



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:14 am BST

PDB ID : 2F16
Title : Crystal structure of the yeast 20S proteasome in complex with bortezomib
Authors : Groll, M.
Deposited on : 2005-11-14
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

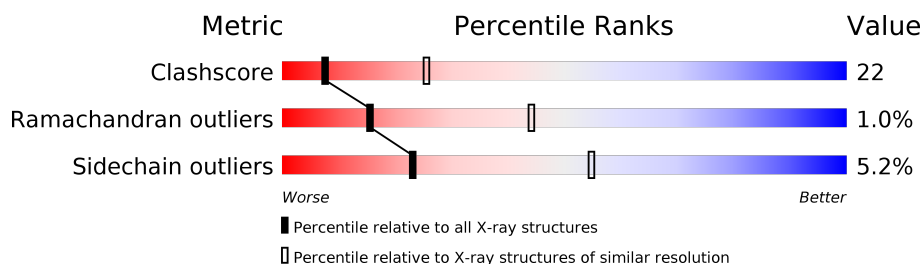
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 3569 (2.80-2.80) |
| Ramachandran outliers | 138981 | 3498 (2.80-2.80) |
| Sidechain outliers | 138945 | 3500 (2.80-2.80) |


















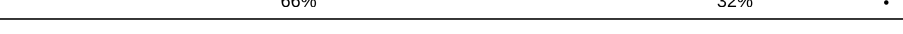

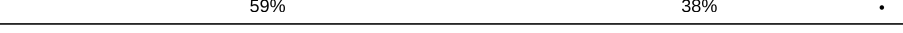
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 250 | 74% 23% . |
| 1 | O | 250 | 75% 23% . |
| 2 | B | 244 | 53% 42% 5% |
| 2 | P | 244 | 55% 41% . |
| 3 | C | 241 | 58% 37% 5% |
| 3 | Q | 241 | 55% 41% . |
| 4 | D | 242 | 70% 28% . |
| 4 | R | 242 | 65% 33% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | E | 233 |  |
| 5 | S | 233 |  |
| 6 | F | 244 |  |
| 6 | T | 244 |  |
| 7 | G | 243 |  |
| 7 | U | 243 |  |
| 8 | H | 222 |  |
| 8 | V | 222 |  |
| 9 | I | 204 |  |
| 9 | W | 204 |  |
| 10 | J | 198 |  |
| 10 | X | 198 |  |
| 11 | K | 212 |  |
| 11 | Y | 212 |  |
| 12 | L | 222 |  |
| 12 | Z | 222 |  |
| 13 | 1 | 233 |  |
| 13 | M | 233 |  |
| 14 | 2 | 196 |  |
| 14 | N | 196 |  |

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50753 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |
| 1 | O | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |

- Molecule 2 is a protein called Proteasome component Y13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1905 | 1201 | 321 | 380 | 3 | | | |
| 2 | P | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1905 | 1201 | 321 | 380 | 3 | | | |

- Molecule 3 is a protein called Proteasome component PRE6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1891 | 1181 | 331 | 375 | 4 | | | |
| 3 | Q | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1891 | 1181 | 331 | 375 | 4 | | | |

- Molecule 4 is a protein called Proteasome component PUP2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1862 | 1162 | 314 | 379 | 7 | | | |
| 4 | R | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1862 | 1162 | 314 | 379 | 7 | | | |

- Molecule 5 is a protein called Proteasome component PRE5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | E | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |
| 5 | S | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |

- Molecule 6 is a protein called Proteasome component C1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | F | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1897 | 1205 | 330 | 358 | 4 | | | |
| 6 | T | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1897 | 1205 | 330 | 358 | 4 | | | |

- Molecule 7 is a protein called Proteasome component C7-alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7 | G | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | | |
| 7 | U | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | | |

- Molecule 8 is a protein called Proteasome component PUP1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8 | H | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1685 | 1061 | 293 | 324 | 7 | | | |
| 8 | V | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1685 | 1061 | 293 | 324 | 7 | | | |

- Molecule 9 is a protein called Proteasome component PUP3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9 | I | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1010 | 258 | 305 | 8 | | | |
| 9 | W | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1010 | 258 | 305 | 8 | | | |

- Molecule 10 is a protein called Proteasome component C11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | J | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | X | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

- Molecule 11 is a protein called Proteasome component PRE2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 11 | K | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1644 | 1045 | 280 | 312 | 7 | | | |
| 11 | Y | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1644 | 1045 | 280 | 312 | 7 | | | |

- Molecule 12 is a protein called Proteasome component C5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 12 | L | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1757 | 1115 | 303 | 335 | 4 | | | |
| 12 | Z | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1757 | 1115 | 303 | 335 | 4 | | | |

- Molecule 13 is a protein called Proteasome component PRE4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | M | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1154 | 312 | 351 | 7 | | | |
| 13 | 1 | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1154 | 312 | 351 | 7 | | | |

- Molecule 14 is a protein called Proteasome component PRE3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | N | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1512 | 955 | 250 | 300 | 7 | | | |
| 14 | 2 | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1512 | 955 | 250 | 300 | 7 | | | |

- Molecule 15 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|--------|---------|--------|--------|---------|---------|
| 15 | H | 1 | Total 28 | B 1 | C 19 | N 4 | O 4 | 0 | 0 |
| 15 | K | 1 | Total 28 | B 1 | C 19 | N 4 | O 4 | 0 | 0 |
| 15 | N | 1 | Total 28 | B 1 | C 19 | N 4 | O 4 | 0 | 0 |
| 15 | V | 1 | Total 28 | B 1 | C 19 | N 4 | O 4 | 0 | 0 |
| 15 | Y | 1 | Total 28 | B 1 | C 19 | N 4 | O 4 | 0 | 0 |
| 15 | 2 | 1 | Total 28 | B 1 | C 19 | N 4 | O 4 | 0 | 0 |

- Molecule 16 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 16 | A | 46 | Total O 46 46 | 0 | 0 |
| 16 | B | 31 | Total O 31 31 | 0 | 0 |
| 16 | C | 33 | Total O 33 33 | 0 | 0 |
| 16 | D | 26 | Total O 26 26 | 0 | 0 |
| 16 | E | 14 | Total O 14 14 | 0 | 0 |
| 16 | F | 36 | Total O 36 36 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 16 | G | 48 | Total 48 | O 48 | 0 | 0 |
| 16 | H | 42 | Total 42 | O 42 | 0 | 0 |
| 16 | I | 50 | Total 50 | O 50 | 0 | 0 |
| 16 | J | 45 | Total 45 | O 45 | 0 | 0 |
| 16 | K | 33 | Total 33 | O 33 | 0 | 0 |
| 16 | L | 42 | Total 42 | O 42 | 0 | 0 |
| 16 | M | 52 | Total 52 | O 52 | 0 | 0 |
| 16 | N | 43 | Total 43 | O 43 | 0 | 0 |
| 16 | O | 23 | Total 23 | O 23 | 0 | 0 |
| 16 | P | 21 | Total 21 | O 21 | 0 | 0 |
| 16 | Q | 21 | Total 21 | O 21 | 0 | 0 |
| 16 | R | 20 | Total 20 | O 20 | 0 | 0 |
| 16 | S | 16 | Total 16 | O 16 | 0 | 0 |
| 16 | T | 32 | Total 32 | O 32 | 0 | 0 |
| 16 | U | 56 | Total 56 | O 56 | 0 | 0 |
| 16 | V | 34 | Total 34 | O 34 | 0 | 0 |
| 16 | W | 46 | Total 46 | O 46 | 0 | 0 |
| 16 | X | 39 | Total 39 | O 39 | 0 | 0 |
| 16 | Y | 32 | Total 32 | O 32 | 0 | 0 |
| 16 | Z | 42 | Total 42 | O 42 | 0 | 0 |
| 16 | 1 | 63 | Total 63 | O 63 | 0 | 0 |

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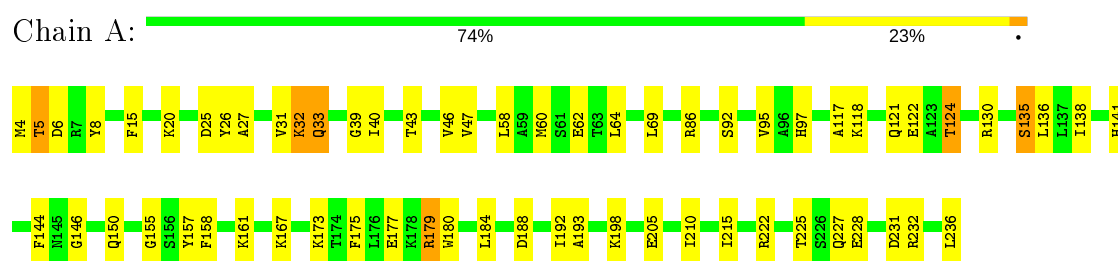
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16 | 2 | 51 | Total | O | 0 | 0 |
| | | | 51 | 51 | | |

3 Residue-property plots

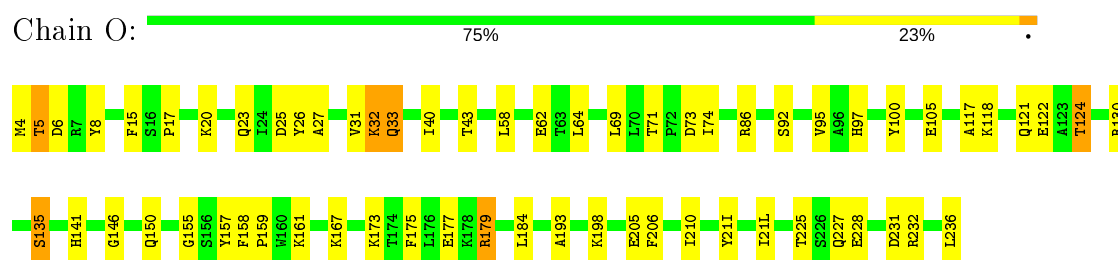
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

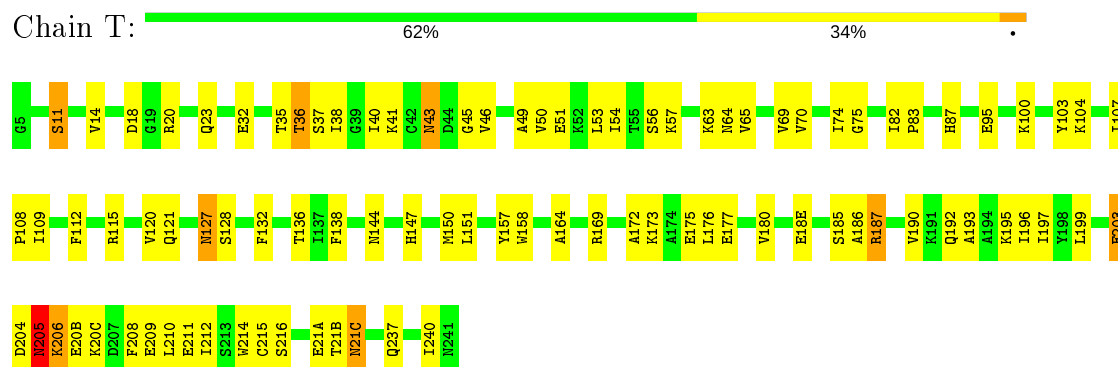


• Molecule 2: Proteasome component Y13

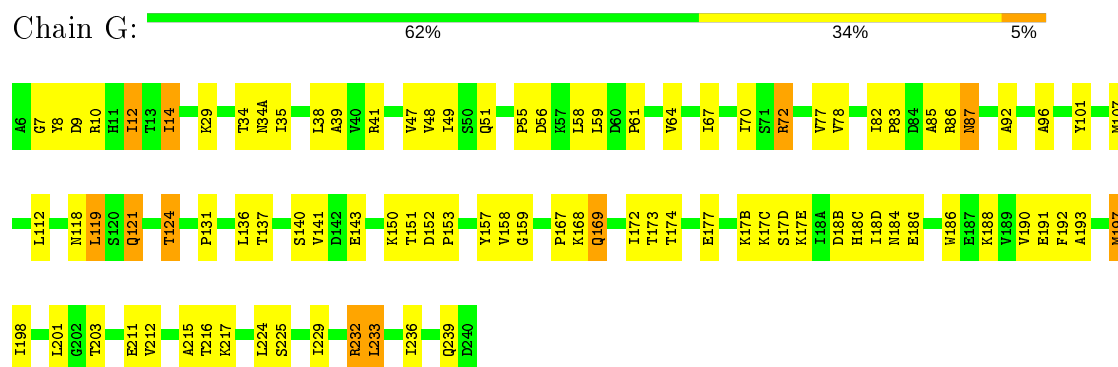


• Molecule 2: Proteasome component Y13

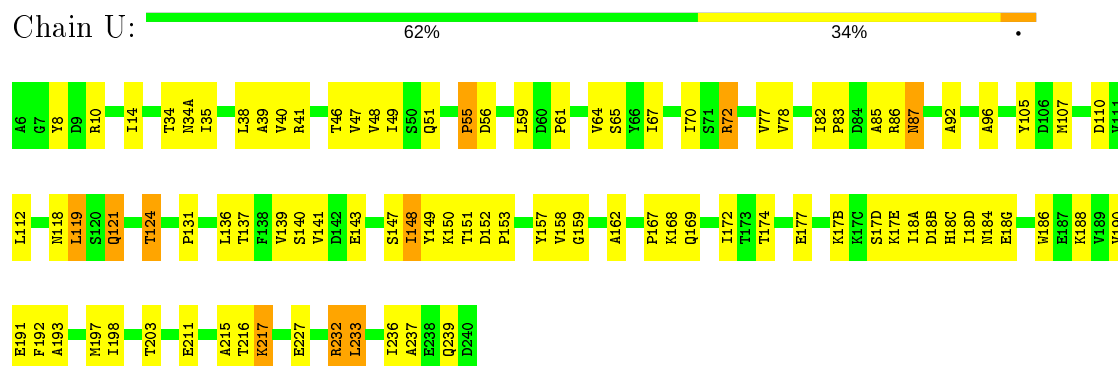




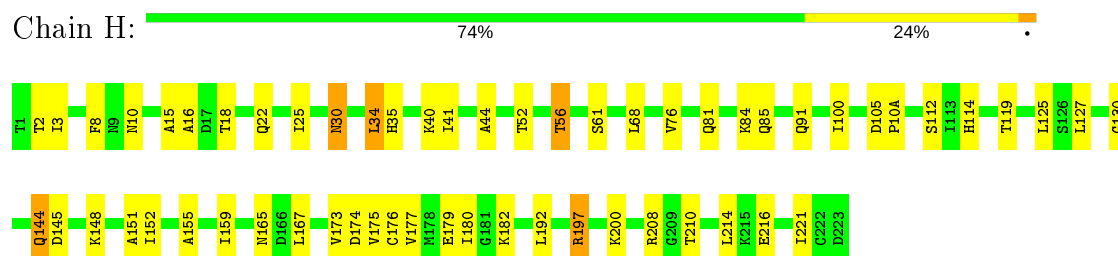
- Molecule 7: Proteasome component C7-alpha



- Molecule 7: Proteasome component C7-alpha

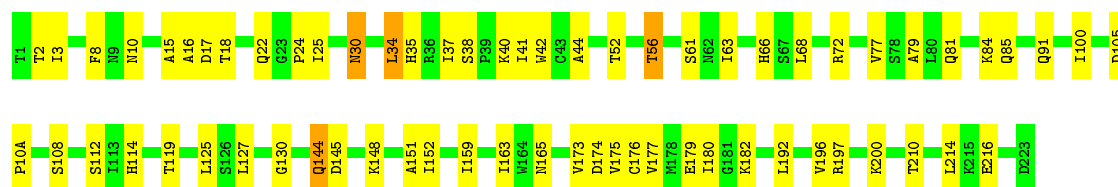


- Molecule 8: Proteasome component PUP1



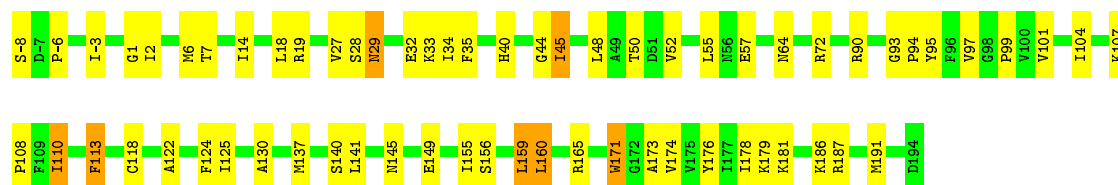
- Molecule 8: Proteasome component PUP1

Chain V:  70% 28%



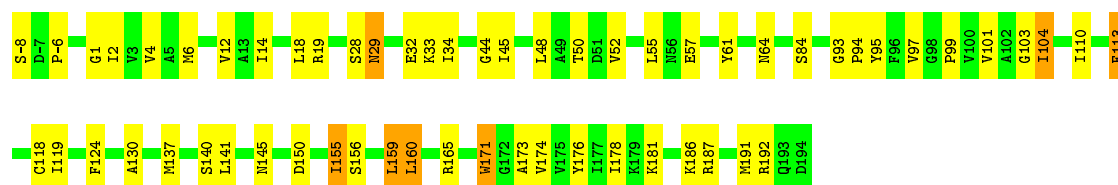
- Molecule 9: Proteasome component PUP3

Chain I:  69% 28%



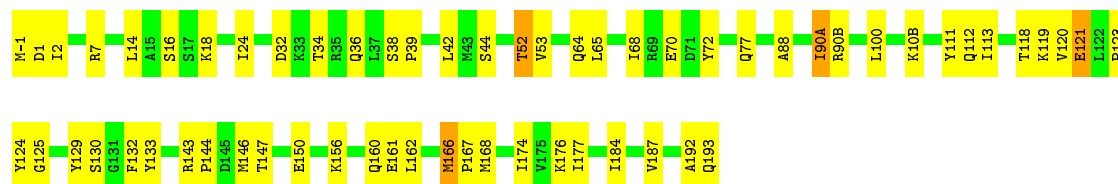
- Molecule 9: Proteasome component PUP3

Chain W:  71% 25%



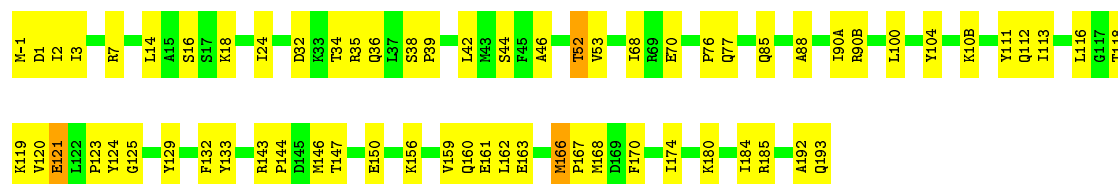
- Molecule 10: Proteasome component C11

Chain J:  69% 29%



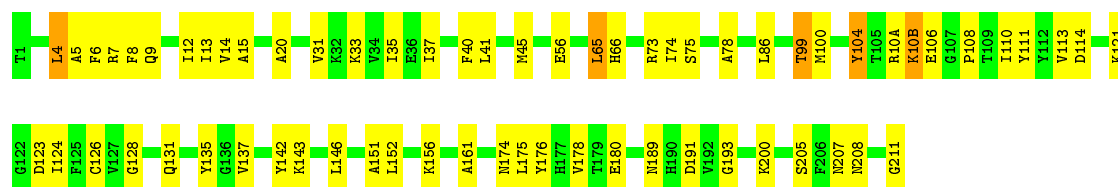
- Molecule 10: Proteasome component C11

Chain X:  67% 32%



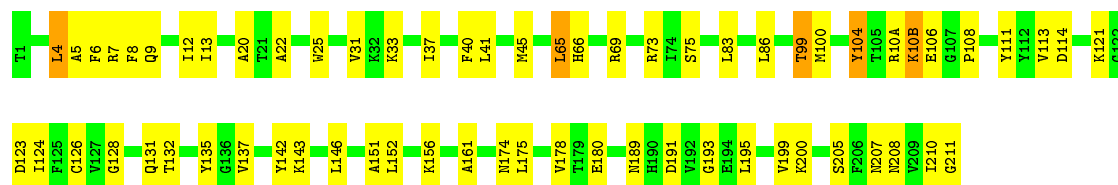
- Molecule 11: Proteasome component PRE2

Chain K:  69% 28%



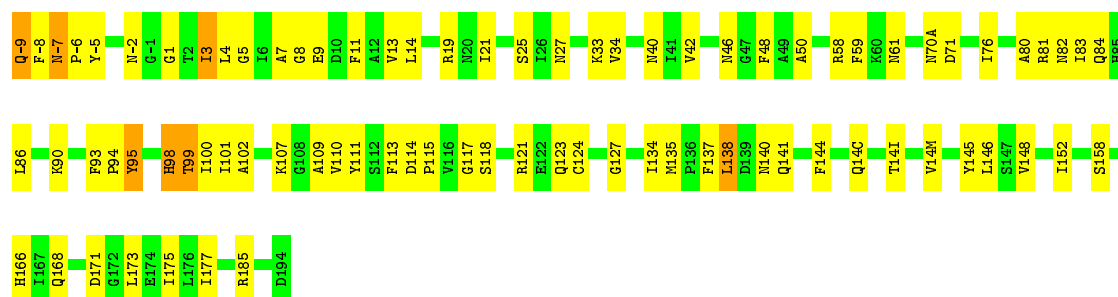
• Molecule 11: Proteasome component PRE2

