| 8:H:12:UNK:O | 8:H:15:UNK:CB | 3.73 | 0.46 |
| 8:H:195:UNK:HA | 8:H:198:UNK:HA | 1.96 | 0.46 |
| 8:H:199:UNK:O | 8:H:200:UNK:CB | 2.63 | 0.46 |
| 12:L:271:UNK:O | 12:L:274:UNK:N | 2.49 | 0.46 |
| 12:L:545:UNK:C | 12:L:547:UNK:N | 2.74 | 0.46 |
| 12:L:545:UNK:O | 12:L:548:UNK:N | 2.49 | 0.46 |
| 13:M:140:UNK:C | 13:M:142:UNK:N | 2.74 | 0.46 |
| 13:M:273:UNK:O | 13:M:277:UNK:N | 2.48 | 0.46 |
| 14:N:10:UNK:O | 14:N:13:UNK:CB | 3.02 | 0.46 |
| 22:V:32:UNK:O | 22:V:36:UNK:N | 2.48 | 0.46 |
| 26:Z:57:UNK:O | 26:Z:60:UNK:CB | 2.64 | 0.46 |
| 4:D:101:UNK:O | 4:D:104:UNK:N | 2.48 | 0.46 |
| 7:G:564:UNK:CB | 7:G:568:UNK:CB | 2.93 | 0.46 |
| 9:I:99:UNK:C | 9:I:104:UNK:CB | 2.93 | 0.46 |
| 12:L:108:UNK:O | 12:L:111:UNK:N | 2.49 | 0.46 |
| 12:L:225:UNK:C | 12:L:229:UNK:CB | 2.93 | 0.46 |
| 13:M:106:UNK:HA | 13:M:109:UNK:CB | 2.45 | 0.46 |
| 13:M:188:UNK:CB | 13:M:189:UNK:CA | 2.93 | 0.46 |
| 13:M:281:UNK:O | 13:M:284:UNK:C | 2.64 | 0.46 |
| 22:V:19:UNK:O | 22:V:23:UNK:N | 7.29 | 0.46 |
| 10:J:149:UNK:C | 10:J:150:UNK:O | 2.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 10:J:33:UNK:O | 10:J:37:UNK:N | 2.48 | 0.46 |
| 12:L:396:UNK:O | 12:L:399:UNK:N | 2.48 | 0.46 |
| 15:O:25:UNK:O | 15:O:124:UNK:N | 2.48 | 0.46 |
| 15:O:85:UNK:O | 15:O:86:UNK:C | 2.61 | 0.46 |
| 19:S:64:UNK:HA | 19:S:77:UNK:C | 2.44 | 0.46 |
| 19:S:63:UNK:CA | 19:S:78:UNK:CB | 2.94 | 0.46 |
| 1:A:103:UNK:C | 1:A:106:UNK:N | 2.79 | 0.46 |
| 5:E:112:UNK:C | 5:E:114:UNK:N | 2.72 | 0.46 |
| 7:G:248:UNK:O | 7:G:249:UNK:CB | 2.63 | 0.46 |
| 7:G:398:UNK:C | 7:G:400:UNK:N | 2.77 | 0.46 |
| 7:G:427:UNK:O | 7:G:431:UNK:N | 2.48 | 0.46 |
| 13:M:168:UNK:CB | 13:M:174:UNK:CB | 2.93 | 0.46 |
| 13:M:178:UNK:O | 13:M:179:UNK:C | 2.62 | 0.46 |
| 14:N:168:UNK:O | 14:N:169:UNK:C | 2.61 | 0.46 |
| 16:P:161:UNK:O | 16:P:162:UNK:O | 2.34 | 0.46 |
| 16:P:233:UNK:N | 16:P:234:UNK:HA | 2.31 | 0.46 |
| 2:B:41:UNK:O | 2:B:42:UNK:C | 2.99 | 0.46 |
| 3:C:89:UNK:CA | 3:C:112:UNK:O | 2.63 | 0.46 |
| 8:H:125:UNK:O | 8:H:129:UNK:CB | 2.64 | 0.46 |
| 24:X:93:UNK:HA | 24:X:94:UNK:CB | 2.46 | 0.46 |
| 2:B:118:UNK:O | 2:B:122:UNK:CA | 2.62 | 0.46 |
| 2:B:147:UNK:O | 2:B:151:UNK:CB | 2.64 | 0.46 |
| 7:G:162:UNK:O | 7:G:166:UNK:N | 2.49 | 0.46 |
| 16:P:173:UNK:O | 16:P:176:UNK:CB | 2.63 | 0.46 |
| 24:X:111:UNK:O | 24:X:112:UNK:C | 2.63 | 0.46 |
| 2:B:90:UNK:C | 2:B:119:CYS:HB3 | 2.46 | 0.46 |
| 7:G:9:UNK:O | 7:G:12:UNK:CB | 10.16 | 0.46 |
| 12:L:316:UNK:O | 12:L:319:UNK:CA | 2.64 | 0.46 |
| 13:M:341:UNK:C | 13:M:342:UNK:O | 2.56 | 0.46 |
| 13:M:433:UNK:O | 13:M:434:UNK:C | 2.63 | 0.46 |
| 25:Y:62:UNK:O | 25:Y:63:UNK:CB | 2.63 | 0.46 |
| 10:J:56:UNK:O | 10:J:60:UNK:CB | 2.64 | 0.46 |
| 14:N:73:UNK:C | 14:N:75:UNK:N | 2.71 | 0.46 |
| 15:O:42:UNK:C | 15:O:44:UNK:N | 2.76 | 0.46 |
| 16:P:145:UNK:O | 16:P:148:UNK:CA | 2.64 | 0.46 |
| 4:D:296:UNK:O | 4:D:299:UNK:CB | 2.64 | 0.45 |
| 6:F:215:UNK:O | 6:F:216:UNK:C | 2.64 | 0.45 |
| 7:G:155:UNK:O | 7:G:156:CYS:O | 2.33 | 0.45 |
| 7:G:455:UNK:O | 7:G:456:UNK:CB | 2.62 | 0.45 |
| 10:J:72:UNK:HA | 10:J:75:UNK:CB | 2.46 | 0.45 |
| 11:K:41:UNK:O | 11:K:42:UNK:C | 2.58 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 12:L:151:UNK:O | 12:L:155:UNK:CA | 2.64 | 0.45 |
| 12:L:169:UNK:O | 12:L:173:UNK:N | 2.49 | 0.45 |
| 12:L:314:UNK:O | 12:L:317:UNK:N | 2.49 | 0.45 |
| 16:P:21:UNK:CB | 16:P:45:UNK:CA | 2.85 | 0.45 |
| 19:S:23:UNK:O | 19:S:26:UNK:N | 6.35 | 0.45 |
| 4:D:234:UNK:O | 4:D:235:UNK:C | 2.63 | 0.45 |
| 7:G:382:UNK:CB | 7:G:454:UNK:CA | 2.90 | 0.45 |
| 12:L:207:UNK:HA | 12:L:208:UNK:C | 2.45 | 0.45 |
| 13:M:14:UNK:O | 13:M:15:UNK:C | 2.60 | 0.45 |
| 13:M:157:UNK:O | 13:M:160:UNK:N | 2.48 | 0.45 |
| 16:P:145:UNK:O | 16:P:148:UNK:N | 2.49 | 0.45 |
| 18:R:82:UNK:O | 18:R:90:UNK:HA | 2.16 | 0.45 |
| 22:V:10:UNK:O | 22:V:13:UNK:N | 3.28 | 0.45 |
| 3:C:120:UNK:O | 3:C:121:UNK:C | 2.64 | 0.45 |
| 4:D:179:UNK:O | 4:D:183:UNK:N | 2.50 | 0.45 |
| 19:S:64:UNK:CA | 19:S:78:UNK:CB | 2.94 | 0.45 |
| 21:U:55:UNK:O | 21:U:58:UNK:O | 2.34 | 0.45 |
| 4:D:109:UNK:O | 4:D:111:UNK:N | 2.50 | 0.45 |
| 5:E:33:UNK:C | 5:E:35:UNK:N | 2.74 | 0.45 |
| 11:K:21:UNK:O | 11:K:22:UNK:C | 2.63 | 0.45 |
| 13:M:273:UNK:O | 13:M:276:UNK:N | 2.49 | 0.45 |
| 13:M:87:UNK:HA | 13:M:89:UNK:HA | 1.98 | 0.45 |
| 14:N:135:UNK:C | 14:N:137:UNK:N | 2.77 | 0.45 |
| 14:N:320:UNK:O | 14:N:321:UNK:C | 2.62 | 0.45 |
| 14:N:72:UNK:HA | 14:N:75:UNK:CB | 2.46 | 0.45 |
| 4:D:146:UNK:O | 4:D:147:UNK:C | 2.62 | 0.45 |
| 7:G:311:UNK:O | 7:G:314:UNK:N | 2.50 | 0.45 |
| 8:H:18:UNK:O | 8:H:21:UNK:N | 2.50 | 0.45 |
| 10:J:44:UNK:CB | 10:J:53:UNK:CB | 2.94 | 0.45 |
| 12:L:246:UNK:O | 12:L:250:UNK:CA | 2.65 | 0.45 |
| 13:M:118:UNK:O | 13:M:121:UNK:N | 2.50 | 0.45 |
| 13:M:327:UNK:O | 13:M:330:UNK:N | 2.49 | 0.45 |
| 15:O:138:UNK:O | 15:O:141:UNK:N | 2.49 | 0.45 |
| 17:Q:109:UNK:CA | 17:Q:110:UNK:CB | 2.84 | 0.45 |
| 3:C:133:UNK:O | 3:C:136:UNK:CB | 2.65 | 0.45 |
| 5:E:165:UNK:O | 5:E:166:UNK:C | 2.65 | 0.45 |
| 6:F:61:UNK:O | 6:F:64:UNK:CB | 2.64 | 0.45 |
| 7:G:175:UNK:CB | 7:G:182:UNK:N | 2.80 | 0.45 |
| 10:J:45:UNK:O | 10:J:46:UNK:CB | 2.63 | 0.45 |
| 12:L:4:UNK:HA | 12:L:7:UNK:CB | 3.88 | 0.45 |
| 13:M:114:UNK:CA | 13:M:177:UNK:CB | 2.95 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 13:M:54:UNK:HA | 13:M:55:UNK:HA | 1.65 | 0.45 |
| 22:V:56:UNK:O | 22:V:60:UNK:N | 2.49 | 0.45 |
| 25:Y:94:UNK:O | 25:Y:97:UNK:CB | 2.65 | 0.45 |
| 5:E:107:UNK:O | 5:E:110:UNK:N | 2.50 | 0.45 |
| 6:F:352:UNK:C | 6:F:355:UNK:N | 2.79 | 0.45 |
| 7:G:229:UNK:O | 7:G:235:UNK:HA | 2.16 | 0.45 |
| 7:G:86:UNK:O | 7:G:87:UNK:C | 2.65 | 0.45 |
| 13:M:432:UNK:O | 13:M:435:UNK:N | 2.49 | 0.45 |
| 19:S:64:UNK:N | 19:S:78:UNK:CB | 2.78 | 0.45 |
| 26:Z:88:UNK:O | 26:Z:91:UNK:CB | 2.65 | 0.45 |
| 1:A:76:UNK:C | 1:A:78:UNK:N | 2.71 | 0.45 |
| 4:D:117:UNK:O | 4:D:120:UNK:N | 2.49 | 0.45 |
| 4:D:383:UNK:CB | 4:D:384:UNK:C | 2.95 | 0.45 |
| 7:G:41:CYS:SG | 7:G:49:UNK:O | 2.74 | 0.45 |
| 7:G:89:UNK:O | 7:G:90:UNK:C | 2.64 | 0.45 |
| 12:L:309:UNK:O | 12:L:313:UNK:N | 2.50 | 0.45 |
| 13:M:30:UNK:O | 13:M:33:UNK:N | 2.50 | 0.45 |
| 13:M:347:UNK:C | 13:M:351:UNK:CB | 2.92 | 0.45 |
| 13:M:406:UNK:O | 13:M:407:UNK:C | 2.64 | 0.45 |
| 14:N:163:UNK:O | 14:N:164:UNK:C | 2.62 | 0.45 |
| 14:N:91:UNK:CA | 14:N:92:UNK:CB | 2.94 | 0.45 |
| 2:B:166:UNK:CA | 2:B:169:UNK:O | 2.63 | 0.45 |
| 4:D:137:UNK:O | 4:D:138:UNK:C | 2.63 | 0.45 |
| 4:D:421:UNK:C | 4:D:423:UNK:N | 2.79 | 0.45 |
| 7:G:11:UNK:CB | 7:G:76:UNK:C | 2.95 | 0.45 |
| 12:L:288:UNK:CB | 12:L:308:UNK:HA | 2.47 | 0.45 |
| 13:M:38:UNK:O | 13:M:41:UNK:N | 2.49 | 0.45 |
| 13:M:61:UNK:N | 13:M:63:UNK:N | 2.65 | 0.45 |
| 15:O:101:UNK:O | 15:O:105:UNK:N | 2.50 | 0.45 |
| 22:V:4:UNK:O | 22:V:5:UNK:C | 3.22 | 0.45 |
| 25:Y:81:UNK:O | 25:Y:84:UNK:O | 2.34 | 0.45 |
| 2:B:162:UNK:O | 2:B:165:UNK:CB | 2.65 | 0.44 |
| 3:C:23:UNK:O | 3:C:26:UNK:CB | 2.66 | 0.44 |
| 4:D:228:UNK:O | 4:D:232:UNK:CB | 2.65 | 0.44 |
| 6:F:315:UNK:CA | 6:F:316:UNK:C | 2.95 | 0.44 |
| 7:G:491:UNK:C | 7:G:493:UNK:N | 2.78 | 0.44 |
| 8:H:298:UNK:O | 8:H:302:UNK:N | 2.50 | 0.44 |
| 11:K:10:UNK:O | 11:K:13:UNK:N | 2.51 | 0.44 |
| 12:L:155:UNK:O | 12:L:239:UNK:CB | 2.65 | 0.44 |
| 12:L:211:UNK:HA | 12:L:214:UNK:CB | 2.47 | 0.44 |
| 13:M:225:UNK:CB | 13:M:228:UNK:CB | 2.95 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 13:M:448:UNK:O | 13:M:449:UNK:C | 2.61 | 0.44 |
| 14:N:5:UNK:O | 14:N:8:UNK:CA | 3.77 | 0.44 |
| 6:F:275:UNK:O | 6:F:279:UNK:N | 2.50 | 0.44 |
| 7:G:572:UNK:HA | 7:G:581:UNK:O | 2.17 | 0.44 |
| 12:L:165:UNK:HA | 12:L:168:UNK:CB | 2.47 | 0.44 |
| 12:L:316:UNK:O | 12:L:317:UNK:C | 2.63 | 0.44 |
| 13:M:62:UNK:N | 13:M:63:UNK:CA | 2.77 | 0.44 |
| 13:M:91:UNK:O | 13:M:94:UNK:CB | 2.66 | 0.44 |
| 15:O:26:UNK:CB | 15:O:124:UNK:O | 2.65 | 0.44 |
| 21:U:9:UNK:O | 21:U:12:UNK:N | 2.50 | 0.44 |
| 3:C:132:UNK:O | 3:C:133:UNK:C | 2.63 | 0.44 |
| 4:D:70:UNK:O | 4:D:72:UNK:N | 2.50 | 0.44 |
| 6:F:430:UNK:O | 6:F:433:UNK:N | 2.50 | 0.44 |
| 6:F:52:UNK:O | 6:F:55:UNK:CA | 2.66 | 0.44 |
| 8:H:283:UNK:O | 8:H:287:UNK:N | 2.51 | 0.44 |
| 9:I:22:UNK:O | 9:I:24:UNK:N | 3.27 | 0.44 |
| 12:L:124:UNK:O | 12:L:125:UNK:C | 2.63 | 0.44 |
| 16:P:203:UNK:CB | 16:P:234:UNK:HA | 2.48 | 0.44 |
| 23:W:3:UNK:O | 23:W:6:UNK:CB | 6.51 | 0.44 |
| 4:D:254:UNK:O | 4:D:256:UNK:N | 2.50 | 0.44 |