Chain Y:  69% 28%



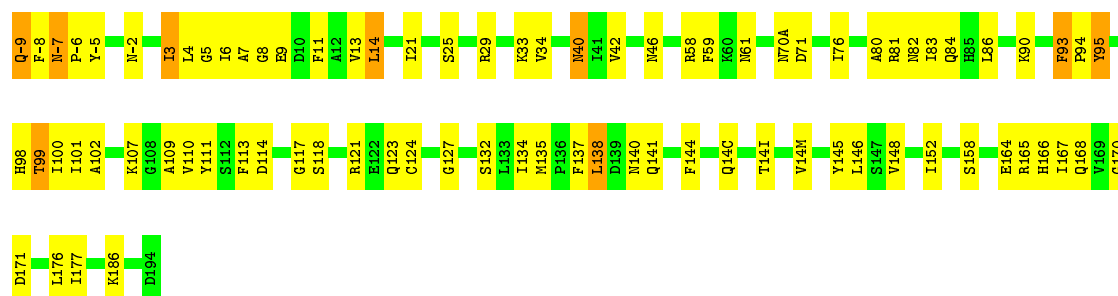
• Molecule 12: Proteasome component C5

Chain L:  63% 34%



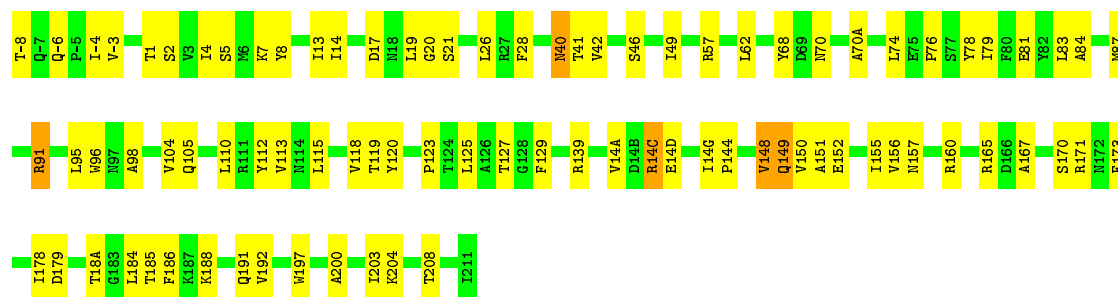
• Molecule 12: Proteasome component C5

Chain Z:  63% 33%

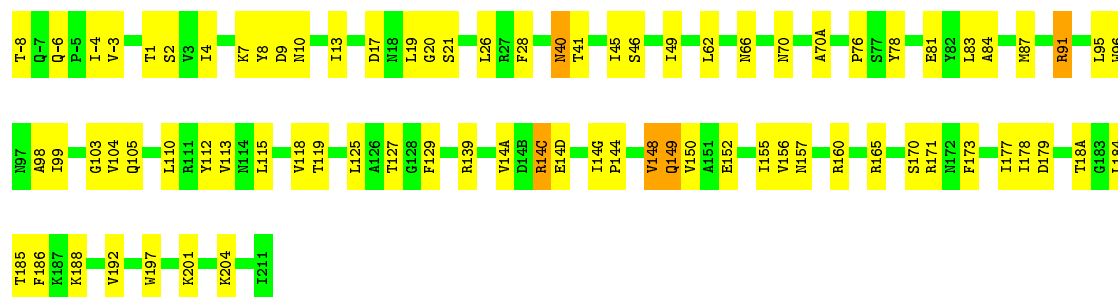


• Molecule 13: Proteasome component PRE4

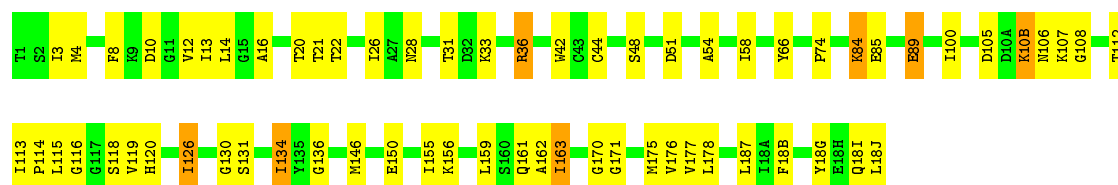
Chain M:  63% 35%



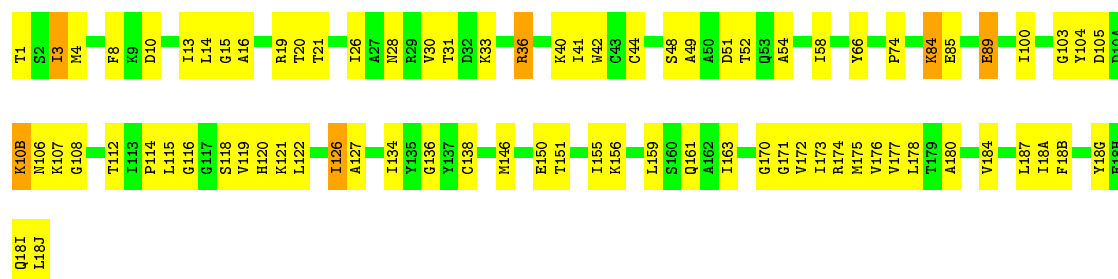
• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

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

| Property | Value | Source |
|--|--|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 136.18Å 300.72Å 144.66Å 90.00° 113.28° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 2.80 | Depositor |
| % Data completeness (in resolution range) | 96.4 (15.00-2.80) | Depositor |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.231 , 0.264 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 50753 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

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: BO2

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.37 | 0/1952 | 0.62 | 0/2642 |
| 1 | O | 0.37 | 0/1952 | 0.62 | 0/2642 |
| 2 | B | 0.36 | 0/1935 | 0.64 | 0/2618 |
| 2 | P | 0.37 | 0/1935 | 0.63 | 0/2618 |
| 3 | C | 0.36 | 0/1920 | 0.62 | 0/2598 |
| 3 | Q | 0.35 | 0/1920 | 0.62 | 0/2598 |
| 4 | D | 0.35 | 0/1887 | 0.63 | 0/2541 |
| 4 | R | 0.36 | 0/1887 | 0.62 | 0/2541 |
| 5 | E | 0.37 | 0/1823 | 0.61 | 0/2463 |
| 5 | S | 0.38 | 0/1823 | 0.61 | 0/2463 |
| 6 | F | 0.37 | 0/1937 | 0.62 | 0/2614 |
| 6 | T | 0.37 | 0/1937 | 0.63 | 0/2614 |
| 7 | G | 0.40 | 0/1959 | 0.64 | 0/2652 |
| 7 | U | 0.39 | 0/1959 | 0.64 | 0/2652 |
| 8 | H | 0.38 | 0/1716 | 0.67 | 0/2326 |
| 8 | V | 0.36 | 0/1716 | 0.67 | 0/2326 |
| 9 | I | 0.39 | 0/1611 | 0.67 | 0/2174 |
| 9 | W | 0.40 | 0/1611 | 0.68 | 0/2174 |
| 10 | J | 0.38 | 0/1613 | 0.65 | 0/2173 |
| 10 | X | 0.37 | 0/1613 | 0.65 | 0/2173 |
| 11 | K | 0.41 | 0/1681 | 0.65 | 0/2274 |
| 11 | Y | 0.39 | 0/1681 | 0.65 | 0/2274 |
| 12 | L | 0.39 | 0/1795 | 0.67 | 1/2420 (0.0%) |
| 12 | Z | 0.38 | 0/1795 | 0.67 | 1/2420 (0.0%) |
| 13 | 1 | 0.41 | 0/1855 | 0.69 | 1/2514 (0.0%) |
| 13 | M | 0.39 | 0/1855 | 0.67 | 1/2514 (0.0%) |
| 14 | 2 | 0.41 | 0/1541 | 0.65 | 0/2087 |
| 14 | N | 0.41 | 0/1541 | 0.65 | 0/2087 |
| All | All | 0.38 | 0/50450 | 0.64 | 4/68192 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 13 | 1 | 95 | LEU | N-CA-C | -5.76 | 95.45 | 111.00 |
| 13 | M | 95 | LEU | N-CA-C | -5.66 | 95.72 | 111.00 |
| 12 | L | 95 | TYR | N-CA-C | -5.23 | 96.89 | 111.00 |
| 12 | Z | 95 | TYR | N-CA-C | -5.23 | 96.89 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1915 | 0 | 1926 | 56 | 0 |
| 1 | O | 1915 | 0 | 1926 | 58 | 0 |
| 2 | B | 1905 | 0 | 1901 | 139 | 0 |
| 2 | P | 1905 | 0 | 1901 | 118 | 0 |
| 3 | C | 1891 | 0 | 1900 | 117 | 0 |
| 3 | Q | 1891 | 0 | 1900 | 122 | 0 |
| 4 | D | 1862 | 0 | 1836 | 71 | 0 |
| 4 | R | 1862 | 0 | 1836 | 84 | 0 |
| 5 | E | 1795 | 0 | 1797 | 120 | 0 |
| 5 | S | 1795 | 0 | 1797 | 128 | 0 |
| 6 | F | 1897 | 0 | 1886 | 88 | 0 |
| 6 | T | 1897 | 0 | 1886 | 87 | 0 |
| 7 | G | 1921 | 0 | 1910 | 90 | 0 |
| 7 | U | 1921 | 0 | 1910 | 104 | 0 |
| 8 | H | 1685 | 0 | 1687 | 59 | 0 |
| 8 | V | 1685 | 0 | 1687 | 62 | 0 |
| 9 | I | 1581 | 0 | 1574 | 76 | 0 |
| 9 | W | 1581 | 0 | 1574 | 65 | 0 |
| 10 | J | 1585 | 0 | 1590 | 77 | 0 |
| 10 | X | 1585 | 0 | 1590 | 76 | 0 |
| 11 | K | 1644 | 0 | 1594 | 74 | 0 |
| 11 | Y | 1644 | 0 | 1594 | 69 | 0 |
| 12 | L | 1757 | 0 | 1711 | 76 | 0 |
| 12 | Z | 1757 | 0 | 1711 | 80 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13 | 1 | 1824 | 0 | 1832 | 83 | 0 |
| 13 | M | 1824 | 0 | 1832 | 79 | 0 |
| 14 | 2 | 1512 | 0 | 1480 | 92 | 0 |
| 14 | N | 1512 | 0 | 1480 | 71 | 0 |
| 15 | 2 | 28 | 0 | 25 | 8 | 0 |
| 15 | H | 28 | 0 | 25 | 2 | 0 |
| 15 | K | 28 | 0 | 25 | 0 | 0 |
| 15 | N | 28 | 0 | 25 | 5 | 0 |
| 15 | V | 28 | 0 | 25 | 2 | 0 |
| 15 | Y | 28 | 0 | 25 | 1 | 0 |
| 16 | 1 | 63 | 0 | 0 | 4 | 0 |
| 16 | 2 | 51 | 0 | 0 | 6 | 0 |
| 16 | A | 46 | 0 | 0 | 1 | 0 |
| 16 | B | 31 | 0 | 0 | 5 | 0 |
| 16 | C | 33 | 0 | 0 | 1 | 0 |
| 16 | D | 26 | 0 | 0 | 1 | 0 |
| 16 | E | 14 | 0 | 0 | 0 | 0 |
| 16 | F | 36 | 0 | 0 | 2 | 0 |
| 16 | G | 48 | 0 | 0 | 3 | 0 |
| 16 | H | 42 | 0 | 0 | 1 | 0 |
| 16 | I | 50 | 0 | 0 | 0 | 0 |
| 16 | J | 45 | 0 | 0 | 5 | 0 |
| 16 | K | 33 | 0 | 0 | 3 | 0 |
| 16 | L | 42 | 0 | 0 | 4 | 0 |
| 16 | M | 52 | 0 | 0 | 3 | 0 |
| 16 | N | 43 | 0 | 0 | 1 | 0 |
| 16 | O | 23 | 0 | 0 | 0 | 0 |
| 16 | P | 21 | 0 | 0 | 1 | 0 |
| 16 | Q | 21 | 0 | 0 | 5 | 0 |
| 16 | R | 20 | 0 | 0 | 2 | 0 |
| 16 | S | 16 | 0 | 0 | 3 | 0 |
| 16 | T | 32 | 0 | 0 | 2 | 0 |
| 16 | U | 56 | 0 | 0 | 5 | 0 |
| 16 | V | 34 | 0 | 0 | 2 | 0 |
| 16 | W | 46 | 0 | 0 | 2 | 0 |
| 16 | X | 39 | 0 | 0 | 4 | 0 |
| 16 | Y | 32 | 0 | 0 | 7 | 0 |
| 16 | Z | 42 | 0 | 0 | 3 | 0 |
| All | All | 50753 | 0 | 49398 | 2178 | 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 22.