| 4:D:298:UNK:O | 4:D:299:UNK:C | 2.65 | 0.44 |
| 5:E:96:UNK:CB | 5:E:98:UNK:O | 2.66 | 0.44 |
| 1:A:78:UNK:CB | 10:J:146:UNK:O | 2.65 | 0.44 |
| 12:L:541:UNK:O | 12:L:545:UNK:N | 2.50 | 0.44 |
| 13:M:127:UNK:O | 13:M:128:UNK:C | 2.60 | 0.44 |
| 13:M:159:UNK:O | 13:M:160:UNK:C | 2.64 | 0.44 |
| 13:M:32:UNK:C | 13:M:34:UNK:N | 2.79 | 0.44 |
| 15:O:105:UNK:O | 15:O:108:UNK:N | 2.50 | 0.44 |
| 16:P:48:UNK:CB | 16:P:73:UNK:CB | 2.95 | 0.44 |
| 19:S:84:UNK:O | 19:S:85:UNK:C | 2.64 | 0.44 |
| 1:A:53:UNK:O | 1:A:56:UNK:N | 2.50 | 0.44 |
| 6:F:247:UNK:O | 6:F:250:UNK:O | 2.35 | 0.44 |
| 6:F:423:UNK:C | 6:F:426:UNK:N | 2.81 | 0.44 |
| 7:G:305:UNK:O | 7:G:308:UNK:N | 2.51 | 0.44 |
| 13:M:315:UNK:O | 13:M:316:UNK:C | 2.64 | 0.44 |
| 16:P:71:UNK:O | 16:P:73:UNK:N | 2.50 | 0.44 |
| 25:Y:98:UNK:O | 25:Y:99:UNK:C | 2.64 | 0.44 |
| 26:Z:72:UNK:O | 26:Z:76:UNK:N | 2.51 | 0.44 |
| 3:C:110:UNK:O | 3:C:111:UNK:C | 2.65 | 0.44 |
| 5:E:113:UNK:O | 5:E:116:UNK:N | 2.50 | 0.44 |
| 6:F:58:UNK:O | 6:F:61:UNK:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:F:76:UNK:O | 6:F:80:UNK:CB | 2.66 | 0.44 |
| 7:G:482:UNK:O | 7:G:576:UNK:CB | 2.66 | 0.44 |
| 9:I:112:UNK:O | 9:I:115:UNK:CB | 2.66 | 0.44 |
| 9:I:112:UNK:O | 9:I:115:UNK:N | 2.50 | 0.44 |
| 9:I:27:UNK:O | 9:I:28:UNK:C | 2.87 | 0.44 |
| 12:L:297:UNK:CA | 12:L:356:UNK:N | 2.73 | 0.44 |
| 16:P:180:UNK:O | 16:P:181:UNK:C | 2.65 | 0.44 |
| 16:P:203:UNK:CA | 16:P:234:UNK:CA | 2.85 | 0.44 |
| 1:A:106:UNK:O | 1:A:107:UNK:C | 2.63 | 0.44 |
| 3:C:21:UNK:O | 3:C:22:UNK:C | 2.66 | 0.44 |
| 6:F:351:UNK:O | 6:F:355:UNK:N | 2.51 | 0.44 |
| 8:H:41:UNK:CB | 8:H:44:UNK:C | 2.96 | 0.44 |
| 13:M:124:UNK:O | 13:M:125:UNK:C | 2.64 | 0.44 |
| 14:N:91:UNK:N | 14:N:93:UNK:N | 2.60 | 0.44 |
| 16:P:136:UNK:CA | 16:P:137:UNK:C | 2.93 | 0.44 |
| 24:X:42:UNK:O | 24:X:45:UNK:CB | 2.66 | 0.44 |
| 3:C:162:UNK:O | 3:C:163:UNK:C | 2.65 | 0.44 |
| 6:F:300:UNK:CB | 6:F:329:UNK:C | 2.95 | 0.44 |
| 7:G:425:UNK:O | 7:G:428:UNK:CA | 2.66 | 0.44 |
| 9:I:76:UNK:O | 9:I:77:CYS:C | 2.54 | 0.44 |
| 12:L:209:UNK:O | 12:L:210:UNK:C | 2.66 | 0.44 |
| 26:Z:56:UNK:O | 26:Z:57:UNK:C | 2.66 | 0.44 |
| 2:B:63:UNK:HA | 2:B:69:UNK:CB | 2.48 | 0.44 |
| 5:E:54:UNK:O | 5:E:57:UNK:N | 2.51 | 0.44 |
| 6:F:213:UNK:HA | 6:F:214:UNK:HA | 1.67 | 0.44 |
| 6:F:394:UNK:O | 6:F:395:UNK:C | 2.66 | 0.44 |
| 8:H:68:UNK:C | 8:H:70:UNK:N | 2.79 | 0.44 |
| 14:N:337:UNK:O | 14:N:341:UNK:N | 2.51 | 0.44 |
| 14:N:91:UNK:O | 14:N:95:UNK:CB | 2.65 | 0.44 |
| 19:S:84:UNK:C | 19:S:87:UNK:N | 2.80 | 0.44 |
| 25:Y:14:UNK:CB | 25:Y:44:UNK:O | 2.66 | 0.44 |
| 2:B:55:CYS:SG | 2:B:117:UNK:CB | 3.06 | 0.43 |
| 4:D:95:UNK:CB | 4:D:98:UNK:CB | 2.96 | 0.43 |
| 8:H:291:UNK:C | 8:H:293:UNK:N | 2.81 | 0.43 |
| 5:E:54:UNK:O | 5:E:55:UNK:C | 2.65 | 0.43 |
| 5:E:65:UNK:O | 5:E:66:UNK:C | 2.63 | 0.43 |
| 6:F:433:UNK:O | 6:F:437:UNK:N | 2.51 | 0.43 |
| 10:J:149:UNK:O | 10:J:150:UNK:C | 2.65 | 0.43 |
| 10:J:14:UNK:O | 10:J:17:UNK:N | 2.94 | 0.43 |
| 10:J:18:UNK:HA | 10:J:21:UNK:CB | 2.49 | 0.43 |
| 13:M:62:UNK:CB | 13:M:65:UNK:N | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 7:G:565:UNK:C | 7:G:567:UNK:N | 2.78 | 0.43 |
| 8:H:277:UNK:O | 8:H:278:UNK:CB | 2.66 | 0.43 |
| 12:L:250:UNK:O | 12:L:254:UNK:CB | 2.67 | 0.43 |
| 12:L:571:UNK:C | 12:L:573:UNK:N | 2.76 | 0.43 |
| 16:P:158:UNK:O | 16:P:161:UNK:N | 2.51 | 0.43 |
| 16:P:64:UNK:CB | 16:P:65:UNK:HA | 2.46 | 0.43 |
| 23:W:71:UNK:O | 23:W:72:UNK:C | 2.65 | 0.43 |
| 4:D:297:UNK:O | 4:D:298:UNK:C | 2.63 | 0.43 |
| 4:D:342:UNK:O | 4:D:343:UNK:C | 2.65 | 0.43 |
| 13:M:52:UNK:HA | 13:M:53:UNK:HA | 1.71 | 0.43 |
| 24:X:46:UNK:O | 24:X:49:UNK:N | 2.51 | 0.43 |
| 5:E:69:UNK:O | 5:E:73:UNK:N | 2.51 | 0.43 |
| 9:I:31:UNK:O | 9:I:34:UNK:CB | 2.66 | 0.43 |
| 13:M:191:UNK:CB | 13:M:192:UNK:CA | 2.92 | 0.43 |
| 13:M:123:UNK:CB | 14:N:255:UNK:CB | 2.96 | 0.43 |
| 15:O:38:UNK:O | 15:O:41:UNK:N | 2.51 | 0.43 |
| 16:P:129:UNK:O | 16:P:163:UNK:CB | 2.66 | 0.43 |
| 16:P:48:UNK:C | 16:P:73:UNK:CB | 2.97 | 0.43 |
| 17:Q:50:UNK:N | 17:Q:51:UNK:CA | 2.82 | 0.43 |
| 18:R:63:UNK:C | 18:R:65:UNK:N | 2.72 | 0.43 |
| 21:U:35:UNK:CB | 21:U:39:UNK:N | 2.82 | 0.43 |
| 2:B:149:CYS:CA | 2:B:150:UNK:C | 2.93 | 0.43 |
| 3:C:25:UNK:O | 3:C:26:UNK:C | 2.70 | 0.43 |
| 3:C:22:UNK:O | 3:C:26:UNK:CB | 2.66 | 0.43 |
| 5:E:96:UNK:C | 5:E:136:UNK:O | 2.67 | 0.43 |
| 8:H:10:UNK:C | 8:H:12:UNK:N | 3.38 | 0.43 |
| 8:H:195:UNK:HA | 8:H:198:UNK:CA | 2.48 | 0.43 |
| 20:T:31:UNK:O | 20:T:32:UNK:C | 2.85 | 0.43 |
| 2:B:121:UNK:C | 2:B:135:UNK:CA | 2.92 | 0.43 |
| 4:D:311:UNK:O | 4:D:315:UNK:N | 2.52 | 0.43 |
| 7:G:31:UNK:O | 7:G:34:UNK:HA | 2.18 | 0.43 |
| 9:I:100:UNK:O | 9:I:104:UNK:N | 2.52 | 0.43 |
| 10:J:100:UNK:O | 10:J:101:UNK:C | 2.62 | 0.43 |
| 10:J:88:UNK:O | 10:J:91:UNK:CB | 2.67 | 0.43 |
| 12:L:343:UNK:O | 12:L:347:UNK:N | 2.51 | 0.43 |
| 14:N:253:UNK:CA | 14:N:259:UNK:CB | 2.96 | 0.43 |
| 2:B:166:UNK:O | 2:B:169:UNK:N | 2.52 | 0.43 |
| 6:F:74:UNK:O | 6:F:77:UNK:N | 2.52 | 0.43 |
| 7:G:30:UNK:O | 7:G:34:UNK:N | 2.51 | 0.43 |
| 9:I:25:UNK:O | 9:I:28:UNK:CB | 6.36 | 0.43 |
| 9:I:50:UNK:HA | 9:I:53:UNK:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 12:L:63:UNK:CB | 12:L:78:UNK:CB | 2.97 | 0.43 |
| 14:N:12:UNK:O | 14:N:16:UNK:N | 2.52 | 0.43 |
| 15:O:25:UNK:O | 15:O:123:UNK:CA | 2.66 | 0.43 |
| 2:B:117:UNK:O | 2:B:118:UNK:C | 2.62 | 0.43 |
| 3:C:78:UNK:HA | 3:C:93:UNK:O | 2.18 | 0.43 |
| 6:F:56:UNK:C | 6:F:59:UNK:CB | 2.96 | 0.43 |
| 7:G:594:UNK:CA | 7:G:595:UNK:CB | 2.85 | 0.43 |
| 8:H:110:UNK:C | 8:H:112:UNK:N | 2.78 | 0.43 |
| 8:H:12:UNK:O | 8:H:15:UNK:N | 3.25 | 0.43 |
| 8:H:272:UNK:O | 8:H:276:UNK:CB | 2.67 | 0.43 |
| 20:T:31:UNK:O | 20:T:34:UNK:N | 3.08 | 0.43 |
| 12:L:34:UNK:O | 12:L:37:UNK:N | 2.52 | 0.43 |
| 14:N:65:UNK:O | 14:N:68:UNK:N | 2.52 | 0.43 |
| 16:P:120:UNK:O | 16:P:121:UNK:C | 2.67 | 0.43 |
| 22:V:30:UNK:O | 22:V:31:UNK:C | 2.67 | 0.43 |
| 3:C:112:UNK:CB | 3:C:113:UNK:HA | 2.49 | 0.42 |
| 7:G:12:UNK:O | 7:G:78:UNK:CA | 2.65 | 0.42 |
| 7:G:558:UNK:O | 7:G:559:UNK:CB | 2.67 | 0.42 |
| 7:G:567:UNK:O | 7:G:586:UNK:CB | 2.66 | 0.42 |
| 12:L:32:UNK:HA | 12:L:35:UNK:CB | 2.48 | 0.42 |
| 13:M:30:UNK:O | 13:M:32:UNK:N | 3.11 | 0.42 |
| 17:Q:40:UNK:CB | 17:Q:41:UNK:CA | 2.93 | 0.42 |
| 23:W:58:UNK:O | 23:W:59:UNK:C | 2.66 | 0.42 |
| 1:A:103:UNK:O | 1:A:106:UNK:CA | 2.67 | 0.42 |
| 1:A:98:UNK:O | 1:A:101:UNK:N | 2.52 | 0.42 |
| 2:B:117:UNK:O | 2:B:120:UNK:CA | 2.67 | 0.42 |
| 5:E:106:UNK:O | 5:E:109:UNK:N | 2.51 | 0.42 |
| 6:F:229:UNK:O | 6:F:230:UNK:C | 2.67 | 0.42 |
| 10:J:58:UNK:O | 10:J:63:UNK:N | 2.52 | 0.42 |
| 12:L:431:UNK:O | 12:L:432:UNK:CB | 2.67 | 0.42 |
| 12:L:462:UNK:O | 12:L:465:UNK:N | 2.52 | 0.42 |
| 12:L:544:UNK:O | 12:L:547:UNK:CB | 2.67 | 0.42 |
| 15:O:209:UNK:O | 15:O:210:UNK:C | 2.66 | 0.42 |
| 15:O:22:UNK:CB | 15:O:23:UNK:CA | 2.97 | 0.42 |
| 19:S:83:UNK:O | 19:S:86:UNK:CA | 2.67 | 0.42 |
| 2:B:149:CYS:HA | 2:B:150:UNK:HA | 1.94 | 0.42 |
| 6:F:115:UNK:O | 6:F:116:UNK:C | 2.67 | 0.42 |
| 7:G:326:UNK:O | 7:G:327:UNK:C | 2.67 | 0.42 |
| 12:L:108:UNK:O | 12:L:111:UNK:CB | 2.67 | 0.42 |
| 6:F:62:UNK:C | 6:F:64:UNK:N | 2.79 | 0.42 |
| 6:F:73:UNK:O | 6:F:74:UNK:C | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 8:H:68:UNK:O | 8:H:71:UNK:N | 2.52 | 0.42 |
| 12:L:241:UNK:O | 12:L:242:UNK:C | 2.67 | 0.42 |
| 16:P:311:UNK:C | 16:P:313:UNK:N | 2.80 | 0.42 |
| 16:P:53:UNK:O | 16:P:57:UNK:N | 2.53 | 0.42 |
| 1:A:84:UNK:O | 1:A:87:UNK:N | 2.52 | 0.42 |
| 4:D:296:UNK:O | 4:D:297:UNK:C | 2.66 | 0.42 |
| 6:F:183:UNK:CB | 6:F:186:UNK:N | 2.82 | 0.42 |
| 7:G:586:UNK:C | 7:G:588:UNK:N | 2.80 | 0.42 |
| 8:H:9:UNK:O | 8:H:12:UNK:CA | 3.91 | 0.42 |
| 14:N:126:UNK:O | 14:N:127:UNK:C | 2.67 | 0.42 |
| 15:O:50:UNK:O | 15:O:51:UNK:CB | 2.68 | 0.42 |
| 15:O:80:UNK:O | 15:O:83:UNK:N | 2.53 | 0.42 |
| 23:W:56:UNK:O | 23:W:59:UNK:N | 2.52 | 0.42 |
| 6:F:150:UNK:O | 6:F:153:UNK:CA | 2.67 | 0.42 |
| 6:F:56:UNK:O | 6:F:59:UNK:N | 2.53 | 0.42 |
| 7:G:243:UNK:O | 7:G:244:UNK:C | 2.67 | 0.42 |
| 7:G:426:UNK:HA | 7:G:429:UNK:CB | 2.50 | 0.42 |
| 12:L:128:UNK:O | 12:L:132:UNK:N | 2.53 | 0.42 |
| 12:L:379:UNK:O | 12:L:388:UNK:CB | 2.66 | 0.42 |
| 14:N:76:UNK:O | 14:N:80:UNK:N | 2.53 | 0.42 |
| 25:Y:103:UNK:O | 25:Y:105:UNK:N | 2.51 | 0.42 |
| 25:Y:92:UNK:O | 25:Y:95:UNK:N | 2.52 | 0.42 |