All (2178) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:N:13:ILE:CD1 | 14:N:177:VAL:HG13 | 1.58 | 1.31 |
| 3:Q:197:LEU:HD13 | 3:Q:210:ILE:HD12 | 1.22 | 1.20 |
| 5:S:49:VAL:HG13 | 5:S:212:ILE:CD1 | 1.72 | 1.19 |
| 3:C:197:LEU:HD13 | 3:C:210:ILE:HD12 | 1.20 | 1.16 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:HD21 | 1.20 | 1.16 |
| 3:C:201:VAL:HG21 | 3:C:210:ILE:HD11 | 1.17 | 1.14 |
| 3:Q:201:VAL:HG21 | 3:Q:210:ILE:HD11 | 1.18 | 1.13 |
| 9:W:6:MET:HE3 | 9:W:155:ILE:HD13 | 1.18 | 1.13 |
| 4:R:162:ALA:HB3 | 5:S:58:LEU:HD23 | 1.30 | 1.12 |
| 11:Y:10(B):LYS:HD2 | 11:Y:10(B):LYS:H | 1.06 | 1.11 |
| 8:H:15:ALA:CB | 8:H:159:ILE:HD11 | 1.80 | 1.11 |
| 8:H:15:ALA:HB3 | 8:H:159:ILE:HD11 | 1.20 | 1.11 |
| 11:K:10(B):LYS:H | 11:K:10(B):LYS:HD2 | 1.04 | 1.10 |
| 14:N:13:ILE:HD11 | 14:N:177:VAL:HG13 | 1.23 | 1.10 |
| 2:P:40:ILE:HD12 | 2:P:162:ALA:HB1 | 1.30 | 1.09 |
| 7:G:9:ASP:HA | 7:G:14:ILE:HD11 | 1.32 | 1.08 |
| 14:N:136:GLY:HA2 | 14:2:161:GLN:HE21 | 1.17 | 1.08 |
| 2:B:108:PRO:HB2 | 2:B:111:ILE:HD13 | 1.31 | 1.07 |
| 14:N:161:GLN:HE21 | 14:2:136:GLY:HA2 | 1.14 | 1.06 |
| 2:B:124:THR:HG22 | 3:C:130:ARG:HH21 | 1.20 | 1.04 |
| 14:N:13:ILE:HD12 | 14:N:177:VAL:HG13 | 1.35 | 1.04 |
| 13:1:13:ILE:HD12 | 13:1:177:ILE:HG12 | 1.37 | 1.03 |
| 2:B:202:THR:HG22 | 2:B:204:SER:H | 1.22 | 1.03 |
| 8:H:41:ILE:HD12 | 8:H:76:VAL:HG22 | 1.39 | 1.03 |
| 4:R:31:ILE:HD11 | 4:R:134:VAL:HA | 1.39 | 1.02 |
| 13:1:45:ILE:HG12 | 13:1:99:ILE:HD12 | 1.40 | 1.01 |
| 2:P:202:THR:HG22 | 2:P:204:SER:H | 1.22 | 1.01 |
| 6:F:38:ILE:HD12 | 6:F:40:ILE:HD11 | 1.44 | 0.99 |
| 7:G:96:ALA:HA | 7:G:107:MET:HE2 | 1.44 | 0.99 |
| 8:V:38:SER:OG | 8:V:41:ILE:HD13 | 1.63 | 0.98 |
| 1:A:15:PHE:H | 2:B:23:GLN:HE22 | 1.08 | 0.98 |
| 5:E:68:ILE:HD11 | 5:E:78:LEU:HD23 | 1.43 | 0.98 |
| 13:M:200:ALA:HA | 13:M:203:ILE:HD12 | 1.42 | 0.97 |
| 13:1:13:ILE:CD1 | 13:1:177:ILE:HG23 | 1.95 | 0.96 |
| 7:U:147:SER:C | 7:U:148:ILE:HD12 | 1.85 | 0.96 |
| 3:C:163:GLN:HE21 | 3:C:164:THR:H | 1.07 | 0.96 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:CD2 | 1.95 | 0.95 |
| 5:S:214:ILE:HD12 | 5:S:219:THR:HG21 | 1.49 | 0.95 |
| 12:L:3:ILE:HD12 | 12:L:46:ASN:HB2 | 1.48 | 0.95 |
| 4:D:229:THR:O | 4:D:233:ILE:HD13 | 1.67 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:15:PHE:H | 3:C:23:GLN:HE22 | 1.14 | 0.94 |
| 3:Q:201:VAL:CG2 | 3:Q:210:ILE:HD11 | 1.98 | 0.94 |
| 3:C:163:GLN:NE2 | 3:C:164:THR:H | 1.65 | 0.94 |
| 5:S:49:VAL:HG13 | 5:S:212:ILE:HD12 | 1.49 | 0.94 |
| 5:E:213:ALA:HB2 | 5:E:223:ILE:HD12 | 1.49 | 0.94 |
| 4:R:31:ILE:HD11 | 4:R:134:VAL:CA | 1.98 | 0.94 |
| 12:Z:3:ILE:HD12 | 12:Z:46:ASN:HB2 | 1.50 | 0.94 |
| 3:Q:163:GLN:HE21 | 3:Q:164:THR:H | 1.11 | 0.93 |
| 2:B:194:LEU:HD11 | 2:B:232:ILE:CD1 | 1.99 | 0.93 |
| 1:O:15:PHE:H | 2:P:23:GLN:HE22 | 1.14 | 0.93 |
| 6:T:49:ALA:CB | 6:T:197:ILE:HD11 | 1.99 | 0.93 |
| 13:M:-4:ILE:HD12 | 14:N:116:GLY:N | 1.84 | 0.92 |
| 2:P:40:ILE:HD12 | 2:P:162:ALA:CB | 1.98 | 0.92 |
| 3:C:201:VAL:CG2 | 3:C:210:ILE:HD11 | 1.98 | 0.92 |
| 3:Q:15:PHE:H | 4:R:23:GLN:HE22 | 1.09 | 0.92 |
| 14:N:13:ILE:CD1 | 14:N:177:VAL:CG1 | 2.48 | 0.92 |
| 4:R:31:ILE:CD1 | 4:R:134:VAL:HA | 1.99 | 0.92 |
| 6:T:49:ALA:HB1 | 6:T:197:ILE:HD11 | 1.52 | 0.92 |
| 7:U:96:ALA:HA | 7:U:107:MET:HE2 | 1.52 | 0.92 |
| 11:Y:10(B):LYS:CD | 11:Y:10(B):LYS:H | 1.82 | 0.92 |
| 7:U:40:VAL:HB | 7:U:18(D):ILE:HD11 | 1.49 | 0.91 |
| 2:B:194:LEU:HD11 | 2:B:232:ILE:HD12 | 1.53 | 0.91 |
| 3:Q:163:GLN:NE2 | 3:Q:164:THR:H | 1.69 | 0.91 |
| 7:G:18(G):GLU:HG2 | 7:G:188:LYS:HB2 | 1.53 | 0.90 |
| 10:J:177:ILE:HD11 | 10:J:187:VAL:CG2 | 2.01 | 0.90 |
| 7:U:18(A):ILE:HD13 | 7:U:18(C):HIS:H | 1.33 | 0.90 |
| 14:N:134:ILE:HD12 | 14:N:162:ALA:HB2 | 1.52 | 0.90 |
| 2:B:11:ARG:O | 2:B:14:ILE:HD12 | 1.70 | 0.90 |
| 5:S:49:VAL:HG13 | 5:S:212:ILE:HD11 | 1.51 | 0.90 |
| 7:U:18(G):GLU:HG2 | 7:U:188:LYS:HB2 | 1.53 | 0.90 |
| 2:P:61:GLN:OE1 | 2:P:208:ASP:HA | 1.71 | 0.90 |
| 2:P:40:ILE:CD1 | 2:P:162:ALA:HB1 | 2.02 | 0.90 |
| 13:M:157:ASN:HD22 | 13:M:160:ARG:HH11 | 0.97 | 0.90 |
| 2:P:71:ASN:ND2 | 2:P:72:ASP:H | 1.68 | 0.90 |
| 11:K:10(B):LYS:H | 11:K:10(B):LYS:CD | 1.81 | 0.90 |
| 2:B:83:ALA:O | 2:B:87:ILE:HD13 | 1.72 | 0.90 |
| 11:K:7:ARG:HG3 | 11:K:12:ILE:CD1 | 2.03 | 0.89 |
| 2:B:61:GLN:OE1 | 2:B:208:ASP:HA | 1.72 | 0.89 |
| 2:B:71:ASN:ND2 | 2:B:72:ASP:H | 1.70 | 0.89 |
| 14:N:131:SER:HA | 14:N:134:ILE:HD11 | 1.53 | 0.89 |
| 13:1:157:ASN:HD22 | 13:1:160:ARG:HH11 | 0.95 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:H:165:ASN:HD22 | 13:1:139:ARG:HH11 | 1.20 | 0.89 |
| 5:S:213:ALA:HB2 | 5:S:223:ILE:HD12 | 1.52 | 0.88 |
| 2:B:71:ASN:HD22 | 2:B:72:ASP:H | 1.19 | 0.88 |
| 5:E:48:LEU:HD11 | 5:E:139:ILE:HD12 | 1.55 | 0.88 |
| 2:P:71:ASN:HD22 | 2:P:72:ASP:H | 1.18 | 0.88 |
| 13:M:139:ARG:HH11 | 8:V:165:ASN:HD22 | 1.17 | 0.88 |
| 13:1:-4:ILE:HD12 | 14:2:116:GLY:N | 1.88 | 0.87 |
| 11:K:10(B):LYS:N | 11:K:10(B):LYS:HD2 | 1.89 | 0.87 |
| 1:O:130:ARG:HH21 | 7:U:124:THR:CG2 | 1.88 | 0.87 |
| 14:2:21:THR:CG2 | 14:2:26:ILE:HD13 | 2.04 | 0.86 |
| 5:S:198:SER:HA | 5:S:201:LEU:HG | 1.57 | 0.86 |
| 3:C:201:VAL:HG21 | 3:C:210:ILE:CD1 | 2.03 | 0.86 |
| 5:E:139:ILE:HD11 | 5:E:221:PHE:HE2 | 1.40 | 0.85 |
| 3:C:15:PHE:H | 4:D:23:GLN:HE22 | 1.25 | 0.85 |
| 5:S:207:LEU:HD23 | 5:S:207:LEU:H | 1.40 | 0.85 |
| 10:X:2:ILE:C | 10:X:3:ILE:HD12 | 1.96 | 0.85 |
| 3:C:163:GLN:HE21 | 3:C:164:THR:N | 1.74 | 0.85 |
| 6:F:193:ALA:O | 6:F:197:ILE:CD1 | 2.25 | 0.85 |
| 14:2:21:THR:HG22 | 14:2:26:ILE:HD13 | 1.58 | 0.84 |
| 6:T:95:GLU:HG2 | 6:T:115:ARG:HB3 | 1.59 | 0.84 |
| 3:Q:201:VAL:HG21 | 3:Q:210:ILE:CD1 | 2.04 | 0.84 |
| 1:O:124:THR:HG22 | 2:P:130:ARG:HH21 | 1.43 | 0.84 |
| 3:Q:185:THR:HG22 | 3:Q:187:GLU:H | 1.42 | 0.84 |
| 4:R:97:VAL:HG21 | 11:Y:65:LEU:HD13 | 1.58 | 0.84 |
| 13:1:13:ILE:HD13 | 13:1:177:ILE:HG23 | 1.59 | 0.84 |
| 2:B:38:ILE:HD13 | 2:B:164:SER:HB3 | 1.58 | 0.84 |
| 9:I:110:ILE:HD13 | 9:I:110:ILE:H | 1.43 | 0.84 |
| 3:Q:185:THR:HB | 3:Q:188:GLU:HG2 | 1.59 | 0.83 |
| 7:U:67:ILE:HD12 | 7:U:211:GLU:HG2 | 1.60 | 0.83 |
| 2:B:90:ASN:O | 2:B:94:ILE:HD13 | 1.78 | 0.83 |
| 5:E:207:LEU:HD23 | 5:E:207:LEU:H | 1.42 | 0.83 |
| 1:A:20:LYS:HE3 | 1:A:25:ASP:OD1 | 1.79 | 0.83 |
| 4:D:229:THR:HG22 | 4:D:233:ILE:HD11 | 1.60 | 0.83 |
| 6:T:54:ILE:HD11 | 6:T:209:GLU:HB2 | 1.59 | 0.83 |
| 5:E:198:SER:HA | 5:E:201:LEU:HG | 1.58 | 0.83 |
| 5:E:28:LEU:HA | 5:E:31:ILE:HD13 | 1.58 | 0.82 |
| 3:C:185:THR:HG22 | 3:C:187:GLU:H | 1.43 | 0.82 |
| 5:E:15:PHE:H | 6:F:23:GLN:HE22 | 1.27 | 0.82 |
| 6:F:54:ILE:HD11 | 6:F:209:GLU:HB2 | 1.59 | 0.82 |
| 14:N:13:ILE:HD12 | 14:N:177:VAL:HA | 1.59 | 0.82 |
| 10:X:32:ASP:OD2 | 10:X:34:THR:HG22 | 1.79 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 11:Y:143:LYS:HB2 | 11:Y:146:LEU:CD1 | 2.10 | 0.82 |
| 3:C:185:THR:HB | 3:C:188:GLU:HG2 | 1.59 | 0.82 |
| 9:I:44:GLY:C | 9:I:45:ILE:HD12 | 1.99 | 0.82 |
| 14:N:13:ILE:HD11 | 14:N:177:VAL:CG1 | 2.06 | 0.82 |
| 16:Q:245:HOH:O | 10:X:68:ILE:HD13 | 1.78 | 0.82 |
| 13:1:3:VAL:HG12 | 13:1:49:ILE:HD12 | 1.61 | 0.82 |
| 4:D:97:VAL:HG21 | 11:K:65:LEU:HD13 | 1.62 | 0.82 |
| 2:B:116:LEU:HD23 | 2:B:119:ILE:HD12 | 1.61 | 0.81 |
| 11:K:7:ARG:HG3 | 11:K:12:ILE:HD11 | 1.61 | 0.81 |
| 12:L:3:ILE:HD12 | 12:L:46:ASN:CB | 2.10 | 0.81 |
| 9:W:6:MET:CE | 9:W:155:ILE:HD13 | 2.07 | 0.81 |
| 2:B:124:THR:CG2 | 3:C:130:ARG:HH21 | 1.91 | 0.81 |
| 1:O:20:LYS:HE3 | 1:O:25:ASP:OD1 | 1.80 | 0.81 |
| 3:Q:65:SER:HB2 | 16:Q:247:HOH:O | 1.78 | 0.81 |
| 5:E:75:GLY:O | 5:E:139:ILE:HD13 | 1.80 | 0.81 |
| 8:H:15:ALA:CB | 8:H:159:ILE:CD1 | 2.58 | 0.81 |
| 11:K:143:LYS:HB2 | 11:K:146:LEU:CD1 | 2.10 | 0.81 |
| 3:Q:163:GLN:HE21 | 3:Q:164:THR:N | 1.77 | 0.81 |
| 13:M:-4:ILE:HD13 | 14:N:115:LEU:HB3 | 1.62 | 0.81 |
| 14:N:161:GLN:NE2 | 14:2:136:GLY:HA2 | 1.94 | 0.81 |
| 8:H:155:ALA:O | 8:H:159:ILE:HD12 | 1.80 | 0.81 |
| 9:I:35:PHE:CE1 | 9:I:45:ILE:HD13 | 2.16 | 0.81 |
| 9:W:6:MET:HE3 | 9:W:155:ILE:CD1 | 2.09 | 0.80 |
| 13:1:45:ILE:HG23 | 13:1:99:ILE:CD1 | 2.11 | 0.80 |
| 7:G:67:ILE:HD12 | 7:G:211:GLU:HG2 | 1.61 | 0.80 |
| 13:1:13:ILE:CG2 | 13:1:155:ILE:HD12 | 2.12 | 0.80 |
| 1:O:71:THR:OG1 | 1:O:74:ILE:HD13 | 1.80 | 0.80 |
| 10:J:32:ASP:OD2 | 10:J:34:THR:HG22 | 1.82 | 0.79 |
| 13:M:157:ASN:HD22 | 13:M:160:ARG:NH1 | 1.78 | 0.79 |
| 6:F:95:GLU:HG2 | 6:F:115:ARG:HB3 | 1.61 | 0.79 |
| 2:B:97:GLN:HE22 | 9:I:64:ASN:HD22 | 1.30 | 0.79 |
| 13:M:14(C):ARG:HH11 | 13:M:14(C):ARG:HG3 | 1.46 | 0.79 |
| 12:Z:3:ILE:HD12 | 12:Z:46:ASN:CB | 2.13 | 0.79 |
| 6:T:197:ILE:HD13 | 6:T:210:LEU:HD11 | 1.65 | 0.79 |
| 11:K:35:ILE:HD12 | 11:K:56:GLU:HB2 | 1.63 | 0.79 |
| 7:G:198:ILE:HG23 | 7:G:203:THR:O | 1.82 | 0.79 |
| 14:N:13:ILE:HD12 | 14:N:177:VAL:CG1 | 2.10 | 0.79 |
| 6:F:193:ALA:O | 6:F:197:ILE:HD12 | 1.83 | 0.79 |
| 8:H:40:LYS:O | 8:H:41:ILE:HD13 | 1.82 | 0.79 |
| 2:P:124:THR:HG22 | 3:Q:130:ARG:HH21 | 1.47 | 0.78 |
| 13:1:157:ASN:HD22 | 13:1:160:ARG:NH1 | 1.77 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:P:71:ASN:HD22 | 2:P:72:ASP:N | 1.81 | 0.78 |
| 11:Y:99:THR:HG22 | 11:Y:113:VAL:HB | 1.64 | 0.78 |
| 5:E:139:ILE:HD13 | 5:E:139:ILE:H | 1.47 | 0.78 |
| 11:K:99:THR:HG22 | 11:K:113:VAL:HB | 1.64 | 0.78 |
| 14:N:12:VAL:O | 14:N:13:ILE:HD13 | 1.82 | 0.78 |
| 13:1:14(C):ARG:HG3 | 13:1:14(C):ARG:HH11 | 1.47 | 0.78 |
| 2:B:215:ILE:HD12 | 2:B:221:GLN:HG2 | 1.65 | 0.78 |
| 11:Y:33:LYS:HA | 11:Y:45:MET:HE2 | 1.63 | 0.78 |
| 11:Y:10(B):LYS:N | 11:Y:10(B):LYS:HD2 | 1.90 | 0.78 |
| 14:N:136:GLY:HA2 | 14:2:161:GLN:NE2 | 1.95 | 0.78 |
| 13:M:157:ASN:ND2 | 13:M:160:ARG:HH11 | 1.80 | 0.78 |
| 13:1:40:ASN:HD22 | 13:1:40:ASN:H | 1.29 | 0.77 |
| 2:P:28:LEU:HA | 2:P:31:ILE:HD12 | 1.66 | 0.77 |
| 5:S:214:ILE:HD13 | 5:S:215:VAL:N | 1.99 | 0.77 |
| 9:W:45:ILE:HB | 9:W:52:VAL:HG13 | 1.65 | 0.77 |
| 5:S:15:PHE:H | 6:T:23:GLN:HE22 | 1.29 | 0.77 |
| 7:U:198:ILE:HG23 | 7:U:203:THR:O | 1.83 | 0.77 |
| 13:1:76:PRO:HD2 | 13:1:105:GLN:OE1 | 1.84 | 0.77 |
| 11:K:35:ILE:HD12 | 11:K:56:GLU:CB | 2.15 | 0.77 |
| 12:L:3:ILE:HD13 | 12:L:127:GLY:O | 1.84 | 0.77 |
| 13:M:-4:ILE:CD1 | 14:N:115:LEU:HB3 | 2.14 | 0.77 |
| 13:M:167:ALA:HB2 | 14:2:26:ILE:HD11 | 1.68 | 0.76 |
| 2:B:194:LEU:CD1 | 2:B:232:ILE:CD1 | 2.63 | 0.76 |
| 6:T:74:ILE:HG12 | 6:T:109:ILE:CD1 | 2.15 | 0.76 |
| 1:A:124:THR:CG2 | 2:B:130:ARG:HH21 | 1.98 | 0.76 |
| 12:Z:4:LEU:HD11 | 12:Z:138:LEU:HD21 | 1.67 | 0.76 |
| 9:W:34:ILE:HD13 | 9:W:44:GLY:HA3 | 1.67 | 0.76 |
| 10:X:18:LYS:HD3 | 10:X:174:ILE:HG13 | 1.68 | 0.76 |
| 2:B:71:ASN:HD22 | 2:B:72:ASP:N | 1.83 | 0.76 |
| 13:M:40:ASN:H | 13:M:40:ASN:HD22 | 1.28 | 0.76 |
| 1:O:130:ARG:HH21 | 7:U:124:THR:HG22 | 1.50 | 0.76 |
| 7:G:151:THR:HG22 | 7:G:157:TYR:HB2 | 1.67 | 0.76 |
| 1:O:124:THR:CG2 | 2:P:130:ARG:HH21 | 1.98 | 0.76 |
| 3:Q:85:SER:O | 3:Q:89:ILE:HD13 | 1.85 | 0.76 |
| 12:L:4:LEU:HD11 | 12:L:138:LEU:HD21 | 1.65 | 0.76 |
| 5:E:48:LEU:CD1 | 5:E:139:ILE:HD12 | 2.15 | 0.75 |
| 8:H:3:ILE:HD12 | 8:H:100:ILE:HG12 | 1.68 | 0.75 |
| 12:Z:3:ILE:HD13 | 12:Z:127:GLY:O | 1.86 | 0.75 |
| 7:U:151:THR:HG22 | 7:U:157:TYR:HB2 | 1.67 | 0.75 |
| 13:1:157:ASN:ND2 | 13:1:160:ARG:HH11 | 1.79 | 0.75 |
| 9:I:34:ILE:HD13 | 9:I:44:GLY:HA3 | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:I:35:PHE:HE1 | 9:I:45:ILE:HD13 | 1.50 | 0.75 |
| 10:J:133:TYR:HD1 | 16:Y:1425:HOH:O | 1.69 | 0.75 |
| 5:S:211:SER:O | 5:S:212:ILE:HD13 | 1.87 | 0.75 |
| 9:W:34:ILE:HD13 | 9:W:44:GLY:CA | 2.15 | 0.75 |
| 11:K:33:LYS:HA | 11:K:45:MET:HE2 | 1.67 | 0.75 |
| 7:U:41:ARG:HD3 | 7:U:148:ILE:HD13 | 1.68 | 0.75 |
| 7:G:233:LEU:O | 7:G:236:ILE:HG13 | 1.87 | 0.74 |
| 7:U:41:ARG:HG2 | 7:U:148:ILE:HD11 | 1.67 | 0.74 |
| 4:R:12(D):ALA:HB3 | 4:R:126:ARG:HD3 | 1.69 | 0.74 |
| 3:C:164:THR:HG21 | 3:C:172:VAL:HG13 | 1.69 | 0.74 |
| 3:C:85:SER:O | 3:C:89:ILE:HD13 | 1.87 | 0.74 |
| 2:B:160:TRP:CE2 | 2:B:163:ILE:HD12 | 2.22 | 0.74 |
| 7:G:18(G):GLU:HG2 | 7:G:188:LYS:CB | 2.17 | 0.74 |
| 9:I:34:ILE:HD13 | 9:I:44:GLY:CA | 2.17 | 0.74 |
| 12:L:4:LEU:CD1 | 12:L:138:LEU:HD21 | 2.17 | 0.74 |
| 8:V:3:ILE:HD12 | 8:V:100:ILE:HG12 | 1.70 | 0.74 |
| 12:Z:4:LEU:CD1 | 12:Z:138:LEU:HD21 | 2.17 | 0.74 |
| 2:B:15:PHE:H | 3:C:23:GLN:NE2 | 1.86 | 0.74 |
| 2:P:160:TRP:CE2 | 2:P:163:ILE:HD12 | 2.23 | 0.74 |
| 7:U:18(A):ILE:HD13 | 7:U:18(C):HIS:O | 1.86 | 0.74 |
| 13:1:13:ILE:HG22 | 13:1:155:ILE:HD12 | 1.70 | 0.74 |
| 4:D:229:THR:HG22 | 4:D:233:ILE:CD1 | 2.16 | 0.74 |
| 10:X:3:ILE:CD1 | 10:X:46:ALA:HB2 | 2.17 | 0.73 |
| 12:Z:-7:ASN:ND2 | 12:Z:-5:TYR:H | 1.86 | 0.73 |
| 3:Q:40:VAL:HG12 | 3:Q:162:ALA:HB1 | 1.70 | 0.73 |
| 5:S:220:PRO:O | 5:S:222:THR:HG23 | 1.88 | 0.73 |
| 7:U:59:LEU:O | 7:U:61:PRO:HD3 | 1.88 | 0.73 |
| 3:Q:70:ILE:HD13 | 3:Q:112:LEU:HD11 | 1.69 | 0.73 |
| 9:I:45:ILE:N | 9:I:45:ILE:HD12 | 2.04 | 0.73 |
| 11:K:37:ILE:HB | 11:K:41:LEU:HB3 | 1.70 | 0.73 |
| 7:U:18(A):ILE:O | 7:U:18(A):ILE:HD12 | 1.88 | 0.73 |
| 8:V:40:LYS:C | 8:V:41:ILE:HD12 | 2.09 | 0.73 |
| 5:E:15:PHE:HB2 | 6:F:23:GLN:HE22 | 1.53 | 0.73 |
| 9:I:45:ILE:HB | 9:I:52:VAL:HG13 | 1.70 | 0.73 |
| 10:J:90(A):ILE:O | 10:J:90(A):ILE:HD13 | 1.89 | 0.73 |
| 7:U:18(D):ILE:H | 7:U:18(D):ILE:HD12 | 1.53 | 0.73 |
| 2:P:39:GLY:O | 2:P:40:ILE:HD13 | 1.89 | 0.73 |
| 3:Q:70:ILE:HD11 | 3:Q:76:LEU:HB2 | 1.70 | 0.73 |
| 7:G:59:LEU:O | 7:G:61:PRO:HD3 | 1.89 | 0.72 |
| 9:I:7:THR:CG2 | 9:I:110:ILE:HD12 | 2.19 | 0.72 |
| 3:Q:164:THR:HG21 | 3:Q:172:VAL:HG13 | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:9:ASP:HA | 7:G:14:ILE:CD1 | 2.14 | 0.72 |
| 1:A:124:THR:HG22 | 2:B:130:ARG:HH21 | 1.53 | 0.72 |
| 1:O:121:GLN:O | 1:O:124:THR:HB | 1.88 | 0.72 |
| 14:2:112:THR:HG22 | 14:2:120:HIS:HB2 | 1.70 | 0.72 |
| 3:C:40:VAL:HG12 | 3:C:162:ALA:HB1 | 1.71 | 0.72 |
| 10:J:177:ILE:HD11 | 10:J:187:VAL:HG23 | 1.71 | 0.72 |
| 13:M:139:ARG:HH11 | 8:V:165:ASN:ND2 | 1.87 | 0.72 |
| 9:I:124:PHE:C | 9:I:125:ILE:HD12 | 2.09 | 0.72 |
| 13:1:-4:ILE:HD13 | 14:2:115:LEU:HB3 | 1.71 | 0.71 |
| 12:L:-7:ASN:ND2 | 12:L:-5:TYR:H | 1.88 | 0.71 |
| 7:U:18(G):GLU:HG2 | 7:U:188:LYS:CB | 2.19 | 0.71 |
| 9:W:4:VAL:CG1 | 9:W:155:ILE:HD11 | 2.20 | 0.71 |
| 10:X:3:ILE:HD11 | 10:X:46:ALA:HB2 | 1.72 | 0.71 |
| 10:J:18:LYS:HD3 | 10:J:174:ILE:HG13 | 1.71 | 0.71 |
| 13:M:203:ILE:HD13 | 14:2:30:VAL:HG21 | 1.73 | 0.71 |
| 6:F:67:ILE:HD13 | 6:F:77:VAL:HB | 1.72 | 0.71 |
| 2:P:185:LYS:HD3 | 2:P:186:VAL:N | 2.05 | 0.71 |
| 8:V:159:ILE:O | 8:V:163:ILE:HD13 | 1.90 | 0.71 |
| 4:R:161:ASN:N | 5:S:58:LEU:O | 2.21 | 0.71 |
| 6:T:193:ALA:O | 6:T:197:ILE:HD12 | 1.90 | 0.71 |
| 4:D:12(D):ALA:HB3 | 4:D:126:ARG:HD3 | 1.70 | 0.71 |
| 7:G:172:ILE:HD11 | 7:G:201:LEU:HD21 | 1.72 | 0.71 |
| 8:H:15:ALA:HB1 | 8:H:159:ILE:CD1 | 2.20 | 0.71 |
| 1:A:121:GLN:O | 1:A:124:THR:HB | 1.91 | 0.71 |
| 2:B:121:GLN:O | 2:B:124:THR:HB | 1.90 | 0.71 |
| 5:E:220:PRO:O | 5:E:222:THR:HG23 | 1.91 | 0.71 |
| 9:W:192:ARG:HG3 | 16:W:200:HOH:O | 1.89 | 0.71 |
| 14:N:12:VAL:C | 14:N:13:ILE:HD13 | 2.12 | 0.71 |
| 2:B:185:LYS:HD3 | 2:B:186:VAL:N | 2.06 | 0.70 |
| 11:Y:37:ILE:HB | 11:Y:41:LEU:HB3 | 1.73 | 0.70 |
| 13:1:4:ILE:HD11 | 13:1:155:ILE:HG23 | 1.73 | 0.70 |
| 7:U:18(A):ILE:CD1 | 7:U:18(C):HIS:O | 2.39 | 0.70 |
| 1:O:225:THR:OG1 | 1:O:228:GLU:HG3 | 1.90 | 0.70 |
| 5:S:201:LEU:HD11 | 5:S:207:LEU:HD22 | 1.73 | 0.70 |
| 7:U:40:VAL:HB | 7:U:18(D):ILE:CD1 | 2.21 | 0.70 |
| 14:2:19:ARG:CD | 14:2:26:ILE:HD12 | 2.22 | 0.70 |
| 3:Q:33:ARG:HB2 | 3:Q:33:ARG:NH1 | 2.06 | 0.70 |
| 11:K:142:TYR:O | 11:K:143:LYS:HD2 | 1.92 | 0.70 |
| 13:M:76:PRO:HD2 | 13:M:105:GLN:OE1 | 1.92 | 0.70 |
| 10:J:168:MET:HE1 | 10:X:167:PRO:HB2 | 1.74 | 0.70 |
| 7:U:217:LYS:HE3 | 7:U:217:LYS:HA | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:U:227:GLU:HG2 | 16:U:292:HOH:O | 1.92 | 0.70 |
| 12:Z:59:PHE:CD1 | 12:Z:83:ILE:HD11 | 2.27 | 0.70 |
| 11:Y:10(A):ARG:HB3 | 11:Y:10(B):LYS:HE3 | 1.74 | 0.70 |
| 6:F:193:ALA:O | 6:F:197:ILE:HD13 | 1.92 | 0.70 |
| 3:Q:163:GLN:HE22 | 3:Q:173:ARG:HE | 1.40 | 0.70 |
| 1:A:225:THR:OG1 | 1:A:228:GLU:HG3 | 1.91 | 0.69 |
| 11:K:10(A):ARG:HB3 | 11:K:10(B):LYS:HE3 | 1.72 | 0.69 |
| 6:T:49:ALA:HB1 | 6:T:197:ILE:CD1 | 2.21 | 0.69 |
| 5:E:201:LEU:HD11 | 5:E:207:LEU:HD22 | 1.73 | 0.69 |
| 14:N:112:THR:HG22 | 14:N:120:HIS:HB2 | 1.74 | 0.69 |
| 6:F:37:SER:HB3 | 6:F:50:VAL:HG23 | 1.73 | 0.69 |
| 11:Y:142:TYR:O | 11:Y:143:LYS:HD2 | 1.93 | 0.69 |
| 9:I:27:VAL:HG13 | 16:J:230:HOH:O | 1.92 | 0.69 |
| 10:J:156:LYS:O | 10:J:160:GLN:HG3 | 1.93 | 0.69 |
| 12:L:76:ILE:HD11 | 12:L:101:ILE:HD13 | 1.73 | 0.69 |
| 8:H:216:GLU:HG3 | 9:I:187:ARG:HG2 | 1.73 | 0.69 |
| 11:K:180:GLU:HB2 | 16:K:1426:HOH:O | 1.93 | 0.69 |
| 1:O:86:ARG:HE | 7:U:118:ASN:HD21 | 1.40 | 0.69 |
| 8:H:22:GLN:HG3 | 15:H:1400:BO2:H6 | 1.75 | 0.69 |
| 2:B:65:GLU:HG3 | 2:B:66:LYS:HG3 | 1.74 | 0.69 |
| 8:H:41:ILE:HD12 | 8:H:76:VAL:CG2 | 2.19 | 0.69 |
| 10:X:156:LYS:O | 10:X:160:GLN:HG3 | 1.93 | 0.69 |
| 2:B:15:PHE:N | 3:C:23:GLN:HE22 | 1.90 | 0.69 |
| 7:G:12:ILE:HD13 | 7:G:12:ILE:H | 1.57 | 0.69 |
| 7:G:217:LYS:HE3 | 7:G:217:LYS:HA | 1.73 | 0.69 |
| 5:S:45:HIS:HD2 | 5:S:214:ILE:HD11 | 1.58 | 0.69 |
| 6:T:37:SER:HB3 | 6:T:50:VAL:HG23 | 1.74 | 0.69 |
| 7:U:121:GLN:O | 7:U:124:THR:HB | 1.93 | 0.69 |
| 10:J:2:ILE:HD13 | 10:J:130:SER:OG | 1.93 | 0.69 |
| 2:P:65:GLU:HG3 | 2:P:66:LYS:HG3 | 1.74 | 0.69 |
| 13:1:19:LEU:HD21 | 13:1:26:LEU:HD22 | 1.75 | 0.68 |
| 3:C:163:GLN:HE22 | 3:C:173:ARG:HE | 1.41 | 0.68 |
| 3:C:41:LYS:HG2 | 3:C:161:SER:O | 1.93 | 0.68 |
| 5:E:15:PHE:HB2 | 6:F:23:GLN:NE2 | 2.08 | 0.68 |
| 6:F:35:THR:HG21 | 6:F:51:GLU:O | 1.93 | 0.68 |
| 14:N:159:LEU:O | 14:N:163:ILE:HD13 | 1.93 | 0.68 |
| 1:O:73:ASP:C | 1:O:74:ILE:HD12 | 2.14 | 0.68 |
| 3:Q:52:ARG:HB2 | 3:Q:209:ASN:HA | 1.75 | 0.68 |
| 8:V:37:ILE:CG2 | 8:V:63:ILE:HD12 | 2.24 | 0.68 |
| 3:C:175:PHE:O | 3:C:179:ASN:HB2 | 1.94 | 0.68 |
| 2:P:121:GLN:O | 2:P:124:THR:HB | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:T:35:THR:HG21 | 6:T:51:GLU:O | 1.94 | 0.68 |
| 8:V:22:GLN:HG3 | 15:V:1401:BO2:H6 | 1.75 | 0.68 |
| 14:2:134:ILE:HD13 | 14:2:138:CYS:SG | 2.33 | 0.68 |
| 9:W:155:ILE:O | 9:W:155:ILE:HD12 | 1.93 | 0.68 |
| 12:Z:99:THR:HG22 | 16:Z:202:HOH:O | 1.94 | 0.68 |
| 2:B:6:ARG:HG2 | 3:C:10:ARG:HH21 | 1.59 | 0.68 |
| 3:C:33:ARG:HB2 | 3:C:33:ARG:NH1 | 2.08 | 0.67 |
| 13:M:19:LEU:HD21 | 13:M:26:LEU:HD22 | 1.77 | 0.67 |
| 2:P:6:ARG:HG2 | 3:Q:10:ARG:NH2 | 2.08 | 0.67 |
| 1:A:130:ARG:HH21 | 7:G:124:THR:CG2 | 2.06 | 0.67 |
| 9:I:97:VAL:HG23 | 9:I:99:PRO:HD3 | 1.75 | 0.67 |
| 4:R:70:ILE:HD12 | 4:R:74:ILE:CG2 | 2.24 | 0.67 |
| 5:S:92:LEU:HD11 | 5:S:112:ALA:HB1 | 1.77 | 0.67 |
| 8:V:35:HIS:HB3 | 8:V:56:THR:HG21 | 1.75 | 0.67 |
| 9:W:4:VAL:HG13 | 9:W:155:ILE:HD11 | 1.75 | 0.67 |
| 8:H:165:ASN:ND2 | 13:1:139:ARG:HH11 | 1.92 | 0.67 |
| 14:2:100:ILE:HD11 | 14:2:127:ALA:HB3 | 1.77 | 0.67 |
| 2:P:4:GLY:HA3 | 5:S:127:TYR:CE1 | 2.28 | 0.67 |
| 2:B:161:LYS:HG3 | 3:C:59:GLN:O | 1.94 | 0.67 |
| 2:B:41:MET:HE3 | 16:B:240:HOH:O | 1.94 | 0.67 |
| 13:M:74:LEU:HD13 | 13:M:79:ILE:HD11 | 1.75 | 0.67 |
| 2:P:28:LEU:HD23 | 2:P:31:ILE:HD12 | 1.76 | 0.67 |
| 5:S:221:PHE:CE1 | 5:S:223:ILE:HD11 | 2.30 | 0.67 |
| 10:J:167:PRO:HB2 | 10:X:168:MET:HE1 | 1.76 | 0.67 |
| 13:1:-4:ILE:CD1 | 14:2:115:LEU:HB3 | 2.24 | 0.67 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:CG | 2.25 | 0.67 |
| 2:P:159:GLY:HA3 | 3:Q:62(A):ILE:CD1 | 2.25 | 0.67 |
| 5:S:226:GLY:O | 5:S:229:VAL:HG22 | 1.95 | 0.67 |
| 5:E:213:ALA:HB2 | 5:E:223:ILE:CD1 | 2.25 | 0.66 |
| 8:H:200:LYS:HE3 | 9:I:140:SER:O | 1.94 | 0.66 |
| 12:L:59:PHE:CD1 | 12:L:83:ILE:HD11 | 2.29 | 0.66 |
| 5:S:141:TYR:CE2 | 5:S:217:LYS:HA | 2.29 | 0.66 |
| 4:R:160:TYR:CE2 | 5:S:59:SER:HB3 | 2.29 | 0.66 |
| 9:W:97:VAL:HG23 | 9:W:99:PRO:HD3 | 1.76 | 0.66 |
| 5:E:67:ILE:CD1 | 5:E:77:SER:HB3 | 2.26 | 0.66 |
| 3:C:226:SER:HB2 | 3:C:227:GLU:OE1 | 1.95 | 0.66 |
| 2:P:97:GLN:HE22 | 9:W:64:ASN:HD22 | 1.42 | 0.66 |
| 8:H:35:HIS:HB3 | 8:H:56:THR:HG21 | 1.75 | 0.66 |
| 9:I:110:ILE:N | 9:I:110:ILE:HD13 | 2.08 | 0.66 |
| 3:Q:226:SER:HB2 | 3:Q:227:GLU:OE1 | 1.96 | 0.66 |
| 14:2:13:ILE:HG12 | 14:2:177:VAL:HG13 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:194:LEU:HD21 | 4:D:233:ILE:HD12 | 1.77 | 0.66 |
| 5:E:213:ALA:CB | 5:E:223:ILE:HD12 | 2.22 | 0.66 |
| 13:M:41:THR:OG1 | 13:M:76:PRO:HG3 | 1.95 | 0.66 |
| 13:M:203:ILE:HD13 | 14:2:30:VAL:CG2 | 2.26 | 0.66 |
| 2:B:181:LYS:O | 2:B:184:MET:HG3 | 1.95 | 0.66 |
| 8:V:38:SER:HG | 8:V:41:ILE:HD13 | 1.60 | 0.66 |
| 3:C:52:ARG:HB2 | 3:C:209:ASN:HA | 1.78 | 0.66 |
| 5:S:18(C):PHE:HA | 5:S:18(F):ILE:HG12 | 1.78 | 0.66 |
| 5:S:221:PHE:CZ | 5:S:223:ILE:HD11 | 2.30 | 0.66 |
| 4:D:229:THR:O | 4:D:233:ILE:CD1 | 2.42 | 0.66 |
| 9:I:104:ILE:HD11 | 9:I:178:ILE:HG22 | 1.78 | 0.66 |
| 2:B:97:GLN:NE2 | 9:I:64:ASN:HD22 | 1.92 | 0.66 |
| 4:D:192:LEU:O | 4:D:196:ILE:HD13 | 1.96 | 0.65 |
| 5:E:221:PHE:CE1 | 5:E:223:ILE:HD11 | 2.31 | 0.65 |
| 14:N:126:ILE:HD13 | 14:N:126:ILE:H | 1.59 | 0.65 |
| 2:P:101:LYS:NZ | 10:X:85:GLN:NE2 | 2.43 | 0.65 |
| 4:R:156:THR:HG22 | 5:S:83:PRO:HD3 | 1.77 | 0.65 |
| 14:2:126:ILE:H | 14:2:126:ILE:HD13 | 1.62 | 0.65 |
| 3:C:206:GLY:HA3 | 3:C:209:ASN:HB2 | 1.78 | 0.65 |
| 6:F:237:GLN:O | 6:F:240:ILE:HG22 | 1.96 | 0.65 |
| 2:P:159:GLY:HA3 | 3:Q:62(A):ILE:HD11 | 1.79 | 0.65 |
| 3:Q:172:VAL:HG23 | 3:Q:196:SER:HB2 | 1.78 | 0.65 |
| 5:E:141:TYR:CE2 | 5:E:217:LYS:HA | 2.31 | 0.65 |
| 3:Q:33:ARG:HH11 | 3:Q:33:ARG:CB | 2.09 | 0.65 |
| 6:T:237:GLN:O | 6:T:240:ILE:HG22 | 1.95 | 0.65 |
| 8:V:196:VAL:HG23 | 16:V:1418:HOH:O | 1.95 | 0.65 |
| 8:H:167:LEU:HB3 | 12:Z:167:ILE:HD13 | 1.78 | 0.65 |
| 5:E:139:ILE:HD11 | 5:E:221:PHE:CE2 | 2.28 | 0.65 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:CG | 2.25 | 0.65 |
| 2:P:15:PHE:H | 3:Q:23:GLN:HE22 | 1.43 | 0.65 |
| 13:1:-3:VAL:CG1 | 13:1:49:ILE:HD12 | 2.26 | 0.65 |
| 12:Z:76:ILE:HD11 | 12:Z:101:ILE:HD13 | 1.78 | 0.65 |
| 2:B:163:ILE:HG12 | 2:B:164:SER:H | 1.61 | 0.65 |
| 2:B:147:GLN:HG2 | 3:C:62(A):ILE:HD13 | 1.78 | 0.65 |
| 12:L:148:VAL:O | 12:L:152:ILE:HG12 | 1.95 | 0.65 |
| 5:S:18(D):ILE:HD13 | 5:S:18(D):ILE:O | 1.96 | 0.65 |
| 2:B:213:ALA:HB2 | 2:B:223:ILE:HD13 | 1.79 | 0.65 |
| 5:E:221:PHE:CZ | 5:E:223:ILE:HD11 | 2.31 | 0.65 |
| 6:F:69:VAL:HG12 | 16:F:248:HOH:O | 1.97 | 0.65 |
| 8:V:216:GLU:HG3 | 9:W:187:ARG:HG2 | 1.79 | 0.65 |
| 3:C:14:ILE:H | 3:C:14:ILE:HD13 | 1.61 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:232:ILE:HD13 | 2:B:232:ILE:O | 1.96 | 0.65 |
| 2:B:8:TYR:CE2 | 7:G:12:ILE:HD12 | 2.32 | 0.65 |
| 13:1:41:THR:OG1 | 13:1:76:PRO:HG3 | 1.96 | 0.64 |
| 7:G:96:ALA:CA | 7:G:107:MET:HE2 | 2.25 | 0.64 |
| 5:E:226:GLY:O | 5:E:229:VAL:HG22 | 1.97 | 0.64 |
| 5:E:2(B):THR:H | 5:E:2(E):ASN:HD22 | 1.44 | 0.64 |
| 7:G:12:ILE:HG12 | 7:G:14:ILE:HD12 | 1.79 | 0.64 |
| 7:G:8:TYR:O | 7:G:12:ILE:HD13 | 1.97 | 0.64 |
| 9:I:104:ILE:HD13 | 9:I:181:LYS:N | 2.12 | 0.64 |
| 9:I:33:LYS:O | 9:I:44:GLY:HA2 | 1.98 | 0.64 |
| 9:I:45:ILE:N | 9:I:45:ILE:CD1 | 2.61 | 0.64 |