| 5:E:50:UNK:O | 5:E:51:UNK:C | 2.67 | 0.42 |
| 6:F:61:UNK:O | 6:F:64:UNK:HA | 2.15 | 0.42 |
| 7:G:377:UNK:O | 7:G:450:UNK:N | 2.53 | 0.42 |
| 7:G:604:UNK:O | 7:G:609:UNK:N | 2.53 | 0.42 |
| 2:B:71:UNK:CB | 8:H:37:UNK:N | 2.83 | 0.42 |
| 12:L:109:UNK:O | 12:L:110:UNK:CB | 2.67 | 0.42 |
| 14:N:90:UNK:HA | 14:N:91:UNK:CB | 2.50 | 0.42 |
| 15:O:114:UNK:O | 15:O:117:UNK:N | 2.53 | 0.42 |
| 16:P:301:UNK:C | 16:P:303:UNK:N | 2.82 | 0.42 |
| 4:D:419:UNK:O | 4:D:420:UNK:C | 2.67 | 0.42 |
| 6:F:303:UNK:O | 6:F:414:UNK:CA | 2.67 | 0.42 |
| 7:G:12:UNK:HA | 7:G:17:UNK:CA | 2.47 | 0.42 |
| 9:I:151:UNK:O | 9:I:152:UNK:C | 2.66 | 0.42 |
| 12:L:82:UNK:O | 12:L:86:UNK:N | 2.52 | 0.42 |
| 14:N:45:UNK:O | 14:N:49:UNK:CB | 6.84 | 0.42 |
| 15:O:231:UNK:O | 15:O:234:UNK:N | 2.53 | 0.42 |
| 16:P:229:UNK:N | 16:P:299:UNK:CB | 2.83 | 0.42 |
| 22:V:33:UNK:O | 22:V:37:UNK:N | 2.53 | 0.42 |
| 2:B:67:UNK:N | 2:B:68:UNK:CA | 2.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:D:182:UNK:O | 4:D:186:UNK:HA | 2.20 | 0.42 |
| 4:D:383:UNK:CA | 4:D:384:UNK:C | 2.98 | 0.42 |
| 6:F:190:UNK:CB | 6:F:203:UNK:CA | 2.83 | 0.42 |
| 10:J:25:UNK:O | 10:J:28:UNK:CB | 2.68 | 0.42 |
| 12:L:369:UNK:O | 12:L:372:UNK:N | 2.53 | 0.42 |
| 13:M:131:UNK:O | 13:M:132:UNK:C | 2.63 | 0.42 |
| 13:M:393:UNK:C | 13:M:395:UNK:N | 2.79 | 0.42 |
| 13:M:399:UNK:O | 13:M:403:UNK:N | 2.53 | 0.42 |
| 2:B:65:UNK:CA | 2:B:68:UNK:CB | 2.94 | 0.42 |
| 2:B:47:UNK:HA | 2:B:85:UNK:O | 2.20 | 0.42 |
| 6:F:121:UNK:CA | 6:F:232:UNK:CB | 2.97 | 0.42 |
| 7:G:187:UNK:N | 7:G:188:UNK:CA | 2.73 | 0.42 |
| 7:G:380:UNK:O | 7:G:409:UNK:C | 2.67 | 0.42 |
| 7:G:12:UNK:N | 7:G:77:UNK:O | 2.53 | 0.42 |
| 12:L:297:UNK:HA | 12:L:355:UNK:CA | 2.48 | 0.42 |
| 13:M:408:UNK:O | 13:M:412:UNK:N | 2.52 | 0.42 |
| 14:N:43:UNK:O | 14:N:45:UNK:N | 2.91 | 0.42 |
| 2:B:109:UNK:O | 2:B:111:UNK:N | 2.53 | 0.41 |
| 4:D:151:UNK:O | 4:D:152:UNK:C | 2.66 | 0.41 |
| 4:D:250:UNK:O | 4:D:251:UNK:C | 2.68 | 0.41 |
| 4:D:324:UNK:O | 4:D:325:UNK:C | 2.68 | 0.41 |
| 5:E:59:UNK:O | 5:E:60:UNK:C | 2.66 | 0.41 |
| 5:E:78:UNK:HA | 5:E:81:UNK:CB | 2.50 | 0.41 |
| 7:G:624:UNK:O | 7:G:627:UNK:CA | 2.68 | 0.41 |
| 12:L:140:UNK:O | 12:L:143:UNK:N | 2.53 | 0.41 |
| 12:L:420:UNK:O | 12:L:423:UNK:N | 2.53 | 0.41 |
| 12:L:530:UNK:C | 12:L:532:UNK:N | 2.78 | 0.41 |
| 13:M:175:UNK:C | 13:M:177:UNK:HA | 2.47 | 0.41 |
| 14:N:29:UNK:O | 14:N:32:UNK:N | 2.53 | 0.41 |
| 22:V:44:UNK:O | 22:V:47:UNK:CA | 2.67 | 0.41 |
| 25:Y:18:UNK:CB | 25:Y:44:UNK:CB | 2.97 | 0.41 |
| 2:B:121:UNK:CA | 2:B:135:UNK:CA | 2.87 | 0.41 |
| 7:G:456:UNK:CB | 7:G:457:UNK:C | 2.98 | 0.41 |
| 8:H:110:UNK:O | 8:H:111:UNK:C | 2.68 | 0.41 |
| 8:H:310:UNK:O | 8:H:311:UNK:CB | 2.68 | 0.41 |
| 9:I:27:UNK:C | 9:I:28:UNK:O | 3.84 | 0.41 |
| 12:L:274:UNK:O | 12:L:275:UNK:C | 2.67 | 0.41 |
| 12:L:582:UNK:O | 12:L:586:UNK:N | 2.53 | 0.41 |
| 13:M:111:UNK:O | 13:M:112:UNK:CB | 2.68 | 0.41 |
| 1:A:105:UNK:O | 1:A:109:UNK:HA | 2.20 | 0.41 |
| 2:B:38:UNK:O | 2:B:39:UNK:C | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 7:G:621:UNK:O | 7:G:622:UNK:C | 2.64 | 0.41 |
| 10:J:69:UNK:HA | 10:J:72:UNK:CB | 2.50 | 0.41 |
| 12:L:158:UNK:O | 12:L:159:UNK:C | 2.65 | 0.41 |
| 13:M:139:UNK:CA | 13:M:140:UNK:CB | 2.98 | 0.41 |
| 15:O:130:UNK:O | 15:O:132:UNK:N | 2.50 | 0.41 |
| 15:O:43:UNK:O | 15:O:44:UNK:C | 2.67 | 0.41 |
| 16:P:313:UNK:O | 16:P:314:UNK:C | 2.67 | 0.41 |
| 2:B:163:UNK:C | 2:B:165:UNK:N | 2.78 | 0.41 |
| 4:D:163:UNK:CA | 8:H:278:UNK:CA | 2.94 | 0.41 |
| 5:E:127:UNK:C | 5:E:129:UNK:N | 2.84 | 0.41 |
| 6:F:181:UNK:O | 6:F:182:UNK:CB | 2.68 | 0.41 |
| 6:F:276:UNK:N | 6:F:315:UNK:O | 2.54 | 0.41 |
| 6:F:322:UNK:CB | 6:F:327:UNK:C | 2.99 | 0.41 |
| 7:G:185:UNK:C | 7:G:188:UNK:CB | 2.96 | 0.41 |
| 7:G:594:UNK:CB | 7:G:596:UNK:N | 2.83 | 0.41 |
| 9:I:113:UNK:O | 9:I:115:UNK:N | 2.53 | 0.41 |
| 13:M:164:UNK:O | 13:M:167:UNK:N | 2.53 | 0.41 |
| 14:N:124:UNK:O | 14:N:127:UNK:CB | 2.69 | 0.41 |
| 7:G:143:UNK:CB | 7:G:190:UNK:CB | 2.98 | 0.41 |
| 7:G:457:UNK:O | 7:G:458:UNK:CB | 2.68 | 0.41 |
| 7:G:567:UNK:O | 7:G:586:UNK:N | 2.54 | 0.41 |
| 9:I:63:UNK:CB | 9:I:134:UNK:O | 2.69 | 0.41 |
| 9:I:83:CYS:HB2 | 9:I:122:CYS:HB2 | 2.02 | 0.41 |