| 6:T:173:LYS:O | 6:T:177:GLU:HG3 | 1.97 | 0.64 |
| 4:D:45:GLY:HA2 | 4:D:146:TYR:CE1 | 2.32 | 0.64 |
| 5:S:74:MET:HE1 | 5:S:96:CYS:SG | 2.38 | 0.64 |
| 10:J:-1:MET:HG2 | 10:J:1:ASP:H | 1.62 | 0.64 |
| 2:P:163:ILE:HG12 | 2:P:164:SER:N | 2.12 | 0.64 |
| 2:P:163:ILE:HG12 | 2:P:164:SER:H | 1.61 | 0.64 |
| 10:X:10(B):LYS:NZ | 10:X:10(B):LYS:HB2 | 2.13 | 0.64 |
| 4:D:196:ILE:N | 4:D:196:ILE:CD1 | 2.60 | 0.64 |
| 6:F:173:LYS:O | 6:F:177:GLU:HG3 | 1.97 | 0.64 |
| 2:B:186:VAL:HG21 | 2:B:216:ARG:HD3 | 1.80 | 0.64 |
| 10:J:68:ILE:HG12 | 16:J:227:HOH:O | 1.98 | 0.64 |
| 11:K:7:ARG:HG3 | 11:K:12:ILE:HD13 | 1.78 | 0.64 |
| 14:N:146:MET:HE3 | 14:N:150:GLU:HB3 | 1.79 | 0.64 |
| 7:U:87:ASN:HD22 | 7:U:87:ASN:C | 1.99 | 0.64 |
| 1:A:130:ARG:HH21 | 7:G:124:THR:HG22 | 1.62 | 0.64 |
| 1:O:71:THR:OG1 | 1:O:74:ILE:CD1 | 2.46 | 0.64 |
| 5:S:207:LEU:H | 5:S:207:LEU:CD2 | 2.10 | 0.64 |
| 7:U:34(A):ASN:HD22 | 7:U:167:PRO:HG2 | 1.63 | 0.64 |
| 8:V:34:LEU:HB2 | 16:V:1415:HOH:O | 1.98 | 0.64 |
| 1:A:33:GLN:HA | 1:A:33:GLN:HE21 | 1.63 | 0.64 |
| 2:B:149:TYR:CZ | 3:C:62(A):ILE:HD12 | 2.33 | 0.64 |
| 2:B:163:ILE:HG12 | 2:B:164:SER:N | 2.13 | 0.64 |
| 2:B:219:GLU:HG2 | 2:B:21(E):VAL:N | 2.13 | 0.64 |
| 1:A:179:ARG:HB3 | 1:A:179:ARG:HH11 | 1.63 | 0.63 |
| 5:S:75:GLY:HA3 | 5:S:221:PHE:CE2 | 2.32 | 0.63 |
| 12:Z:59:PHE:CG | 12:Z:83:ILE:HD11 | 2.33 | 0.63 |
| 7:G:87:ASN:HD22 | 7:G:87:ASN:C | 2.02 | 0.63 |
| 10:J:168:MET:HE3 | 10:X:168:MET:HE3 | 1.80 | 0.63 |
| 9:W:33:LYS:O | 9:W:44:GLY:HA2 | 1.98 | 0.63 |
| 4:D:186:LEU:O | 4:D:190:GLU:HG3 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:92:LEU:HD11 | 5:E:112:ALA:HB1 | 1.79 | 0.63 |
| 9:I:110:ILE:HD11 | 9:I:122:ALA:O | 1.98 | 0.63 |
| 3:C:40:VAL:HG12 | 3:C:162:ALA:CB | 2.28 | 0.63 |
| 6:F:20(B):GLU:HG3 | 6:F:20(C):LYS:HG3 | 1.80 | 0.63 |
| 2:P:219:GLU:HG2 | 2:P:21(E):VAL:N | 2.12 | 0.63 |
| 3:Q:175:PHE:O | 3:Q:179:ASN:HB2 | 1.97 | 0.63 |
| 7:U:148:ILE:N | 7:U:148:ILE:HD12 | 2.12 | 0.63 |
| 14:2:175:MET:HB2 | 14:2:187:LEU:HB2 | 1.79 | 0.63 |
| 2:B:77:ALA:HB3 | 2:B:137:ILE:HB | 1.80 | 0.63 |
| 3:C:33:ARG:CB | 3:C:33:ARG:HH11 | 2.11 | 0.63 |
| 7:G:151:THR:HG22 | 7:G:157:TYR:CB | 2.29 | 0.63 |
| 7:U:39:ALA:HB2 | 7:U:48:VAL:HG12 | 1.81 | 0.63 |
| 14:2:44:CYS:HB2 | 14:2:100:ILE:HB | 1.80 | 0.63 |
| 6:F:38:ILE:HG22 | 6:F:164:ALA:HB2 | 1.79 | 0.63 |
| 6:T:40:ILE:HD12 | 6:T:193:ALA:HB2 | 1.80 | 0.63 |
| 11:Y:210:ILE:HD12 | 16:Y:1432:HOH:O | 1.97 | 0.63 |
| 11:Y:66:HIS:HA | 16:Y:1433:HOH:O | 1.97 | 0.63 |
| 14:N:175:MET:HB2 | 14:N:187:LEU:HB2 | 1.79 | 0.63 |
| 4:R:186:LEU:O | 4:R:190:GLU:HG3 | 1.99 | 0.63 |
| 7:U:41:ARG:CG | 7:U:148:ILE:CD1 | 2.77 | 0.63 |
| 11:Y:180:GLU:N | 16:Y:1428:HOH:O | 2.19 | 0.63 |
| 13:1:13:ILE:CD1 | 13:1:177:ILE:HG12 | 2.21 | 0.63 |
| 3:C:160:TRP:CE2 | 4:D:59:LEU:HD23 | 2.34 | 0.63 |
| 5:E:207:LEU:CD2 | 5:E:207:LEU:H | 2.11 | 0.63 |
| 5:E:67:ILE:HD13 | 5:E:77:SER:HB3 | 1.80 | 0.63 |
| 2:P:181:LYS:O | 2:P:184:MET:HG3 | 1.98 | 0.63 |
| 2:P:186:VAL:HG21 | 2:P:216:ARG:HD3 | 1.81 | 0.63 |
| 2:P:6:ARG:HD2 | 4:R:9:ASP:N | 2.14 | 0.63 |
| 3:Q:41:LYS:HG2 | 3:Q:161:SER:O | 1.98 | 0.63 |
| 3:C:172:VAL:HG23 | 3:C:196:SER:HB2 | 1.80 | 0.63 |
| 7:G:121:GLN:O | 7:G:124:THR:HB | 1.98 | 0.63 |
| 12:L:59:PHE:CG | 12:L:83:ILE:HD11 | 2.34 | 0.63 |
| 1:O:177:GLU:HG2 | 2:P:58:LEU:HD21 | 1.80 | 0.63 |
| 3:Q:206:GLY:HA3 | 3:Q:209:ASN:HB2 | 1.79 | 0.63 |
| 3:Q:160:TRP:CE2 | 4:R:59:LEU:HD23 | 2.34 | 0.63 |
| 4:R:102:TYR:O | 12:Z:81:ARG:HG3 | 1.98 | 0.63 |
| 8:H:35:HIS:CB | 8:H:56:THR:HG21 | 2.29 | 0.62 |
| 14:N:131:SER:HA | 14:N:134:ILE:CD1 | 2.28 | 0.62 |
| 2:P:70:LEU:HD21 | 2:P:89:ILE:HD12 | 1.80 | 0.62 |
| 5:S:213:ALA:HB2 | 5:S:223:ILE:CD1 | 2.25 | 0.62 |
| 6:T:38:ILE:HG22 | 6:T:164:ALA:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:W:104:ILE:CD1 | 9:W:104:ILE:N | 2.61 | 0.62 |
| 12:Z:83:ILE:HD13 | 12:Z:86:LEU:HD12 | 1.81 | 0.62 |
| 14:N:44:CYS:HB2 | 14:N:100:ILE:HB | 1.80 | 0.62 |
| 4:R:31:ILE:HD11 | 4:R:134:VAL:N | 2.14 | 0.62 |
| 13:M:139:ARG:NH1 | 8:V:165:ASN:HD22 | 1.94 | 0.62 |
| 2:B:219:GLU:HG2 | 2:B:21(E):VAL:H | 1.64 | 0.62 |
| 4:D:102:TYR:O | 12:L:81:ARG:HG3 | 1.99 | 0.62 |
| 13:M:4:ILE:HG13 | 13:M:155:ILE:HD12 | 1.81 | 0.62 |
| 1:O:27:ALA:O | 1:O:31:VAL:HG23 | 1.99 | 0.62 |
| 2:P:76:VAL:HG21 | 2:P:89:ILE:HD11 | 1.81 | 0.62 |
| 8:V:35:HIS:CB | 8:V:56:THR:HG21 | 2.28 | 0.62 |
| 7:G:34(A):ASN:HD22 | 7:G:167:PRO:HG2 | 1.64 | 0.62 |
| 8:H:173:VAL:HB | 8:H:192:LEU:HB2 | 1.81 | 0.62 |
| 12:L:-9:GLN:HE21 | 13:M:-8:THR:HG21 | 1.64 | 0.62 |
| 4:R:177:LEU:HA | 5:S:58:LEU:HD11 | 1.81 | 0.62 |
| 13:1:13:ILE:HD11 | 13:1:177:ILE:HG23 | 1.82 | 0.62 |
| 14:2:13:ILE:HD12 | 14:2:151:THR:CG2 | 2.30 | 0.62 |
| 1:O:179:ARG:HH11 | 1:O:179:ARG:HB3 | 1.65 | 0.62 |
| 1:O:33:GLN:HA | 1:O:33:GLN:HE21 | 1.63 | 0.62 |
| 3:Q:55:THR:HG22 | 3:Q:56:LEU:HD22 | 1.82 | 0.62 |
| 5:S:143:LYS:HE3 | 16:1:254:HOH:O | 1.99 | 0.62 |
| 10:J:10(B):LYS:HB2 | 10:J:10(B):LYS:NZ | 2.14 | 0.62 |
| 2:P:219:GLU:HG2 | 2:P:21(E):VAL:H | 1.65 | 0.62 |
| 7:U:41:ARG:CG | 7:U:148:ILE:HD11 | 2.29 | 0.62 |
| 14:2:126:ILE:N | 14:2:126:ILE:HD13 | 2.15 | 0.62 |
| 2:B:124:THR:HG22 | 3:C:130:ARG:NH2 | 2.03 | 0.62 |
| 2:P:77:ALA:HB3 | 2:P:137:ILE:HB | 1.80 | 0.62 |
| 3:Q:41:LYS:HD3 | 3:Q:161:SER:HA | 1.82 | 0.62 |
| 5:S:2(B):THR:H | 5:S:2(E):ASN:HD22 | 1.45 | 0.62 |
| 8:H:10:ASN:OD1 | 8:H:180:ILE:HD12 | 1.98 | 0.62 |
| 5:E:15:PHE:H | 6:F:23:GLN:NE2 | 1.98 | 0.62 |
| 5:E:75:GLY:HA3 | 5:E:221:PHE:CE2 | 2.34 | 0.62 |
| 12:L:33:LYS:HD2 | 12:L:46:ASN:ND2 | 2.15 | 0.62 |
| 2:P:6:ARG:HG2 | 3:Q:10:ARG:HH21 | 1.63 | 0.62 |
| 3:Q:70:ILE:HD13 | 3:Q:112:LEU:CD1 | 2.29 | 0.62 |
| 2:B:14:ILE:H | 2:B:14:ILE:HD13 | 1.65 | 0.62 |
| 2:B:6:ARG:HG2 | 3:C:10:ARG:NH2 | 2.15 | 0.62 |
| 3:C:41:LYS:HD3 | 3:C:161:SER:HA | 1.81 | 0.62 |
| 11:K:191:ASP:OD2 | 11:K:193:GLY:N | 2.32 | 0.62 |
| 5:S:207:LEU:N | 5:S:207:LEU:HD23 | 2.14 | 0.62 |
| 2:P:97:GLN:NE2 | 9:W:64:ASN:HD22 | 1.97 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:179:ARG:HB3 | 1:A:179:ARG:NH1 | 2.15 | 0.61 |
| 3:Q:40:VAL:HG12 | 3:Q:162:ALA:CB | 2.29 | 0.61 |
| 4:R:45:GLY:HA2 | 4:R:146:TYR:CE1 | 2.34 | 0.61 |
| 10:X:7:ARG:HG2 | 10:X:7:ARG:HH11 | 1.65 | 0.61 |
| 5:E:213:ALA:CB | 5:E:223:ILE:CD1 | 2.78 | 0.61 |
| 7:G:39:ALA:HB2 | 7:G:48:VAL:HG12 | 1.81 | 0.61 |
| 10:J:133:TYR:HE1 | 16:X:221:HOH:O | 1.83 | 0.61 |
| 7:G:86:ARG:HD2 | 16:G:257:HOH:O | 2.00 | 0.61 |
| 6:T:35:THR:HG23 | 6:T:51:GLU:HB3 | 1.82 | 0.61 |
| 8:V:173:VAL:HB | 8:V:192:LEU:HB2 | 1.83 | 0.61 |
| 3:C:35:THR:HB | 3:C:51:GLU:HG3 | 1.82 | 0.61 |
| 4:R:67:ILE:HD12 | 4:R:211:GLN:HE21 | 1.65 | 0.61 |
| 12:Z:-6:PRO:O | 13:1:91:ARG:NH1 | 2.32 | 0.61 |
| 13:M:167:ALA:HB2 | 14:2:26:ILE:CD1 | 2.30 | 0.61 |
| 5:S:213:ALA:CB | 5:S:223:ILE:CD1 | 2.78 | 0.61 |
| 7:U:107:MET:HE3 | 7:U:112:LEU:HB2 | 1.82 | 0.61 |
| 1:A:27:ALA:O | 1:A:31:VAL:HG23 | 2.00 | 0.61 |
| 2:B:141:TYR:CD1 | 2:B:21(E):VAL:HG21 | 2.34 | 0.61 |
| 3:C:55:THR:HG22 | 3:C:56:LEU:HD22 | 1.81 | 0.61 |
| 7:U:151:THR:HG22 | 7:U:157:TYR:CB | 2.31 | 0.61 |
| 7:U:8:TYR:C | 7:U:10:ARG:H | 2.04 | 0.61 |
| 10:X:-1:MET:HG2 | 10:X:1:ASP:H | 1.64 | 0.61 |
| 4:R:160:TYR:HA | 5:S:59:SER:HA | 1.83 | 0.61 |
| 5:S:74:MET:CE | 5:S:96:CYS:SG | 2.88 | 0.61 |
| 10:X:143:ARG:HG2 | 10:X:143:ARG:HH11 | 1.66 | 0.61 |
| 2:B:149:TYR:OH | 3:C:62(A):ILE:HB | 2.01 | 0.61 |
| 5:E:207:LEU:HD23 | 5:E:207:LEU:N | 2.15 | 0.61 |
| 9:I:2:ILE:HG21 | 9:I:130:ALA:HB3 | 1.83 | 0.61 |
| 9:I:6:MET:HE3 | 9:I:155:ILE:HG13 | 1.81 | 0.61 |
| 12:L:99:THR:HG23 | 12:L:113:PHE:HB2 | 1.82 | 0.61 |
| 6:T:203:GLU:O | 6:T:206:LYS:HD2 | 2.01 | 0.61 |
| 14:2:107:LYS:HG2 | 14:2:108:GLY:H | 1.64 | 0.60 |
| 12:L:114:ASP:HB2 | 12:L:118:SER:HB3 | 1.82 | 0.60 |
| 12:Z:114:ASP:HB2 | 12:Z:118:SER:HB3 | 1.83 | 0.60 |
| 14:2:146:MET:HE3 | 14:2:150:GLU:HB3 | 1.80 | 0.60 |
| 6:F:35:THR:HG23 | 6:F:51:GLU:HB3 | 1.82 | 0.60 |
| 6:T:20(B):GLU:HG3 | 6:T:20(C):LYS:HG3 | 1.82 | 0.60 |
| 6:T:197:ILE:HD13 | 6:T:210:LEU:CD1 | 2.31 | 0.60 |
| 12:Z:134:ILE:HD11 | 12:Z:158:SER:O | 2.00 | 0.60 |
| 5:E:139:ILE:CD1 | 5:E:139:ILE:H | 2.13 | 0.60 |
| 8:V:112:SER:HB3 | 8:V:125:LEU:HD13 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:1:-4:ILE:HD12 | 14:2:116:GLY:CA | 2.32 | 0.60 |
| 14:2:49:ALA:HA | 16:2:1423:HOH:O | 1.99 | 0.60 |
| 12:L:7:ALA:HB2 | 12:L:110:VAL:HG23 | 1.84 | 0.60 |
| 9:W:2:ILE:HG21 | 9:W:130:ALA:HB3 | 1.82 | 0.60 |
| 10:X:133:TYR:CE2 | 10:X:166:MET:HG3 | 2.35 | 0.60 |
| 12:Z:7:ALA:HB2 | 12:Z:110:VAL:HG23 | 1.83 | 0.60 |
| 5:E:73:HIS:HE1 | 5:E:107:LEU:O | 1.84 | 0.60 |
| 14:N:107:LYS:HG2 | 14:N:108:GLY:H | 1.66 | 0.60 |
| 2:P:141:TYR:CD1 | 2:P:21(E):VAL:HG21 | 2.36 | 0.60 |
| 2:B:215:ILE:HD12 | 2:B:221:GLN:HA | 1.84 | 0.60 |
| 7:G:212:VAL:HB | 7:G:229:ILE:HD11 | 1.84 | 0.60 |
| 3:Q:35:THR:HB | 3:Q:51:GLU:HG3 | 1.82 | 0.60 |
| 5:S:213:ALA:CB | 5:S:223:ILE:HD12 | 2.28 | 0.60 |
| 11:K:104:TYR:CD1 | 11:K:180:GLU:HG3 | 2.36 | 0.60 |
| 12:L:98:HIS:HD2 | 16:L:199:HOH:O | 1.82 | 0.60 |
| 1:O:179:ARG:NH1 | 1:O:179:ARG:HB3 | 2.16 | 0.60 |
| 3:Q:14:ILE:O | 3:Q:21:ILE:HD13 | 2.01 | 0.60 |
| 6:T:69:VAL:HG12 | 16:T:261:HOH:O | 2.02 | 0.60 |
| 7:U:41:ARG:HG2 | 7:U:148:ILE:CD1 | 2.31 | 0.60 |
| 7:U:35:ILE:HG23 | 7:U:51:GLN:HB2 | 1.84 | 0.60 |
| 5:E:210:LEU:HD22 | 5:E:233:ILE:HD11 | 1.84 | 0.60 |
| 7:G:131:PRO:HB3 | 16:G:244:HOH:O | 2.00 | 0.60 |
| 9:I:48:LEU:HG | 9:I:50:THR:HG22 | 1.84 | 0.60 |
| 13:M:14(D):GLU:O | 13:M:14(G):ILE:HG12 | 2.01 | 0.60 |
| 14:N:18(G):TYR:HA | 14:N:18(J):LEU:HG | 1.84 | 0.60 |
| 7:U:18(D):ILE:HD12 | 7:U:18(D):ILE:N | 2.16 | 0.60 |
| 8:V:200:LYS:HE3 | 9:W:140:SER:O | 2.02 | 0.60 |
| 11:Y:104:TYR:CD1 | 11:Y:180:GLU:HG3 | 2.36 | 0.60 |
| 11:Y:7:ARG:HD2 | 11:Y:108:PRO:O | 2.02 | 0.60 |
| 15:2:1405:BO2:H241 | 16:2:1423:HOH:O | 2.02 | 0.59 |
| 2:B:101:LYS:HG3 | 9:I:57:GLU:HB3 | 1.84 | 0.59 |
| 4:D:12(G):GLU:HG2 | 4:D:125:GLU:H | 1.66 | 0.59 |
| 7:G:8:TYR:C | 7:G:10:ARG:H | 2.04 | 0.59 |
| 11:K:208:ASN:HD21 | 9:W:29:ASN:HD21 | 1.50 | 0.59 |
| 14:N:126:ILE:HD13 | 14:N:126:ILE:N | 2.16 | 0.59 |
| 14:N:8:PHE:CE1 | 14:N:10:ASP:HB2 | 2.37 | 0.59 |
| 4:R:159:ARG:HB3 | 5:S:60:SER:HB3 | 1.84 | 0.59 |
| 5:S:73:HIS:HE1 | 5:S:107:LEU:O | 1.85 | 0.59 |
| 7:U:148:ILE:N | 7:U:148:ILE:CD1 | 2.65 | 0.59 |
| 4:D:45:GLY:HA2 | 4:D:146:TYR:CD1 | 2.37 | 0.59 |
| 11:K:20:ALA:HB2 | 11:K:31:VAL:HG21 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 12:L:134:ILE:HD11 | 12:L:158:SER:O | 2.02 | 0.59 |
| 12:L:83:ILE:HD13 | 12:L:86:LEU:HD12 | 1.83 | 0.59 |
| 4:R:159:ARG:O | 5:S:60:SER:N | 2.35 | 0.59 |
| 7:U:18(A):ILE:CD1 | 7:U:18(C):HIS:H | 2.11 | 0.59 |
| 10:X:2:ILE:O | 10:X:3:ILE:HD12 | 2.01 | 0.59 |
| 13:1:14(D):GLU:O | 13:1:14(G):ILE:HG12 | 2.02 | 0.59 |
| 7:G:152:ASP:HB2 | 7:G:153:PRO:CD | 2.33 | 0.59 |
| 13:M:7:LYS:HG3 | 13:M:14(G):ILE:HD12 | 1.83 | 0.59 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:HG3 | 1.85 | 0.59 |
| 11:Y:10(A):ARG:H | 11:Y:10(B):LYS:HZ2 | 1.50 | 0.59 |
| 14:2:174:ARG:HG2 | 14:2:18(A):ILE:CD1 | 2.32 | 0.59 |
| 5:S:97:ASN:HD21 | 12:Z:61:ASN:HD21 | 1.48 | 0.59 |
| 7:U:18(A):ILE:C | 7:U:18(A):ILE:HD12 | 2.21 | 0.59 |
| 12:Z:3:ILE:HG13 | 12:Z:100:ILE:HD13 | 1.85 | 0.59 |
| 4:D:67:ILE:HD12 | 4:D:211:GLN:HE21 | 1.67 | 0.59 |
| 12:L:-6:PRO:O | 13:M:91:ARG:NH1 | 2.32 | 0.59 |
| 13:M:-4:ILE:HD12 | 14:N:116:GLY:CA | 2.32 | 0.59 |
| 3:Q:185:THR:HG22 | 3:Q:187:GLU:N | 2.15 | 0.59 |
| 1:O:58:LEU:HB3 | 7:U:162:ALA:O | 2.03 | 0.59 |
| 8:V:114:HIS:CE1 | 15:2:1405:BO2:H5 | 2.38 | 0.59 |
| 1:A:4:MET:SD | 1:A:5:THR:N | 2.64 | 0.59 |
| 7:U:96:ALA:CA | 7:U:107:MET:HE2 | 2.31 | 0.59 |
| 14:2:8:PHE:CE1 | 14:2:10:ASP:HB2 | 2.38 | 0.59 |
| 3:C:185:THR:HG22 | 3:C:187:GLU:N | 2.16 | 0.59 |
| 11:K:10(A):ARG:H | 11:K:10(B):LYS:NZ | 2.01 | 0.59 |
| 4:R:12(G):GLU:HG2 | 4:R:125:GLU:H | 1.67 | 0.59 |
| 5:S:194:VAL:HG13 | 5:S:207:LEU:HD11 | 1.85 | 0.59 |
| 2:B:185:LYS:HD2 | 2:B:187:ASP:H | 1.66 | 0.59 |
| 7:G:186:TRP:O | 7:G:190:VAL:HG23 | 2.03 | 0.59 |
| 11:Y:20:ALA:HB2 | 11:Y:31:VAL:HG21 | 1.84 | 0.59 |
| 8:H:112:SER:HB3 | 8:H:125:LEU:HD13 | 1.85 | 0.58 |
| 6:F:175:GLU:HB3 | 6:F:196:ILE:HD12 | 1.85 | 0.58 |
| 9:I:110:ILE:CD1 | 9:I:110:ILE:N | 2.66 | 0.58 |
| 11:K:208:ASN:ND2 | 9:W:29:ASN:HD21 | 2.01 | 0.58 |
| 13:1:179:ASP:HB3 | 13:1:18(A):THR:OG1 | 2.04 | 0.58 |
| 10:J:2:ILE:CD1 | 10:J:130:SER:OG | 2.51 | 0.58 |
| 1:O:159:PRO:O | 2:P:59:LEU:HD12 | 2.03 | 0.58 |
| 4:R:31:ILE:HD12 | 4:R:79:SER:O | 2.03 | 0.58 |
| 1:A:69:LEU:HD23 | 1:A:69:LEU:C | 2.23 | 0.58 |
| 3:C:158:SER:HB2 | 4:D:59:LEU:HD21 | 1.83 | 0.58 |
| 6:F:203:GLU:O | 6:F:206:LYS:HD2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:2:40:LYS:O | 14:2:41:ILE:HD13 | 2.03 | 0.58 |
| 1:A:86:ARG:HE | 7:G:118:ASN:HD21 | 1.49 | 0.58 |
| 9:I:29:ASN:HD21 | 11:Y:208:ASN:HD21 | 1.51 | 0.58 |
| 10:J:7:ARG:HG2 | 10:J:7:ARG:HH11 | 1.68 | 0.58 |
| 4:D:59:LEU:HD11 | 4:D:64:ILE:HD11 | 1.85 | 0.58 |
| 7:U:152:ASP:HB2 | 7:U:153:PRO:CD | 2.34 | 0.58 |
| 13:1:7:LYS:HG3 | 13:1:14(G):ILE:HD12 | 1.84 | 0.58 |
| 9:I:104:ILE:CD1 | 9:I:178:ILE:HG22 | 2.33 | 0.58 |
| 13:M:19:LEU:HB2 | 13:M:170:SER:HB2 | 1.86 | 0.58 |
| 9:W:48:LEU:HG | 9:W:50:THR:HG22 | 1.85 | 0.58 |
| 14:2:19:ARG:HD3 | 14:2:26:ILE:CD1 | 2.34 | 0.58 |
| 2:B:152:ASN:HB2 | 2:B:153:PRO:HD2 | 1.85 | 0.58 |
| 10:J:-1:MET:HG2 | 10:J:1:ASP:N | 2.18 | 0.58 |
| 1:O:69:LEU:HD23 | 1:O:69:LEU:C | 2.23 | 0.58 |
| 2:P:185:LYS:HD2 | 2:P:187:ASP:H | 1.67 | 0.58 |
| 2:P:38:ILE:HD12 | 2:P:197:LEU:HG | 1.86 | 0.58 |
| 4:R:177:LEU:HD22 | 5:S:58:LEU:HD13 | 1.85 | 0.58 |
| 7:U:72:ARG:HB2 | 7:U:72:ARG:NH1 | 2.19 | 0.58 |
| 8:V:148:LYS:O | 8:V:152:ILE:HG12 | 2.03 | 0.58 |
| 11:K:75:SER:HB2 | 11:K:106:GLU:OE2 | 2.04 | 0.58 |
| 12:Z:-7:ASN:HD22 | 12:Z:-7:ASN:C | 2.07 | 0.58 |
| 2:B:214:THR:O | 2:B:215:ILE:HD13 | 2.04 | 0.58 |
| 11:K:10(A):ARG:HG2 | 11:K:10(A):ARG:HH11 | 1.69 | 0.58 |
| 4:R:70:ILE:HD12 | 4:R:74:ILE:HG22 | 1.85 | 0.58 |
| 5:S:132:TYR:O | 5:S:153:PRO:HB3 | 2.03 | 0.58 |
| 6:T:175:GLU:HB3 | 6:T:196:ILE:HD12 | 1.84 | 0.58 |
| 2:B:202:THR:HG22 | 2:B:204:SER:N | 2.07 | 0.57 |
| 4:D:177:LEU:HD13 | 5:E:58:LEU:HD11 | 1.85 | 0.57 |
| 11:Y:191:ASP:OD2 | 11:Y:193:GLY:N | 2.37 | 0.57 |
| 5:E:194:VAL:HG13 | 5:E:207:LEU:HD11 | 1.86 | 0.57 |
| 7:U:86:ARG:HD2 | 16:U:249:HOH:O | 2.02 | 0.57 |
| 3:C:241:GLN:C | 3:C:243:GLN:H | 2.07 | 0.57 |
| 2:P:239:THR:HG22 | 2:P:239:THR:OXT | 2.03 | 0.57 |
| 2:P:121:GLN:HG3 | 3:Q:83:ALA:HB1 | 1.86 | 0.57 |
| 12:Z:99:THR:HG23 | 12:Z:113:PHE:HB2 | 1.85 | 0.57 |
| 3:C:168:ASN:HB2 | 3:C:200:VAL:HG11 | 1.86 | 0.57 |
| 5:E:207:LEU:HA | 5:E:2(E):ASN:ND2 | 2.19 | 0.57 |
| 12:L:42:VAL:HG23 | 12:L:102:ALA:HB3 | 1.87 | 0.57 |
| 12:L:173:LEU:HG | 12:L:175:ILE:HD11 | 1.86 | 0.57 |
| 6:T:95:GLU:CG | 6:T:115:ARG:HB3 | 2.34 | 0.57 |
| 11:Y:143:LYS:HB2 | 11:Y:146:LEU:HD13 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 10:J:133:TYR:CE2 | 10:J:166:MET:HG3 | 2.39 | 0.57 |
| 13:M:14(C):ARG:CG | 13:M:14(C):ARG:HH11 | 2.15 | 0.57 |
| 2:P:225:LYS:HG3 | 2:P:228:GLU:OE1 | 2.04 | 0.57 |
| 3:Q:186:VAL:O | 3:Q:190:VAL:HG23 | 2.04 | 0.57 |
| 3:Q:168:ASN:HB2 | 3:Q:200:VAL:HG11 | 1.85 | 0.57 |
| 5:S:139:ILE:HD12 | 5:S:215:VAL:HG12 | 1.87 | 0.57 |
| 7:U:186:TRP:O | 7:U:190:VAL:HG23 | 2.04 | 0.57 |
| 14:N:36:ARG:HG3 | 14:N:42:TRP:CE2 | 2.39 | 0.57 |
| 2:P:152:ASN:HB2 | 2:P:153:PRO:HD2 | 1.86 | 0.57 |
| 8:V:37:ILE:HD13 | 8:V:56:THR:O | 2.05 | 0.57 |
| 9:W:84:SER:OG | 9:W:119:ILE:HD11 | 2.05 | 0.57 |
| 9:W:84:SER:CB | 9:W:119:ILE:HD11 | 2.35 | 0.57 |
| 14:2:10(B):LYS:C | 14:2:10(B):LYS:HD3 | 2.25 | 0.57 |
| 3:Q:33:ARG:HH11 | 3:Q:33:ARG:HB2 | 1.69 | 0.57 |
| 5:S:201:LEU:O | 5:S:202:ARG:HB2 | 2.03 | 0.57 |
| 10:X:44:SER:OG | 10:X:100:LEU:HB2 | 2.04 | 0.57 |
| 14:2:172:VAL:HG21 | 14:2:18(A):ILE:HD11 | 1.87 | 0.57 |
| 14:2:18(G):TYR:HA | 14:2:18(J):LEU:HG | 1.85 | 0.57 |
| 6:F:38:ILE:HG22 | 6:F:164:ALA:CB | 2.34 | 0.57 |
| 7:G:35:ILE:HG23 | 7:G:51:GLN:HB2 | 1.87 | 0.57 |
| 9:W:12:VAL:HG22 | 9:W:104:ILE:HD11 | 1.87 | 0.57 |
| 12:Z:166:HIS:HD2 | 12:Z:168:GLN:H | 1.53 | 0.57 |
| 4:D:196:ILE:H | 4:D:196:ILE:HD13 | 1.70 | 0.57 |
| 4:D:229:THR:CG2 | 4:D:233:ILE:HD11 | 2.32 | 0.57 |
| 6:F:120:VAL:HG21 | 6:F:151:LEU:HD21 | 1.87 | 0.57 |
| 3:Q:241:GLN:C | 3:Q:243:GLN:H | 2.07 | 0.57 |
| 12:Z:114:ASP:HB3 | 12:Z:118:SER:H | 1.70 | 0.57 |
| 5:E:201:LEU:O | 5:E:202:ARG:HB2 | 2.05 | 0.57 |
| 13:M:149:GLN:NE2 | 13:M:149:GLN:H | 2.03 | 0.57 |
| 14:N:156:LYS:HG2 | 14:N:18(J):LEU:HD11 | 1.87 | 0.57 |
| 5:S:214:ILE:CD1 | 5:S:219:THR:HG21 | 2.30 | 0.57 |
| 6:T:38:ILE:HD11 | 6:T:49:ALA:HB3 | 1.87 | 0.57 |
| 13:1:103:GLY:HA2 | 13:1:178:ILE:HD13 | 1.86 | 0.56 |
| 14:2:176:VAL:HG12 | 14:2:178:LEU:HD13 | 1.87 | 0.56 |
| 14:2:19:ARG:HG3 | 14:2:26:ILE:HD12 | 1.87 | 0.56 |
| 7:G:107:MET:HE3 | 7:G:112:LEU:HB2 | 1.87 | 0.56 |
| 1:O:86:ARG:HE | 7:U:118:ASN:ND2 | 2.03 | 0.56 |
| 3:Q:182:PRO:O | 3:Q:184:ALA:N | 2.38 | 0.56 |
| 4:R:45:GLY:HA2 | 4:R:146:TYR:CD1 | 2.40 | 0.56 |
| 5:S:207:LEU:HA | 5:S:2(E):ASN:ND2 | 2.19 | 0.56 |
| 13:1:14(C):ARG:CG | 13:1:14(C):ARG:HH11 | 2.17 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:2:36:ARG:HG3 | 14:2:42:TRP:CE2 | 2.40 | 0.56 |
| 3:C:14:ILE:HD13 | 3:C:14:ILE:N | 2.19 | 0.56 |
| 3:C:186:VAL:O | 3:C:190:VAL:HG23 | 2.05 | 0.56 |
| 4:D:50:VAL:HG22 | 4:D:67:ILE:HD11 | 1.87 | 0.56 |
| 11:K:99:THR:CG2 | 11:K:113:VAL:HB | 2.33 | 0.56 |
| 11:K:40:PHE:CD2 | 11:K:73:ARG:HD2 | 2.40 | 0.56 |
| 4:R:50:VAL:HG22 | 4:R:67:ILE:HD11 | 1.86 | 0.56 |
| 7:U:41:ARG:CD | 7:U:148:ILE:HD13 | 2.35 | 0.56 |
| 11:Y:10(A):ARG:H | 11:Y:10(B):LYS:NZ | 2.02 | 0.56 |
| 12:Z:8:GLY:HA3 | 12:Z:11:PHE:CE2 | 2.40 | 0.56 |
| 5:E:15:PHE:N | 6:F:23:GLN:HE22 | 2.01 | 0.56 |
| 13:M:179:ASP:HB3 | 13:M:18(A):THR:OG1 | 2.05 | 0.56 |
| 10:X:147:THR:OG1 | 10:X:150:GLU:HG3 | 2.05 | 0.56 |
| 11:Y:75:SER:HB2 | 11:Y:106:GLU:OE2 | 2.05 | 0.56 |
| 4:D:12(D):ALA:HB3 | 4:D:126:ARG:CD | 2.36 | 0.56 |
| 14:N:10(B):LYS:HD3 | 14:N:10(B):LYS:C | 2.26 | 0.56 |
| 4:R:177:LEU:HD22 | 5:S:58:LEU:CD1 | 2.35 | 0.56 |
| 11:Y:123:ASP:HB2 | 11:Y:124:ILE:HD12 | 1.86 | 0.56 |
| 2:B:239:THR:OXT | 2:B:239:THR:HG22 | 2.05 | 0.56 |
| 2:B:8:TYR:CD2 | 7:G:12:ILE:HD12 | 2.40 | 0.56 |
| 3:C:45:CYS:HA | 3:C:141:PHE:HZ | 1.70 | 0.56 |
| 16:B:256:HOH:O | 3:C:33:ARG:HD2 | 2.04 | 0.56 |
| 7:G:72:ARG:NH1 | 7:G:72:ARG:HB2 | 2.20 | 0.56 |
| 14:N:13:ILE:HD12 | 14:N:177:VAL:CA | 2.33 | 0.56 |
| 3:Q:57:LYS:HD2 | 3:Q:58:LEU:N | 2.20 | 0.56 |
| 8:V:159:ILE:HG22 | 8:V:163:ILE:HD13 | 1.87 | 0.56 |
| 11:Y:40:PHE:CD2 | 11:Y:73:ARG:HD2 | 2.41 | 0.56 |
| 3:C:57:LYS:HD2 | 3:C:58:LEU:N | 2.21 | 0.56 |
| 6:F:11:SER:HB3 | 6:F:14:VAL:HG23 | 1.86 | 0.56 |
| 7:G:172:ILE:HD11 | 7:G:201:LEU:CD2 | 2.35 | 0.56 |
| 10:J:44:SER:OG | 10:J:100:LEU:HB2 | 2.05 | 0.56 |
| 12:L:8:GLY:HA3 | 12:L:11:PHE:CE2 | 2.40 | 0.56 |
| 5:S:179:THR:O | 5:S:179:THR:HG22 | 2.05 | 0.56 |
| 10:X:-1:MET:HG2 | 10:X:1:ASP:N | 2.20 | 0.56 |
| 13:1:19:LEU:HB2 | 13:1:170:SER:HB2 | 1.87 | 0.56 |
| 2:B:152:ASN:HB2 | 2:B:153:PRO:CD | 2.36 | 0.56 |
| 3:C:216:LYS:HD2 | 3:C:220:ASP:OD1 | 2.06 | 0.56 |
| 5:E:73:HIS:CE1 | 5:E:74:MET:HE2 | 2.40 | 0.56 |
| 8:H:167:LEU:HD13 | 12:Z:167:ILE:CD1 | 2.36 | 0.56 |
| 3:Q:149:TYR:CE1 | 3:Q:159:SER:HB3 | 2.41 | 0.56 |
| 6:T:38:ILE:HG22 | 6:T:164:ALA:CB | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:U:140:SER:HA | 7:U:215:ALA:HB1 | 1.88 | 0.56 |
| 12:L:-8:PHE:HB2 | 13:M:-8:THR:HG23 | 1.86 | 0.56 |
| 11:Y:10(A):ARG:HH11 | 11:Y:10(A):ARG:HG2 | 1.70 | 0.56 |
| 11:K:143:LYS:HB2 | 11:K:146:LEU:HD13 | 1.86 | 0.56 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:HG3 | 1.86 | 0.56 |
| 6:T:49:ALA:HB3 | 6:T:197:ILE:HD11 | 1.84 | 0.56 |
| 7:U:18(A):ILE:HD13 | 7:U:18(C):HIS:N | 2.13 | 0.56 |
| 8:V:22:GLN:HG3 | 15:V:1401:BO2:C6 | 2.36 | 0.56 |
| 15:2:1405:BO2:H21 | 16:2:1453:HOH:O | 2.05 | 0.56 |
| 14:2:175:MET:HE3 | 14:2:18(B):PHE:CE2 | 2.41 | 0.56 |
| 2:B:21:LEU:HD13 | 2:B:124:THR:HG23 | 1.87 | 0.56 |
| 2:B:21:LEU:O | 2:B:25:GLU:HG2 | 2.06 | 0.56 |
| 7:G:77:VAL:CG1 | 7:G:137:THR:HB | 2.36 | 0.56 |
| 10:J:143:ARG:HH11 | 10:J:143:ARG:HG2 | 1.71 | 0.56 |
| 12:L:3:ILE:HG13 | 12:L:100:ILE:HD13 | 1.88 | 0.56 |
| 4:R:53:ARG:HG2 | 4:R:53:ARG:O | 2.05 | 0.56 |
| 7:G:140:SER:HA | 7:G:215:ALA:HB1 | 1.87 | 0.56 |
| 9:I:1:GLY:HA3 | 9:I:33:LYS:HE2 | 1.87 | 0.56 |
| 14:N:130:GLY:O | 14:N:134:ILE:HD13 | 2.05 | 0.56 |
| 3:Q:216:LYS:HD2 | 3:Q:220:ASP:OD1 | 2.05 | 0.56 |
| 4:R:173:GLN:CG | 5:S:56:ASP:OD2 | 2.54 | 0.56 |
| 6:T:11:SER:HB3 | 6:T:14:VAL:HG23 | 1.87 | 0.56 |
| 6:T:210:LEU:HD11 | 6:T:212:ILE:HD11 | 1.87 | 0.56 |
| 9:W:150:ASP:HA | 16:W:237:HOH:O | 2.05 | 0.56 |
| 15:2:1405:BO2:H251 | 16:2:1423:HOH:O | 2.06 | 0.55 |
| 14:2:14:LEU:O | 14:2:175:MET:HA | 2.05 | 0.55 |
| 12:L:-7:ASN:C | 12:L:-7:ASN:HD22 | 2.09 | 0.55 |
| 14:N:20:THR:HG22 | 15:N:1404:BO2:H221 | 1.87 | 0.55 |
| 9:W:29:ASN:HB3 | 9:W:171:TRP:CE3 | 2.41 | 0.55 |
| 10:J:144:PRO:CG | 11:Y:207:ASN:ND2 | 2.70 | 0.55 |
| 5:E:132:TYR:O | 5:E:153:PRO:HB3 | 2.06 | 0.55 |
| 11:K:123:ASP:HB2 | 11:K:124:ILE:HD12 | 1.87 | 0.55 |
| 3:Q:45:CYS:HA | 3:Q:141:PHE:HZ | 1.70 | 0.55 |
| 6:T:54:ILE:HG12 | 6:T:208:PHE:HA | 1.88 | 0.55 |
| 7:U:168:LYS:HE3 | 16:U:277:HOH:O | 2.05 | 0.55 |
| 13:1:40:ASN:HD22 | 13:1:40:ASN:N | 1.94 | 0.55 |
| 2:B:214:THR:C | 2:B:215:ILE:HD13 | 2.26 | 0.55 |
| 4:R:12(D):ALA:HB3 | 4:R:126:ARG:CD | 2.35 | 0.55 |
| 5:S:67:ILE:HG21 | 5:S:223:ILE:HD12 | 1.88 | 0.55 |
| 8:V:100:ILE:HD11 | 8:V:127:LEU:HG | 1.87 | 0.55 |
| 3:C:182:PRO:O | 3:C:184:ALA:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 6:F:54:ILE:HG12 | 6:F:208:PHE:HA | 1.88 | 0.55 |
| 9:I:29:ASN:HB3 | 9:I:171:TRP:CE3 | 2.41 | 0.55 |
| 13:M:184:LEU:HD23 | 13:M:185:THR:N | 2.21 | 0.55 |
| 3:Q:159:SER:HB2 | 16:Q:261:HOH:O | 2.06 | 0.55 |
| 2:B:225:LYS:HG3 | 2:B:228:GLU:OE1 | 2.06 | 0.55 |
| 11:K:35:ILE:HD12 | 11:K:56:GLU:HB3 | 1.89 | 0.55 |
| 6:T:192:GLN:NE2 | 6:T:195:LYS:CE | 2.69 | 0.55 |
| 2:B:121:GLN:CG | 3:C:83:ALA:HB1 | 2.36 | 0.55 |
| 8:H:100:ILE:HD11 | 8:H:127:LEU:HG | 1.87 | 0.55 |
| 10:J:147:THR:OG1 | 10:J:150:GLU:HG3 | 2.05 | 0.55 |
| 2:P:71:ASN:ND2 | 2:P:72:ASP:N | 2.43 | 0.55 |
| 7:U:72:ARG:HB2 | 7:U:72:ARG:HH11 | 1.72 | 0.55 |
| 9:W:174:VAL:HG21 | 9:W:186:LYS:HE3 | 1.88 | 0.55 |
| 10:X:14:LEU:HD12 | 10:X:42:LEU:HD23 | 1.89 | 0.55 |
| 13:1:149:GLN:H | 13:1:149:GLN:NE2 | 2.04 | 0.55 |
| 2:B:20:ARG:HH11 | 2:B:20:ARG:HG2 | 1.71 | 0.55 |
| 5:E:75:GLY:O | 5:E:139:ILE:CD1 | 2.54 | 0.55 |
| 6:F:95:GLU:CG | 6:F:115:ARG:HB3 | 2.35 | 0.55 |
| 3:Q:83:ALA:O | 3:Q:87:ILE:HD12 | 2.07 | 0.55 |
| 10:J:24:ILE:HG13 | 10:X:133:TYR:OH | 2.06 | 0.55 |
| 8:H:179:GLU:OE2 | 8:H:182:LYS:HE2 | 2.06 | 0.55 |
| 11:K:7:ARG:HD2 | 11:K:108:PRO:O | 2.06 | 0.55 |
| 14:N:14:LEU:O | 14:N:175:MET:HA | 2.06 | 0.55 |
| 13:1:3:VAL:HG12 | 13:1:49:ILE:CD1 | 2.34 | 0.55 |