| 12:L:182:UNK:O | 12:L:185:UNK:N | 2.54 | 0.41 |
| 13:M:168:UNK:CB | 13:M:174:UNK:CA | 2.97 | 0.41 |
| 13:M:174:UNK:O | 13:M:175:UNK:C | 2.69 | 0.41 |
| 15:O:26:UNK:CA | 15:O:124:UNK:O | 2.68 | 0.41 |
| 16:P:160:UNK:N | 16:P:161:UNK:CA | 2.83 | 0.41 |
| 20:T:62:UNK:O | 20:T:63:UNK:C | 2.64 | 0.41 |
| 21:U:11:UNK:O | 21:U:12:UNK:C | 2.67 | 0.41 |
| 3:C:23:UNK:C | 3:C:26:UNK:CB | 2.98 | 0.41 |
| 4:D:95:UNK:HA | 4:D:385:UNK:CB | 2.51 | 0.41 |
| 6:F:225:UNK:O | 6:F:228:UNK:N | 2.54 | 0.41 |
| 6:F:52:UNK:O | 6:F:55:UNK:C | 2.68 | 0.41 |
| 6:F:90:UNK:O | 6:F:218:UNK:CB | 2.69 | 0.41 |
| 7:G:83:UNK:O | 7:G:86:UNK:N | 2.54 | 0.41 |
| 12:L:275:UNK:O | 12:L:278:UNK:N | 2.54 | 0.41 |
| 12:L:570:UNK:O | 12:L:573:UNK:N | 2.53 | 0.41 |
| 13:M:113:UNK:CA | 13:M:114:UNK:CB | 2.89 | 0.41 |
| 13:M:189:UNK:C | 13:M:191:UNK:O | 2.69 | 0.41 |
| 13:M:225:UNK:O | 13:M:228:UNK:C | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 13:M:345:UNK:O | 13:M:346:UNK:CB | 2.69 | 0.41 |
| 13:M:369:UNK:O | 13:M:372:UNK:CB | 2.68 | 0.41 |
| 14:N:106:UNK:O | 14:N:107:UNK:CB | 2.68 | 0.41 |
| 23:W:71:UNK:O | 23:W:72:UNK:O | 2.38 | 0.41 |
| 2:B:68:UNK:O | 2:B:70:UNK:N | 2.54 | 0.41 |
| 2:B:53:UNK:N | 2:B:90:UNK:CB | 2.83 | 0.41 |
| 4:D:342:UNK:O | 4:D:346:UNK:N | 2.54 | 0.41 |
| 4:D:354:UNK:O | 4:D:355:UNK:CB | 2.68 | 0.41 |
| 5:E:78:UNK:O | 5:E:82:UNK:N | 2.54 | 0.41 |
| 6:F:183:UNK:O | 6:F:186:UNK:CB | 2.69 | 0.41 |
| 6:F:194:UNK:O | 6:F:197:UNK:N | 2.53 | 0.41 |
| 6:F:72:UNK:O | 6:F:73:UNK:C | 2.65 | 0.41 |
| 12:L:193:UNK:O | 12:L:194:UNK:C | 2.69 | 0.41 |
| 12:L:588:UNK:O | 12:L:592:UNK:N | 2.53 | 0.41 |
| 13:M:133:UNK:O | 13:M:224:UNK:CB | 2.69 | 0.41 |
| 14:N:11:UNK:O | 14:N:15:UNK:N | 2.53 | 0.41 |
| 14:N:72:UNK:O | 14:N:75:UNK:N | 2.54 | 0.41 |
| 2:B:75:UNK:O | 2:B:76:UNK:CB | 2.68 | 0.41 |
| 3:C:28:UNK:O | 3:C:29:UNK:C | 2.69 | 0.41 |
| 7:G:210:UNK:O | 7:G:213:UNK:C | 2.69 | 0.41 |
| 12:L:192:UNK:O | 12:L:193:UNK:C | 2.69 | 0.41 |
| 12:L:298:UNK:O | 12:L:301:UNK:CB | 2.69 | 0.41 |
| 12:L:386:UNK:O | 12:L:387:UNK:CB | 2.69 | 0.41 |
| 13:M:327:UNK:O | 13:M:330:UNK:CB | 2.69 | 0.41 |
| 16:P:143:UNK:O | 16:P:144:UNK:CB | 2.67 | 0.41 |
| 19:S:36:UNK:O | 19:S:40:UNK:N | 2.54 | 0.41 |
| 22:V:51:UNK:O | 22:V:52:UNK:CB | 2.68 | 0.41 |
| 8:H:101:UNK:CB | 8:H:162:UNK:N | 2.84 | 0.41 |
| 9:I:22:UNK:O | 9:I:25:UNK:CB | 2.89 | 0.41 |
| 13:M:186:UNK:O | 13:M:253:UNK:CB | 2.69 | 0.41 |
| 14:N:290:UNK:O | 14:N:294:UNK:N | 2.54 | 0.41 |
| 15:O:234:UNK:O | 15:O:237:UNK:CA | 2.69 | 0.41 |
| 16:P:146:UNK:O | 16:P:149:UNK:CA | 2.69 | 0.41 |
| 22:V:66:UNK:O | 22:V:69:UNK:N | 2.54 | 0.41 |
| 1:A:101:UNK:O | 1:A:102:UNK:C | 2.69 | 0.41 |
| 3:C:25:UNK:O | 3:C:28:UNK:N | 2.54 | 0.41 |
| 4:D:110:UNK:O | 4:D:111:UNK:C | 2.67 | 0.41 |
| 6:F:185:UNK:C | 6:F:187:UNK:N | 2.81 | 0.41 |
| 6:F:418:UNK:O | 6:F:423:UNK:CB | 2.68 | 0.41 |
| 7:G:115:UNK:O | 7:G:119:UNK:CB | 2.69 | 0.41 |
| 7:G:193:UNK:CA | 7:G:196:UNK:CB | 2.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 7:G:625:UNK:C | 7:G:627:UNK:N | 2.84 | 0.41 |
| 8:H:101:UNK:CA | 8:H:161:UNK:HA | 2.51 | 0.41 |
| 9:I:167:UNK:O | 9:I:168:UNK:C | 2.69 | 0.41 |
| 12:L:161:UNK:CB | 12:L:163:UNK:N | 2.83 | 0.41 |
| 12:L:184:UNK:O | 12:L:188:UNK:N | 2.54 | 0.41 |
| 13:M:179:UNK:O | 13:M:180:UNK:C | 2.68 | 0.41 |
| 13:M:209:UNK:O | 13:M:210:UNK:C | 2.69 | 0.41 |
| 13:M:251:UNK:O | 13:M:252:UNK:CB | 2.69 | 0.41 |
| 13:M:382:UNK:O | 13:M:383:UNK:C | 2.69 | 0.41 |
| 14:N:18:UNK:O | 14:N:21:UNK:N | 2.54 | 0.41 |
| 14:N:8:UNK:O | 14:N:11:UNK:CB | 3.51 | 0.41 |
| 26:Z:75:UNK:O | 26:Z:76:UNK:C | 2.69 | 0.41 |
| 3:C:27:UNK:O | 3:C:30:UNK:CB | 2.69 | 0.41 |
| 4:D:250:UNK:O | 4:D:253:UNK:CB | 2.69 | 0.41 |
| 4:D:263:UNK:HA | 4:D:288:UNK:CB | 2.51 | 0.41 |
| 4:D:414:UNK:O | 4:D:418:UNK:N | 2.54 | 0.41 |
| 8:H:119:UNK:O | 8:H:122:UNK:CB | 2.69 | 0.41 |
| 8:H:152:UNK:O | 8:H:155:UNK:CB | 2.69 | 0.41 |
| 8:H:94:UNK:O | 8:H:95:UNK:C | 2.68 | 0.41 |
| 9:I:100:UNK:O | 9:I:103:UNK:C | 2.69 | 0.41 |
| 12:L:418:UNK:O | 12:L:421:UNK:CB | 2.69 | 0.41 |
| 13:M:168:UNK:HA | 13:M:174:UNK:HA | 2.02 | 0.41 |
| 13:M:22:UNK:CA | 13:M:23:UNK:CB | 2.97 | 0.41 |