| 5:E:2(C):VAL:HG13 | 5:E:2(D):ASP:N | 2.21 | 0.55 |
| 12:L:166:HIS:HD2 | 12:L:168:GLN:H | 1.55 | 0.55 |
| 5:S:2(C):VAL:HG13 | 5:S:2(D):ASP:N | 2.21 | 0.55 |
| 6:F:38:ILE:HD11 | 6:F:197:ILE:HD11 | 1.88 | 0.55 |
| 8:H:15:ALA:HB1 | 8:H:159:ILE:HD13 | 1.89 | 0.55 |
| 9:I:7:THR:HG21 | 9:I:110:ILE:HD12 | 1.86 | 0.55 |
| 6:F:203:GLU:C | 6:F:205:ASN:H | 2.10 | 0.54 |
| 11:Y:99:THR:CG2 | 11:Y:113:VAL:HB | 2.36 | 0.54 |
| 12:Z:33:LYS:HD2 | 12:Z:46:ASN:ND2 | 2.22 | 0.54 |
| 14:2:20:THR:HG22 | 15:2:1405:BO2:H221 | 1.89 | 0.54 |
| 14:2:174:ARG:HG2 | 14:2:18(A):ILE:HD12 | 1.90 | 0.54 |
| 14:2:156:LYS:HG2 | 14:2:18(J):LEU:HD11 | 1.88 | 0.54 |
| 7:G:158:VAL:HG22 | 7:G:159:GLY:N | 2.22 | 0.54 |
| 7:G:224:LEU:HB2 | 7:G:229:ILE:HD11 | 1.90 | 0.54 |
| 1:O:159:PRO:HB2 | 2:P:60:GLU:HB3 | 1.89 | 0.54 |
| 5:S:198:SER:HA | 5:S:201:LEU:CG | 2.34 | 0.54 |
| 8:V:179:GLU:OE2 | 8:V:182:LYS:HE2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:169:SER:HA | 3:C:172:VAL:CG1 | 2.37 | 0.54 |
| 5:E:179:THR:O | 5:E:179:THR:HG22 | 2.07 | 0.54 |
| 1:O:232:ARG:HH11 | 1:O:232:ARG:HG3 | 1.73 | 0.54 |
| 5:S:86:ARG:HH11 | 5:S:86:ARG:HG3 | 1.72 | 0.54 |
| 9:I:29:ASN:HD21 | 11:Y:208:ASN:ND2 | 2.05 | 0.54 |
| 9:I:165:ARG:NH2 | 12:Z:135:MET:CE | 2.70 | 0.54 |
| 1:O:118:LYS:HE2 | 1:O:122:GLU:OE1 | 2.07 | 0.54 |
| 2:P:20:ARG:HH11 | 2:P:20:ARG:HG2 | 1.73 | 0.54 |
| 2:P:21:LEU:HD13 | 2:P:124:THR:HG23 | 1.89 | 0.54 |
| 14:N:48:SER:HB3 | 14:N:51:ASP:HB2 | 1.90 | 0.54 |
| 5:S:67:ILE:HG21 | 5:S:223:ILE:CD1 | 2.37 | 0.54 |
| 5:E:74:MET:CE | 5:E:96:CYS:SG | 2.95 | 0.54 |
| 11:K:180:GLU:CB | 16:K:1426:HOH:O | 2.53 | 0.54 |
| 11:Y:10(B):LYS:CD | 11:Y:10(B):LYS:N | 2.59 | 0.54 |
| 16:X:221:HOH:O | 11:Y:132:THR:HG22 | 2.06 | 0.54 |
| 2:P:202:THR:HG22 | 2:P:204:SER:N | 2.07 | 0.54 |
| 2:P:87:ILE:O | 2:P:91:THR:HG23 | 2.08 | 0.54 |
| 7:U:107:MET:HE3 | 7:U:112:LEU:HD13 | 1.90 | 0.54 |
| 13:1:184:LEU:HD23 | 13:1:185:THR:N | 2.23 | 0.54 |
| 5:E:58:LEU:HD12 | 5:E:58:LEU:N | 2.23 | 0.54 |
| 6:F:192:GLN:O | 6:F:196:ILE:HG12 | 2.08 | 0.54 |
| 6:F:63:LYS:O | 6:F:65:VAL:HG23 | 2.08 | 0.54 |
| 6:T:186:ALA:O | 6:T:190:VAL:HG23 | 2.07 | 0.54 |
| 6:T:51:GLU:OE1 | 6:T:53:LEU:HD21 | 2.08 | 0.54 |
| 7:U:236:ILE:HG13 | 7:U:237:ALA:N | 2.22 | 0.54 |
| 10:X:113:ILE:HG12 | 10:X:119:LYS:HG3 | 1.89 | 0.54 |
| 1:A:232:ARG:HG3 | 1:A:232:ARG:HH11 | 1.72 | 0.54 |
| 2:B:14:ILE:H | 2:B:14:ILE:CD1 | 2.20 | 0.54 |
| 5:E:210:LEU:HD22 | 5:E:233:ILE:CD1 | 2.37 | 0.54 |
| 5:E:86:ARG:HH11 | 5:E:86:ARG:HG3 | 1.73 | 0.54 |
| 6:F:109:ILE:CD1 | 6:F:142:ASP:HB3 | 2.37 | 0.54 |
| 8:H:22:GLN:HG3 | 15:H:1400:BO2:C6 | 2.36 | 0.54 |
| 4:R:207:LEU:C | 4:R:207:LEU:HD23 | 2.28 | 0.54 |
| 4:R:31:ILE:HD13 | 4:R:80:GLY:HA3 | 1.90 | 0.54 |
| 3:Q:177:GLU:OE2 | 4:R:57:PRO:HD2 | 2.08 | 0.54 |
| 7:U:77:VAL:CG1 | 7:U:137:THR:HB | 2.37 | 0.54 |
| 14:2:163:ILE:HG23 | 14:2:170:GLY:HA2 | 1.88 | 0.54 |
| 1:A:97:HIS:HD2 | 8:H:61:SER:OG | 1.91 | 0.54 |
| 14:N:176:VAL:HG12 | 14:N:178:LEU:HD13 | 1.89 | 0.54 |
| 3:Q:173:ARG:O | 3:Q:177:GLU:HG3 | 2.08 | 0.54 |
| 3:C:33:ARG:HB2 | 3:C:33:ARG:HH11 | 1.71 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:E:198:SER:HA | 5:E:201:LEU:CG | 2.35 | 0.53 |
| 5:E:31:ILE:HD12 | 5:E:31:ILE:H | 1.72 | 0.53 |
| 2:P:20:ARG:NH1 | 2:P:20:ARG:HG2 | 2.23 | 0.53 |
| 8:V:148:LYS:HE3 | 8:V:177:VAL:HG11 | 1.89 | 0.53 |
| 10:J:168:MET:HE1 | 10:X:167:PRO:CB | 2.37 | 0.53 |
| 4:D:40:ILE:HG13 | 4:D:193:VAL:CG2 | 2.38 | 0.53 |
| 6:F:11:SER:HB3 | 6:F:14:VAL:CG2 | 2.38 | 0.53 |
| 2:P:121:GLN:CD | 3:Q:87:ILE:HD11 | 2.28 | 0.53 |
| 9:W:55:LEU:CD1 | 9:W:97:VAL:HG21 | 2.38 | 0.53 |
| 13:1:104:VAL:HG23 | 13:1:178:ILE:HG22 | 1.91 | 0.53 |
| 5:E:2(C):VAL:O | 5:E:226:GLY:HA2 | 2.09 | 0.53 |
| 12:L:175:ILE:HD12 | 12:L:175:ILE:N | 2.23 | 0.53 |
| 14:N:175:MET:HE3 | 14:N:18(B):PHE:CE2 | 2.42 | 0.53 |
| 3:Q:221:ILE:N | 3:Q:221:ILE:HD12 | 2.24 | 0.53 |
| 12:Z:148:VAL:O | 12:Z:152:ILE:HG13 | 2.08 | 0.53 |
| 2:B:20:ARG:HG2 | 2:B:20:ARG:NH1 | 2.23 | 0.53 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:N | 2.06 | 0.53 |
| 2:P:76:VAL:HG21 | 2:P:89:ILE:CD1 | 2.39 | 0.53 |
| 3:Q:52:ARG:HD2 | 3:Q:208:LYS:O | 2.08 | 0.53 |
| 4:R:31:ILE:HD11 | 4:R:133:GLY:C | 2.28 | 0.53 |
| 5:E:95:GLN:HG3 | 5:E:115:LEU:HD13 | 1.91 | 0.53 |
| 13:M:40:ASN:HD22 | 13:M:40:ASN:N | 1.93 | 0.53 |
| 2:P:152:ASN:HB2 | 2:P:153:PRO:CD | 2.38 | 0.53 |
| 2:P:31:ILE:HD11 | 2:P:153:PRO:HG2 | 1.90 | 0.53 |
| 6:T:203:GLU:C | 6:T:205:ASN:H | 2.10 | 0.53 |
| 12:L:135:MET:CE | 9:W:165:ARG:NH2 | 2.72 | 0.53 |
| 11:K:156:LYS:HB2 | 11:K:175:LEU:HD11 | 1.90 | 0.53 |
| 3:Q:169:SER:HA | 3:Q:172:VAL:CG1 | 2.38 | 0.53 |
| 4:R:38:ILE:HD12 | 4:R:197:LEU:HG | 1.91 | 0.53 |
| 5:S:138:ILE:N | 5:S:138:ILE:HD12 | 2.23 | 0.53 |
| 1:A:173:LYS:O | 1:A:177:GLU:HG3 | 2.08 | 0.53 |
| 7:G:14:ILE:HD13 | 7:G:14:ILE:H | 1.72 | 0.53 |
| 10:J:177:ILE:CD1 | 10:J:187:VAL:HG23 | 2.38 | 0.53 |
| 5:S:2(C):VAL:O | 5:S:226:GLY:HA2 | 2.09 | 0.53 |
| 6:T:192:GLN:O | 6:T:196:ILE:HG12 | 2.09 | 0.53 |
| 13:1:45:ILE:HG23 | 13:1:99:ILE:HD11 | 1.91 | 0.53 |
| 14:2:19:ARG:HD3 | 14:2:26:ILE:HD12 | 1.90 | 0.53 |
| 1:A:118:LYS:HE2 | 1:A:122:GLU:OE1 | 2.08 | 0.53 |
| 5:E:68:ILE:HD12 | 5:E:68:ILE:N | 2.24 | 0.53 |
| 6:T:120:VAL:HG21 | 6:T:151:LEU:HD21 | 1.89 | 0.53 |
| 5:E:18(D):ILE:HG23 | 5:E:18(E):LYS:HG3 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:8:PHE:HB3 | 8:H:151:ALA:HB2 | 1.91 | 0.53 |
| 12:L:33:LYS:HD2 | 12:L:46:ASN:HD22 | 1.74 | 0.53 |
| 2:P:101:LYS:HZ2 | 10:X:85:GLN:NE2 | 2.05 | 0.53 |
| 3:Q:33:ARG:CB | 3:Q:33:ARG:NH1 | 2.71 | 0.53 |
| 13:1:84:ALA:HA | 13:1:113:VAL:HG21 | 1.91 | 0.53 |
| 14:2:107:LYS:HG2 | 14:2:108:GLY:N | 2.23 | 0.53 |
| 10:J:168:MET:CE | 10:X:168:MET:HE3 | 2.38 | 0.53 |
| 11:K:66:HIS:CG | 11:K:74:ILE:HD13 | 2.43 | 0.53 |
| 12:L:42:VAL:CG2 | 12:L:102:ALA:HB3 | 2.38 | 0.53 |
| 5:S:12:THR:HG21 | 5:S:124:THR:HA | 1.91 | 0.53 |
| 9:W:1:GLY:HA3 | 9:W:33:LYS:HE2 | 1.90 | 0.53 |
| 12:Z:42:VAL:HG23 | 12:Z:102:ALA:HB3 | 1.90 | 0.53 |
| 2:B:121:GLN:HG3 | 3:C:83:ALA:HB1 | 1.90 | 0.52 |
| 4:D:207:LEU:HD23 | 4:D:207:LEU:C | 2.28 | 0.52 |
| 9:I:174:VAL:HG21 | 9:I:186:LYS:HE3 | 1.90 | 0.52 |
| 7:U:18(A):ILE:CD1 | 7:U:18(A):ILE:C | 2.77 | 0.52 |
| 2:P:137:ILE:HD11 | 2:P:165:VAL:HG22 | 1.89 | 0.52 |
| 6:T:82:ILE:HB | 6:T:83:PRO:HD3 | 1.92 | 0.52 |
| 12:Z:4:LEU:HD11 | 12:Z:6:ILE:HD11 | 1.92 | 0.52 |
| 14:2:19:ARG:CG | 14:2:26:ILE:HD12 | 2.39 | 0.52 |
| 11:K:174:ASN:HD21 | 11:K:189:ASN:HD22 | 1.58 | 0.52 |
| 13:M:84:ALA:HA | 13:M:113:VAL:HG21 | 1.90 | 0.52 |
| 14:N:113:ILE:N | 14:N:113:ILE:HD12 | 2.24 | 0.52 |
| 8:V:108:SER:HB3 | 8:V:180:ILE:HD11 | 1.92 | 0.52 |
| 1:A:215:ILE:HD12 | 1:A:215:ILE:N | 2.24 | 0.52 |
| 2:B:87:ILE:O | 2:B:91:THR:HG23 | 2.09 | 0.52 |
| 3:C:52:ARG:HD2 | 3:C:208:LYS:O | 2.09 | 0.52 |
| 5:E:227:GLU:CD | 5:E:227:GLU:N | 2.63 | 0.52 |
| 5:E:70:CYS:SG | 5:E:92:LEU:HD23 | 2.49 | 0.52 |
| 6:F:186:ALA:O | 6:F:190:VAL:HG23 | 2.09 | 0.52 |
| 5:S:58:LEU:N | 5:S:58:LEU:HD12 | 2.23 | 0.52 |
| 6:T:63:LYS:O | 6:T:65:VAL:HG23 | 2.08 | 0.52 |
| 6:F:158:TRP:CZ3 | 7:G:64:VAL:HA | 2.45 | 0.52 |
| 6:F:210:LEU:HD21 | 6:F:212:ILE:HD11 | 1.91 | 0.52 |
| 7:G:72:ARG:HB2 | 7:G:72:ARG:HH11 | 1.74 | 0.52 |
| 12:L:109:ALA:HB2 | 12:L:121:ARG:NH2 | 2.24 | 0.52 |
| 12:L:93:PHE:N | 12:L:94:PRO:HD3 | 2.24 | 0.52 |
| 2:P:5:SER:O | 2:P:7:ARG:N | 2.43 | 0.52 |
| 7:U:233:LEU:O | 7:U:236:ILE:HG12 | 2.09 | 0.52 |
| 4:D:12(D):ALA:HA | 5:E:129:GLY:HA2 | 1.90 | 0.52 |
| 6:F:21(B):THR:O | 6:F:21(C):ASN:HB2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:101:ILE:HD12 | 12:L:101:ILE:C | 2.30 | 0.52 |
| 13:M:-6:GLN:O | 13:M:-6:GLN:HG3 | 2.09 | 0.52 |
| 14:N:107:LYS:HG2 | 14:N:108:GLY:N | 2.25 | 0.52 |
| 7:U:158:VAL:HG22 | 7:U:159:GLY:N | 2.24 | 0.52 |
| 12:Z:93:PHE:N | 12:Z:94:PRO:HD3 | 2.25 | 0.52 |
| 3:C:216:LYS:HB2 | 3:C:220:ASP:HB3 | 1.92 | 0.52 |
| 4:D:53:ARG:HG2 | 4:D:53:ARG:O | 2.10 | 0.52 |
| 10:J:14:LEU:HD12 | 10:J:42:LEU:HD23 | 1.90 | 0.52 |
| 13:M:19:LEU:HD12 | 13:M:20:GLY:H | 1.75 | 0.52 |
| 2:P:137:ILE:CD1 | 2:P:165:VAL:HG22 | 2.40 | 0.52 |
| 2:P:27:ALA:O | 2:P:30:SER:HB3 | 2.10 | 0.52 |
| 6:T:74:ILE:HG12 | 6:T:109:ILE:HD11 | 1.90 | 0.52 |
| 3:C:173:ARG:O | 3:C:177:GLU:HG3 | 2.10 | 0.52 |
| 4:D:38:ILE:HD12 | 4:D:197:LEU:HG | 1.91 | 0.52 |
| 5:E:54:ASN:ND2 | 5:E:56:ASP:O | 2.41 | 0.52 |
| 4:D:177:LEU:HD22 | 5:E:58:LEU:CD1 | 2.40 | 0.52 |
| 6:F:127:ASN:N | 6:F:127:ASN:HD22 | 2.07 | 0.52 |
| 6:F:192:GLN:NE2 | 6:F:195:LYS:CE | 2.73 | 0.52 |
| 11:K:12:ILE:HD12 | 11:K:110:ILE:CG1 | 2.40 | 0.52 |
| 13:M:171:ARG:HG3 | 13:M:192:VAL:HB | 1.92 | 0.52 |
| 1:O:173:LYS:O | 1:O:177:GLU:HG3 | 2.09 | 0.52 |
| 4:R:160:TYR:CE2 | 4:R:163:LYS:HD3 | 2.45 | 0.52 |
| 14:2:112:THR:CG2 | 14:2:120:HIS:HB2 | 2.38 | 0.52 |
| 2:B:111:ILE:N | 2:B:111:ILE:HD12 | 2.25 | 0.52 |
| 5:S:207:LEU:HA | 5:S:2(E):ASN:HD22 | 1.75 | 0.52 |
| 5:S:52:LYS:CB | 5:S:63:TYR:HB3 | 2.40 | 0.52 |
| 7:U:87:ASN:ND2 | 7:U:87:ASN:C | 2.62 | 0.52 |
| 12:Z:137:PHE:CE1 | 12:Z:141:GLN:HG3 | 2.45 | 0.52 |
| 2:B:71:ASN:ND2 | 2:B:72:ASP:N | 2.45 | 0.52 |
| 3:C:57:LYS:NZ | 3:C:58:LEU:HA | 2.25 | 0.52 |
| 14:N:163:ILE:HG23 | 14:N:170:GLY:HA2 | 1.91 | 0.52 |
| 3:Q:76:LEU:HD12 | 3:Q:138:ILE:HG12 | 1.92 | 0.52 |
| 4:R:70:ILE:HD12 | 4:R:74:ILE:HG21 | 1.92 | 0.52 |
| 8:V:159:ILE:HG22 | 8:V:163:ILE:CD1 | 2.40 | 0.52 |
| 8:V:17:ASP:HB3 | 8:V:163:ILE:HD11 | 1.90 | 0.52 |
| 2:B:234:VAL:HA | 2:B:239:THR:HA | 1.93 | 0.51 |
| 4:D:40:ILE:CD1 | 4:D:193:VAL:HG23 | 2.40 | 0.51 |
| 6:F:51:GLU:OE1 | 6:F:53:LEU:HD21 | 2.10 | 0.51 |
| 4:R:121:LEU:HB2 | 16:R:853:HOH:O | 2.10 | 0.51 |
| 13:1:-6:GLN:O | 13:1:-6:GLN:HG3 | 2.09 | 0.51 |
| 9:I:137:MET:HE3 | 9:I:141:LEU:HD11 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:J:52:THR:HG22 | 10:J:53:VAL:N | 2.25 | 0.51 |
| 5:S:210:LEU:HD11 | 5:S:212:ILE:HD11 | 1.91 | 0.51 |
| 6:T:11:SER:HB3 | 6:T:14:VAL:CG2 | 2.40 | 0.51 |
| 6:T:20(B):GLU:HG3 | 6:T:20(C):LYS:N | 2.25 | 0.51 |
| 7:U:96:ALA:HA | 7:U:107:MET:CE | 2.33 | 0.51 |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:N | 2.07 | 0.51 |
| 13:1:110:LEU:HG | 13:1:125:LEU:HD12 | 1.92 | 0.51 |
| 8:H:148:LYS:O | 8:H:152:ILE:HG13 | 2.09 | 0.51 |
| 10:J:113:ILE:HG12 | 10:J:119:LYS:HG3 | 1.92 | 0.51 |
| 12:L:5:GLY:O | 12:L:124:CYS:HA | 2.11 | 0.51 |
| 5:S:82:ALA:HB3 | 5:S:83:PRO:HD3 | 1.92 | 0.51 |
| 8:V:8:PHE:HB3 | 8:V:151:ALA:HB2 | 1.92 | 0.51 |
| 9:W:19:ARG:HB2 | 9:W:171:TRP:HB2 | 1.92 | 0.51 |
| 4:D:138:ILE:N | 4:D:138:ILE:HD12 | 2.25 | 0.51 |
| 5:E:47:VAL:HG22 | 5:E:214:ILE:HD13 | 1.92 | 0.51 |
| 5:E:67:ILE:HG21 | 5:E:223:ILE:CD1 | 2.41 | 0.51 |
| 7:G:87:ASN:ND2 | 7:G:87:ASN:C | 2.64 | 0.51 |
| 10:J:177:ILE:HD11 | 10:J:187:VAL:HG22 | 1.90 | 0.51 |
| 12:L:-8:PHE:CB | 13:M:-8:THR:HG23 | 2.40 | 0.51 |
| 3:Q:216:LYS:HB2 | 3:Q:220:ASP:HB3 | 1.92 | 0.51 |
| 5:S:18(D):ILE:HG23 | 5:S:18(E):LYS:HG3 | 1.91 | 0.51 |
| 11:K:207:ASN:ND2 | 10:X:144:PRO:CG | 2.73 | 0.51 |
| 10:J:144:PRO:CG | 11:Y:207:ASN:HD21 | 2.24 | 0.51 |
| 2:B:27:ALA:O | 2:B:30:SER:HB3 | 2.11 | 0.51 |
| 3:C:227:GLU:OE1 | 3:C:227:GLU:N | 2.42 | 0.51 |
| 5:E:18(C):PHE:HA | 5:E:18(F):ILE:HG13 | 1.92 | 0.51 |
| 6:F:40:ILE:N | 6:F:40:ILE:HD12 | 2.26 | 0.51 |
| 7:G:12:ILE:HD13 | 7:G:12:ILE:N | 2.26 | 0.51 |
| 11:K:126:CYS:HB2 | 11:K:135:TYR:CE1 | 2.45 | 0.51 |
| 14:N:54:ALA:O | 14:N:58:ILE:HG12 | 2.11 | 0.51 |
| 7:U:41:ARG:CG | 7:U:148:ILE:HD13 | 2.41 | 0.51 |