| 13:M:275:UNK:HA | 13:M:278:UNK:CB | 2.51 | 0.41 |
| 14:N:124:UNK:C | 14:N:126:UNK:N | 2.78 | 0.41 |
| 14:N:200:UNK:O | 14:N:201:UNK:C | 2.68 | 0.41 |
| 16:P:146:UNK:O | 16:P:149:UNK:CB | 2.69 | 0.41 |
| 24:X:43:UNK:HA | 24:X:59:UNK:CB | 2.51 | 0.41 |
| 4:D:262:UNK:O | 4:D:263:UNK:C | 2.69 | 0.40 |
| 4:D:406:UNK:O | 4:D:407:UNK:C | 2.69 | 0.40 |
| 6:F:242:UNK:O | 6:F:252:UNK:CB | 2.70 | 0.40 |
| 6:F:419:UNK:O | 6:F:423:UNK:CB | 2.69 | 0.40 |
| 6:F:71:UNK:O | 6:F:72:UNK:CB | 2.69 | 0.40 |
| 7:G:11:UNK:HA | 7:G:76:UNK:HA | 2.03 | 0.40 |
| 7:G:255:UNK:C | 7:G:257:UNK:N | 2.79 | 0.40 |
| 7:G:397:UNK:O | 7:G:400:UNK:CB | 2.69 | 0.40 |
| 12:L:182:UNK:O | 12:L:183:UNK:C | 2.69 | 0.40 |
| 12:L:203:UNK:HA | 12:L:204:UNK:HA | 1.87 | 0.40 |
| 12:L:600:UNK:O | 12:L:601:UNK:CB | 2.70 | 0.40 |
| 14:N:40:UNK:O | 14:N:41:UNK:C | 2.61 | 0.40 |
| 14:N:42:UNK:O | 14:N:43:UNK:CB | 4.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 15:O:48:UNK:CB | 15:O:121:UNK:O | 2.70 | 0.40 |
| 15:O:129:UNK:O | 15:O:132:UNK:CA | 2.67 | 0.40 |
| 20:T:63:UNK:O | 20:T:64:UNK:C | 2.66 | 0.40 |
| 21:U:48:UNK:O | 21:U:52:UNK:N | 2.55 | 0.40 |
| 25:Y:90:UNK:C | 25:Y:92:UNK:N | 2.85 | 0.40 |
| 4:D:260:UNK:O | 4:D:265:UNK:CB | 2.70 | 0.40 |
| 4:D:308:UNK:O | 4:D:309:UNK:C | 2.67 | 0.40 |
| 4:D:95:UNK:O | 4:D:98:UNK:N | 2.54 | 0.40 |
| 6:F:33:UNK:HA | 6:F:36:UNK:CB | 2.51 | 0.40 |
| 7:G:157:UNK:O | 7:G:161:UNK:CB | 2.69 | 0.40 |
| 9:I:28:UNK:O | 9:I:29:UNK:CB | 4.19 | 0.40 |
| 12:L:560:UNK:O | 12:L:564:UNK:N | 2.54 | 0.40 |
| 13:M:115:UNK:O | 13:M:116:UNK:CB | 2.69 | 0.40 |
| 13:M:167:UNK:O | 13:M:171:UNK:CB | 2.70 | 0.40 |
| 13:M:172:UNK:O | 13:M:173:UNK:CB | 2.70 | 0.40 |
| 14:N:12:UNK:O | 14:N:15:UNK:CB | 2.69 | 0.40 |
| 14:N:139:UNK:O | 14:N:140:UNK:C | 2.69 | 0.40 |
| 19:S:26:UNK:O | 19:S:28:UNK:N | 4.66 | 0.40 |
| 4:D:249:UNK:O | 4:D:252:UNK:CB | 2.69 | 0.40 |
| 4:D:69:UNK:O | 4:D:70:UNK:CB | 2.69 | 0.40 |
| 6:F:322:UNK:CB | 6:F:328:UNK:N | 2.85 | 0.40 |
| 6:F:367:UNK:O | 6:F:368:UNK:C | 2.70 | 0.40 |
| 6:F:430:UNK:O | 6:F:433:UNK:CB | 2.70 | 0.40 |
| 7:G:461:UNK:O | 7:G:464:UNK:N | 2.54 | 0.40 |
| 7:G:491:UNK:O | 7:G:493:UNK:N | 2.53 | 0.40 |
| 7:G:49:UNK:O | 7:G:51:UNK:N | 2.54 | 0.40 |
| 8:H:101:UNK:O | 8:H:102:UNK:C | 2.70 | 0.40 |
| 8:H:303:UNK:O | 8:H:306:UNK:N | 2.54 | 0.40 |
| 12:L:453:UNK:O | 12:L:456:UNK:CB | 2.70 | 0.40 |
| 14:N:25:UNK:HA | 14:N:26:UNK:HA | 1.76 | 0.40 |
| 18:R:60:UNK:O | 18:R:62:UNK:N | 2.54 | 0.40 |
| 23:W:43:UNK:O | 23:W:44:UNK:CB | 2.69 | 0.40 |
| 4:D:398:UNK:O | 4:D:401:UNK:CB | 2.70 | 0.40 |
| 7:G:435:UNK:CB | 7:G:437:UNK:HA | 2.51 | 0.40 |
| 8:H:233:UNK:O | 8:H:236:UNK:N | 2.54 | 0.40 |
| 8:H:266:UNK:O | 8:H:267:UNK:C | 2.69 | 0.40 |
| 8:H:308:UNK:HA | 8:H:312:UNK:CB | 2.52 | 0.40 |
| 8:H:79:UNK:O | 8:H:80:UNK:C | 2.69 | 0.40 |
| 8:H:91:UNK:O | 8:H:94:UNK:CB | 2.70 | 0.40 |
| 11:K:48:UNK:O | 11:K:49:UNK:C | 2.70 | 0.40 |
| 12:L:34:UNK:O | 12:L:37:UNK:CB | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 14:N:146:UNK:N | 14:N:147:UNK:CA | 2.72 | 0.40 |
| 14:N:193:UNK:O | 14:N:194:UNK:C | 2.70 | 0.40 |
| 14:N:52:UNK:O | 14:N:53:UNK:C | 2.69 | 0.40 |
| 15:O:192:UNK:O | 15:O:193:UNK:CB | 2.70 | 0.40 |
| 16:P:31:UNK:O | 16:P:32:UNK:C | 2.68 | 0.40 |
| 16:P:90:UNK:CB | 16:P:128:UNK:O | 2.70 | 0.40 |
| 20:T:33:UNK:O | 20:T:36:UNK:CA | 7.87 | 0.40 |
| 1:A:72:UNK:O | 1:A:75:UNK:CB | 2.69 | 0.40 |
| 6:F:262:UNK:HA | 6:F:286:UNK:N | 2.36 | 0.40 |
| 8:H:283:UNK:O | 8:H:284:UNK:C | 2.70 | 0.40 |
| 8:H:41:UNK:CB | 8:H:45:UNK:N | 2.84 | 0.40 |
| 8:H:90:UNK:O | 8:H:91:UNK:CB | 2.70 | 0.40 |
| 9:I:159:UNK:O | 9:I:162:UNK:N | 2.54 | 0.40 |
| 9:I:167:UNK:O | 9:I:170:UNK:N | 2.55 | 0.40 |
| 10:J:101:UNK:C | 10:J:103:UNK:N | 2.81 | 0.40 |
| 12:L:167:UNK:O | 12:L:170:UNK:CB | 2.69 | 0.40 |
| 12:L:348:UNK:C | 12:L:350:UNK:N | 2.85 | 0.40 |
| 13:M:146:UNK:O | 13:M:147:UNK:C | 2.70 | 0.40 |
| 13:M:20:UNK:O | 13:M:21:UNK:CB | 2.70 | 0.40 |
| 13:M:258:UNK:O | 13:M:262:UNK:CB | 2.70 | 0.40 |
| 13:M:367:UNK:O | 13:M:368:UNK:CB | 2.69 | 0.40 |
| 14:N:141:UNK:O | 14:N:145:UNK:N | 2.51 | 0.40 |
| 14:N:182:UNK:O | 14:N:183:UNK:C | 2.69 | 0.40 |
| 14:N:266:UNK:O | 14:N:270:UNK:N | 2.54 | 0.40 |
| 15:O:187:UNK:O | 15:O:188:UNK:C | 2.70 | 0.40 |
| 26:Z:77:UNK:O | 26:Z:80:UNK:CA | 2.69 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|--------------|----------|---------|----------|-------------|-----|
| 2 | B | 4/143 (3%) | 3 (75%) | 0 | 1 (25%) | 0 | 1 |
| 5 | E | 4/159 (2%) | 3 (75%) | 1 (25%) | 0 | 100 | 100 |
| 6 | F | 4/411 (1%) | 4 (100%) | 0 | 0 | 100 | 100 |
| 7 | G | 12/538 (2%) | 9 (75%) | 1 (8%) | 2 (17%) | 0 | 4 |
| 9 | I | 8/162 (5%) | 7 (88%) | 0 | 1 (12%) | 0 | 7 |
| All | All | 32/1413 (2%) | 26 (81%) | 2 (6%) | 4 (12%) | 1 | 7 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 119 | CYS |
| 7 | G | 105 | CYS |
| 9 | I | 116 | CYS |
| 7 | G | 156 | CYS |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 2 | B | 4/4 (100%) | 2 (50%) | 2 (50%) | 0 | 0 |
| 5 | E | 4/4 (100%) | 4 (100%) | 0 | 100 | 100 |
| 6 | F | 4/4 (100%) | 3 (75%) | 1 (25%) | 1 | 5 |
| 7 | G | 12/12 (100%) | 8 (67%) | 4 (33%) | 0 | 2 |
| 9 | I | 8/8 (100%) | 7 (88%) | 1 (12%) | 5 | 27 |
| All | All | 32/32 (100%) | 24 (75%) | 8 (25%) | 3 | 5 |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 54 | CYS |
| 2 | B | 55 | CYS |
| 6 | F | 405 | CYS |
| 7 | G | 41 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 52 | CYS |
| 7 | G | 55 | CYS |
| 7 | G | 69 | CYS |
| 9 | I | 119 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 44 | SF4 | B | 201 | 2 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 45 | FES | E | 201 | 5 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 44 | SF4 | F | 508 | 6 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 44 | SF4 | G | 801 | 7 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 44 | SF4 | G | 802 | 7 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 45 | FES | G | 804 | 7 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 44 | SF4 | I | 222 | 9 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 44 | SF4 | I | 223 | 9 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 44 | SF4 | B | 201 | 2 | - | 0/0/48/48 | 0/6/5/5 |
| 45 | FES | E | 201 | 5 | - | 0/0/4/4 | 0/1/1/1 |
| 44 | SF4 | F | 508 | 6 | - | 0/0/48/48 | 0/6/5/5 |
| 44 | SF4 | G | 801 | 7 | - | 0/0/48/48 | 0/6/5/5 |
| 44 | SF4 | G | 802 | 7 | - | 0/0/48/48 | 0/6/5/5 |
| 45 | FES | G | 804 | 7 | - | 0/0/4/4 | 0/1/1/1 |
| 44 | SF4 | I | 222 | 9 | - | 0/0/48/48 | 0/6/5/5 |
| 44 | SF4 | I | 223 | 9 | - | 0/0/48/48 | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 44 | B | 201 | SF4 | 4 | 0 |
| 44 | F | 508 | SF4 | 1 | 0 |
| 45 | G | 804 | FES | 2 | 0 |
| 44 | I | 222 | SF4 | 2 | 0 |
| 44 | I | 223 | SF4 | 3 | 0 |

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 |
|-----|-------|------------------|
| 7 | G | 6 |
| 12 | L | 5 |
| 15 | O | 3 |
| 16 | P | 2 |
| 10 | J | 2 |
| 8 | H | 2 |
| 20 | T | 2 |
| 17 | Q | 1 |
| 1 | A | 1 |
| 14 | N | 1 |
| 13 | M | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 23:UNK | C | 52:UNK | N | 39.81 |
| 1 | J | 107:UNK | C | 140:UNK | N | 30.90 |
| 1 | N | 300:UNK | C | 320:UNK | N | 26.56 |
| 1 | P | 250:UNK | C | 285:UNK | N | 26.48 |
| 1 | L | 466:UNK | C | 487:UNK | N | 23.59 |
| 1 | G | 347:UNK | C | 367:UNK | N | 22.81 |
| 1 | M | 415:UNK | C | 430:UNK | N | 22.06 |
| 1 | P | 185:UNK | C | 203:UNK | N | 21.21 |
| 1 | H | 200:UNK | C | 219:UNK | N | 20.56 |
| 1 | J | 76:UNK | C | 85:UNK | N | 19.66 |
| 1 | H | 242:UNK | C | 253:UNK | N | 18.95 |
| 1 | G | 495:UNK | C | 525:UNK | N | 18.00 |
| 1 | L | 513:UNK | C | 520:UNK | N | 17.41 |
| 1 | G | 530:UNK | C | 542:UNK | N | 16.15 |
| 1 | L | 400:UNK | C | 408:UNK | N | 14.38 |
| 1 | Q | 59:UNK | C | 76:UNK | N | 13.51 |
| 1 | O | 54:UNK | C | 79:UNK | N | 12.62 |
| 1 | G | 318:UNK | C | 326:UNK | N | 12.59 |
| 1 | L | 22:UNK | C | 28:UNK | N | 11.17 |
| 1 | O | 167:UNK | C | 172:UNK | N | 11.08 |
| 1 | O | 210:UNK | C | 222:UNK | N | 10.93 |
| 1 | T | 23:UNK | C | 28:UNK | N | 9.73 |
| 1 | L | 358:UNK | C | 363:UNK | N | 8.92 |
| 1 | G | 410:UNK | C | 425:UNK | N | 7.45 |
| 1 | G | 400:UNK | C | 404:UNK | N | 6.25 |
| 1 | T | 8:UNK | C | 9:UNK | N | 1.65 |