| 6:F:109:ILE:H | 6:F:109:ILE:HD12 | 1.75 | 0.51 |
| 6:F:82:ILE:HB | 6:F:83:PRO:HD3 | 1.91 | 0.51 |
| 7:G:18(G):GLU:CG | 7:G:188:LYS:HB2 | 2.34 | 0.51 |
| 8:H:148:LYS:HE3 | 8:H:177:VAL:HG11 | 1.91 | 0.51 |
| 12:L:137:PHE:CE1 | 12:L:141:GLN:HG3 | 2.45 | 0.51 |
| 2:P:51:GLU:OE2 | 2:P:209:ARG:NH2 | 2.44 | 0.51 |
| 5:S:227:GLU:N | 5:S:227:GLU:CD | 2.64 | 0.51 |
| 5:S:40:LEU:HD23 | 5:S:40:LEU:N | 2.26 | 0.51 |
| 5:S:70:CYS:SG | 5:S:92:LEU:HD23 | 2.49 | 0.51 |
| 5:S:73:HIS:CE1 | 5:S:74:MET:HE2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 9:W:103:GLY:C | 9:W:104:ILE:HD12 | 2.31 | 0.51 |
| 12:Z:100:ILE:N | 12:Z:100:ILE:HD12 | 2.26 | 0.51 |
| 13:1:66:ASN:HB3 | 16:1:221:HOH:O | 2.10 | 0.51 |
| 2:P:126:HIS:HB3 | 3:Q:129:VAL:HG12 | 1.92 | 0.51 |
| 2:P:124:THR:CG2 | 3:Q:130:ARG:HH21 | 2.21 | 0.51 |
| 12:Z:42:VAL:CG2 | 12:Z:102:ALA:HB3 | 2.41 | 0.51 |
| 14:2:10(B):LYS:HD3 | 14:2:10(B):LYS:O | 2.10 | 0.51 |
| 2:B:213:ALA:CB | 2:B:223:ILE:HD13 | 2.40 | 0.51 |
| 10:J:168:MET:CE | 10:X:168:MET:CE | 2.89 | 0.51 |
| 5:S:49:VAL:CG1 | 5:S:212:ILE:HD12 | 2.32 | 0.51 |
| 6:T:175:GLU:OE1 | 6:T:199:LEU:HD23 | 2.11 | 0.51 |
| 6:T:192:GLN:NE2 | 6:T:195:LYS:HE3 | 2.26 | 0.51 |
| 7:U:18(G):GLU:CG | 7:U:188:LYS:HB2 | 2.36 | 0.51 |
| 9:W:14:ILE:HG12 | 9:W:34:ILE:HD12 | 1.93 | 0.51 |
| 14:2:48:SER:HB3 | 14:2:51:ASP:HB2 | 1.92 | 0.51 |
| 2:B:137:ILE:HD11 | 2:B:165:VAL:HG22 | 1.92 | 0.51 |
| 9:I:55:LEU:CD1 | 9:I:97:VAL:HG21 | 2.41 | 0.51 |
| 11:K:66:HIS:CD2 | 11:K:74:ILE:HD13 | 2.46 | 0.51 |
| 3:Q:57:LYS:NZ | 3:Q:58:LEU:HA | 2.25 | 0.51 |
| 6:T:63:LYS:O | 6:T:65:VAL:N | 2.44 | 0.51 |
| 10:X:18:LYS:CD | 10:X:174:ILE:HG13 | 2.40 | 0.51 |
| 11:Y:13:ILE:HD12 | 11:Y:152:LEU:HD23 | 1.93 | 0.51 |
| 2:B:27:ALA:O | 2:B:31:ILE:HG12 | 2.12 | 0.51 |
| 12:L:90:LYS:HD3 | 12:L:95:TYR:CZ | 2.46 | 0.51 |
| 7:U:131:PRO:HB3 | 16:U:261:HOH:O | 2.10 | 0.51 |
| 8:V:63:ILE:HD11 | 8:V:79:ALA:HA | 1.93 | 0.51 |
| 12:Z:14(I):THR:HG21 | 12:Z:14(M):VAL:HB | 1.93 | 0.51 |
| 14:2:146:MET:CE | 14:2:150:GLU:HB3 | 2.41 | 0.50 |
| 3:C:136:THR:O | 3:C:150:GLN:HA | 2.11 | 0.50 |
| 3:C:57:LYS:O | 3:C:58:LEU:HB2 | 2.11 | 0.50 |
| 4:D:170:GLU:N | 4:D:170:GLU:OE1 | 2.44 | 0.50 |
| 4:D:215:ILE:HD13 | 4:D:215:ILE:C | 2.31 | 0.50 |
| 5:E:45:HIS:HB3 | 5:E:214:ILE:HD11 | 1.93 | 0.50 |
| 6:F:18:ASP:OD1 | 6:F:20:ARG:HD3 | 2.11 | 0.50 |
| 10:J:64:GLN:NE2 | 16:J:217:HOH:O | 2.33 | 0.50 |
| 14:N:10(B):LYS:O | 14:N:10(B):LYS:HD3 | 2.10 | 0.50 |
| 3:Q:220:ASP:C | 3:Q:221:ILE:HD12 | 2.31 | 0.50 |
| 10:X:10(B):LYS:HB2 | 10:X:10(B):LYS:HZ3 | 1.76 | 0.50 |
| 11:Y:156:LYS:HB2 | 11:Y:175:LEU:HD11 | 1.92 | 0.50 |
| 8:H:18:THR:HB | 8:H:30:ASN:HA | 1.94 | 0.50 |
| 11:K:10(A):ARG:H | 11:K:10(B):LYS:HZ2 | 1.56 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:N:112:THR:CG2 | 14:N:120:HIS:HB2 | 2.39 | 0.50 |
| 7:U:136:LEU:O | 7:U:150:LYS:HA | 2.10 | 0.50 |
| 7:U:78:VAL:HG11 | 7:U:85:ALA:CB | 2.41 | 0.50 |
| 6:F:175:GLU:CB | 6:F:196:ILE:HD12 | 2.42 | 0.50 |
| 9:I:110:ILE:HG12 | 9:I:125:ILE:CD1 | 2.42 | 0.50 |
| 13:M:17:ASP:HA | 13:M:173:PHE:CB | 2.42 | 0.50 |
| 2:P:31:ILE:HD11 | 2:P:153:PRO:CG | 2.42 | 0.50 |
| 4:R:215:ILE:HD13 | 4:R:215:ILE:C | 2.31 | 0.50 |
| 13:1:13:ILE:CD1 | 13:1:177:ILE:CG2 | 2.82 | 0.50 |
| 14:2:159:LEU:HB3 | 14:2:173:ILE:HD12 | 1.92 | 0.50 |
| 14:2:1:THR:HG22 | 14:2:3:ILE:HD12 | 1.93 | 0.50 |
| 3:C:149:TYR:CE1 | 3:C:159:SER:HB3 | 2.46 | 0.50 |
| 5:E:12:THR:HG21 | 5:E:124:THR:HA | 1.92 | 0.50 |
| 6:F:67:ILE:HD13 | 6:F:77:VAL:CB | 2.40 | 0.50 |
| 13:M:14(A):VAL:O | 13:M:14(A):VAL:HG23 | 2.12 | 0.50 |
| 9:W:113:PHE:HA | 9:W:118:CYS:O | 2.11 | 0.50 |
| 10:X:52:THR:CG2 | 10:X:53:VAL:N | 2.75 | 0.50 |
| 13:1:14(A):VAL:O | 13:1:14(A):VAL:HG23 | 2.12 | 0.50 |
| 1:A:150:GLN:O | 1:A:157:TYR:HA | 2.11 | 0.50 |
| 5:E:40:LEU:HD23 | 5:E:40:LEU:N | 2.27 | 0.50 |
| 12:L:14(I):THR:HG21 | 12:L:14(M):VAL:HB | 1.94 | 0.50 |
| 1:O:150:GLN:O | 1:O:157:TYR:HA | 2.11 | 0.50 |
| 2:P:108:PRO:CG | 2:P:111:ILE:HD12 | 2.41 | 0.50 |
| 6:T:127:ASN:HD22 | 6:T:127:ASN:N | 2.08 | 0.50 |
| 12:Z:5:GLY:O | 12:Z:124:CYS:HA | 2.11 | 0.50 |
| 5:E:18(C):PHE:HA | 5:E:18(F):ILE:CD1 | 2.42 | 0.50 |
| 6:F:38:ILE:HD11 | 6:F:197:ILE:CD1 | 2.42 | 0.50 |
| 10:J:52:THR:CG2 | 10:J:53:VAL:N | 2.74 | 0.50 |
| 12:L:84:GLN:HG3 | 12:L:117:GLY:O | 2.12 | 0.50 |
| 13:M:104:VAL:HG23 | 13:M:178:ILE:HG22 | 1.94 | 0.50 |
| 14:N:22:THR:O | 14:N:22:THR:HG22 | 2.11 | 0.50 |
| 1:O:4:MET:SD | 1:O:5:THR:N | 2.67 | 0.50 |
| 3:Q:156:ILE:HD13 | 4:R:83:ALA:HB2 | 1.92 | 0.50 |
| 8:V:84:LYS:HG3 | 8:V:85:GLN:N | 2.26 | 0.50 |
| 9:W:101:VAL:O | 9:W:110:ILE:HA | 2.12 | 0.50 |
| 10:X:113:ILE:HA | 10:X:118:THR:O | 2.12 | 0.50 |
| 2:B:95:HIS:HB2 | 16:B:259:HOH:O | 2.12 | 0.50 |
| 4:D:160:TYR:CE2 | 4:D:163:LYS:HD3 | 2.47 | 0.50 |
| 4:D:194:LEU:HD21 | 4:D:233:ILE:CD1 | 2.42 | 0.50 |
| 2:B:4:GLY:HA3 | 5:E:127:TYR:CE1 | 2.46 | 0.50 |
| 6:F:20(B):GLU:HG3 | 6:F:20(C):LYS:N | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:H:81:GLN:O | 8:H:85:GLN:HG3 | 2.12 | 0.50 |
| 11:K:124:ILE:N | 11:K:124:ILE:HD12 | 2.26 | 0.50 |
| 11:K:211:GLY:HA2 | 8:V:214:LEU:HD13 | 1.94 | 0.50 |
| 12:L:13:VAL:HG12 | 12:L:177:ILE:HG13 | 1.93 | 0.50 |
| 13:M:57:ARG:NE | 16:M:245:HOH:O | 2.44 | 0.50 |
| 4:R:185:THR:OG1 | 4:R:188:GLU:HG3 | 2.12 | 0.50 |
| 5:S:39:GLY:O | 5:S:162:GLY:HA2 | 2.12 | 0.50 |
| 2:P:101:LYS:HZ2 | 10:X:85:GLN:HE21 | 1.59 | 0.50 |
| 4:D:75:GLY:HA3 | 4:D:221:PHE:CD2 | 2.46 | 0.50 |
| 5:E:97:ASN:HD21 | 12:L:61:ASN:HD21 | 1.59 | 0.50 |
| 12:L:177:ILE:N | 12:L:177:ILE:HD12 | 2.27 | 0.50 |
| 4:R:75:GLY:HA3 | 4:R:221:PHE:CD2 | 2.46 | 0.50 |
| 6:T:175:GLU:CB | 6:T:196:ILE:HD12 | 2.41 | 0.50 |
| 6:T:21(B):THR:O | 6:T:21(C):ASN:HB2 | 2.11 | 0.50 |
| 8:V:81:GLN:O | 8:V:85:GLN:HG3 | 2.12 | 0.50 |
| 12:Z:101:ILE:HD12 | 12:Z:101:ILE:C | 2.32 | 0.50 |
| 12:Z:5:GLY:C | 12:Z:6:ILE:HD12 | 2.31 | 0.50 |
| 13:1:19:LEU:HD12 | 13:1:20:GLY:H | 1.77 | 0.49 |
| 2:B:147:GLN:HB3 | 3:C:62(A):ILE:HD13 | 1.94 | 0.49 |
| 7:G:78:VAL:HG11 | 7:G:85:ALA:CB | 2.42 | 0.49 |
| 11:K:13:ILE:HD12 | 11:K:152:LEU:HD23 | 1.94 | 0.49 |
| 12:L:100:ILE:HD12 | 12:L:100:ILE:N | 2.26 | 0.49 |
| 8:V:41:ILE:HD12 | 8:V:41:ILE:N | 2.27 | 0.49 |
| 12:Z:109:ALA:HB2 | 12:Z:121:ARG:NH2 | 2.27 | 0.49 |
| 6:F:175:GLU:OE1 | 6:F:199:LEU:HD23 | 2.11 | 0.49 |
| 7:G:177:GLU:O | 7:G:17(B):LYS:HG3 | 2.12 | 0.49 |
| 8:H:210:THR:CG2 | 12:Z:14(C):GLN:HG2 | 2.42 | 0.49 |
| 8:H:214:LEU:HD13 | 11:Y:211:GLY:HA2 | 1.92 | 0.49 |
| 5:S:38:VAL:HG12 | 5:S:39:GLY:N | 2.27 | 0.49 |
| 6:T:18:ASP:OD1 | 6:T:20:ARG:HD3 | 2.12 | 0.49 |
| 13:1:171:ARG:HG3 | 13:1:192:VAL:HB | 1.95 | 0.49 |
| 14:2:3:ILE:HG22 | 14:2:16:ALA:CB | 2.42 | 0.49 |
| 5:E:52:LYS:CB | 5:E:63:TYR:HB3 | 2.43 | 0.49 |
| 8:H:84:LYS:HG3 | 8:H:85:GLN:N | 2.26 | 0.49 |
| 14:N:84:LYS:HG3 | 14:N:119:VAL:HG22 | 1.94 | 0.49 |
| 3:Q:227:GLU:N | 3:Q:227:GLU:OE1 | 2.44 | 0.49 |
| 11:Y:124:ILE:HD12 | 11:Y:124:ILE:N | 2.26 | 0.49 |
| 14:2:1:THR:HG22 | 14:2:3:ILE:CD1 | 2.43 | 0.49 |
| 2:B:215:ILE:CD1 | 2:B:221:GLN:HG2 | 2.38 | 0.49 |
| 2:B:53:LYS:HG2 | 2:B:54:VAL:HG23 | 1.94 | 0.49 |
| 5:E:2(B):THR:OG1 | 5:E:2(E):ASN:HB3 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:G:136:LEU:O | 7:G:150:LYS:HA | 2.12 | 0.49 |
| 9:I:113:PHE:HA | 9:I:118:CYS:O | 2.11 | 0.49 |
| 13:M:1:THR:HG22 | 16:M:214:HOH:O | 2.12 | 0.49 |
| 1:O:32:LYS:HE2 | 1:O:32:LYS:HA | 1.95 | 0.49 |
| 2:P:101:LYS:HG3 | 9:W:57:GLU:HB3 | 1.94 | 0.49 |
| 3:Q:136:THR:O | 3:Q:150:GLN:HA | 2.12 | 0.49 |
| 5:S:194:VAL:CG1 | 5:S:207:LEU:HD11 | 2.43 | 0.49 |
| 5:S:2(B):THR:OG1 | 5:S:2(E):ASN:HB3 | 2.13 | 0.49 |
| 6:T:18:ASP:N | 6:T:18:ASP:OD2 | 2.40 | 0.49 |
| 10:X:2:ILE:HD13 | 10:X:170:PHE:CG | 2.47 | 0.49 |
| 12:Z:177:ILE:HD12 | 12:Z:177:ILE:N | 2.27 | 0.49 |
| 13:1:19:LEU:HD12 | 13:1:28:PHE:O | 2.12 | 0.49 |
| 3:C:227:GLU:CD | 3:C:227:GLU:H | 2.16 | 0.49 |
| 5:E:38:VAL:HG12 | 5:E:39:GLY:N | 2.28 | 0.49 |
| 10:J:90(B):ARG:HH11 | 10:J:90(B):ARG:HG2 | 1.78 | 0.49 |
| 2:P:95:HIS:HB2 | 16:P:243:HOH:O | 2.13 | 0.49 |
| 5:S:52:LYS:HB2 | 5:S:63:TYR:HB3 | 1.92 | 0.49 |
| 13:1:17:ASP:HA | 13:1:173:PHE:CB | 2.42 | 0.49 |
| 14:2:100:ILE:HD11 | 14:2:127:ALA:CB | 2.40 | 0.49 |
| 1:A:32:LYS:HE2 | 1:A:32:LYS:HA | 1.94 | 0.49 |
| 2:B:107:ILE:HD11 | 2:B:111:ILE:HG22 | 1.95 | 0.49 |
| 2:B:51:GLU:OE2 | 2:B:202:THR:HG23 | 2.12 | 0.49 |
| 6:F:56:SER:OG | 6:F:57:LYS:N | 2.45 | 0.49 |
| 12:L:101:ILE:O | 12:L:101:ILE:HD12 | 2.12 | 0.49 |
| 12:L:135:MET:HE3 | 9:W:165:ARG:NH2 | 2.27 | 0.49 |
| 2:P:4:GLY:HA3 | 5:S:127:TYR:CZ | 2.47 | 0.49 |
| 5:S:11:ASP:OD1 | 5:S:13:VAL:HG12 | 2.12 | 0.49 |
| 5:S:194:VAL:HG13 | 5:S:207:LEU:CD1 | 2.42 | 0.49 |
| 10:X:52:THR:HG22 | 10:X:53:VAL:N | 2.28 | 0.49 |
| 2:B:185:LYS:HE2 | 2:B:187:ASP:OD1 | 2.13 | 0.49 |
| 5:E:116:LEU:CD1 | 5:E:138:ILE:HD11 | 2.42 | 0.49 |
| 9:I:-8:SER:O | 9:I:-6:PRO:HD3 | 2.12 | 0.49 |
| 10:J:111:TYR:CE1 | 10:J:121:GLU:HG3 | 2.48 | 0.49 |
| 13:M:19:LEU:HD12 | 13:M:28:PHE:O | 2.13 | 0.49 |
| 2:P:234:VAL:HA | 2:P:239:THR:HA | 1.94 | 0.49 |
| 7:U:46:THR:HG23 | 7:U:148:ILE:HD11 | 1.95 | 0.49 |
| 10:X:90(A):ILE:CD1 | 10:X:116:LEU:HD23 | 2.42 | 0.49 |
| 11:Y:126:CYS:HB2 | 11:Y:135:TYR:CE1 | 2.47 | 0.49 |
| 2:B:137:ILE:CD1 | 2:B:165:VAL:HG22 | 2.42 | 0.49 |
| 2:B:5:SER:O | 2:B:7:ARG:N | 2.45 | 0.49 |
| 4:D:233:ILE:N | 4:D:233:ILE:HD12 | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:E:207:LEU:HA | 5:E:2(E):ASN:HD22 | 1.76 | 0.49 |
| 7:G:56:ASP:HB3 | 7:G:59:LEU:HG | 1.95 | 0.49 |
| 12:L:76:ILE:HD11 | 12:L:101:ILE:CD1 | 2.42 | 0.49 |
| 5:S:201:LEU:HD11 | 5:S:207:LEU:CD2 | 2.42 | 0.49 |
| 7:U:49:ILE:HD13 | 7:U:193:ALA:HB1 | 1.94 | 0.49 |
| 8:V:18:THR:HB | 8:V:30:ASN:HA | 1.94 | 0.49 |
| 9:W:104:ILE:CD1 | 9:W:178:ILE:HG22 | 2.43 | 0.49 |
| 12:Z:101:ILE:HD12 | 12:Z:101:ILE:O | 2.13 | 0.49 |
| 14:2:84:LYS:HG3 | 14:2:119:VAL:HG22 | 1.94 | 0.49 |
| 14:2:163:ILE:CD1 | 14:2:173:ILE:HD11 | 2.43 | 0.49 |
| 14:2:155:ILE:HG22 | 14:2:175:MET:HE1 | 1.95 | 0.49 |
| 14:2:21:THR:O | 15:2:1405:BO2:H3 | 2.13 | 0.49 |
| 2:B:215:ILE:HD12 | 2:B:221:GLN:CG | 2.39 | 0.49 |
| 5:E:194:VAL:HG13 | 5:E:207:LEU:CD1 | 2.43 | 0.49 |
| 5:E:31:ILE:HD12 | 5:E:31:ILE:N | 2.27 | 0.49 |
| 7:G:225:SER:O | 7:G:229:ILE:HG12 | 2.12 | 0.49 |
| 12:L:145:TYR:CD1 | 12:L:146:LEU:N | 2.81 | 0.49 |
| 12:L:14(C):GLN:HG2 | 8:V:210:THR:CG2 | 2.42 | 0.49 |
| 12:L:185:ARG:NH1 | 16:L:230:HOH:O | 2.45 | 0.49 |
| 13:M:40:ASN:ND2 | 13:M:40:ASN:N | 2.61 | 0.49 |
| 2:P:53:LYS:HG2 | 2:P:54:VAL:HG23 | 1.94 | 0.49 |
| 10:X:123:PRO:HB2 | 10:X:124:TYR:CD1 | 2.47 | 0.49 |
| 11:Y:86:LEU:C | 11:Y:86:LEU:HD13 | 2.33 | 0.49 |
| 13:1:4:ILE:CD1 | 13:1:155:ILE:HG12 | 2.43 | 0.49 |
| 4:D:112:LEU:C | 4:D:112:LEU:HD13 | 2.33 | 0.49 |
| 6:F:36:THR:HG22 | 6:F:51:GLU:OE2 | 2.13 | 0.49 |
| 6:F:63:LYS:O | 6:F:65:VAL:N | 2.45 | 0.49 |
| 11:K:12:ILE:HD12 | 11:K:110:ILE:HD11 | 1.95 | 0.49 |
| 5:S:54:ASN:ND2 | 5:S:56:ASP:O | 2.42 | 0.49 |
| 4:D:229:THR:C | 4:D:233:ILE:HD13 | 2.31 | 0.48 |
| 11:K:7:ARG:CG | 11:K:12:ILE:HD11 | 2.39 | 0.48 |
| 12:L:3:ILE:CD1 | 12:L:46:ASN:CB | 2.88 | 0.48 |
| 6:T:176:LEU:O | 6:T:180:VAL:HG23 | 2.13 | 0.48 |
| 7:U:65:SER:OG | 7:U:211:GLU:OE2 | 2.25 | 0.48 |
| 11:Y:123:ASP:CB | 11:Y:124:ILE:HD12 | 2.43 | 0.48 |
| 11:Y:174:ASN:HD21 | 11:Y:189:ASN:HD22 | 1.60 | 0.48 |
| 13:M:178:ILE:CD1 | 13:M:184:LEU:HG | 2.42 | 0.48 |
| 2:P:107:ILE:HD11 | 2:P:111:ILE:HG22 | 1.95 | 0.48 |
| 14:2:41:ILE:CD1 | 14:2:103:GLY:HA3 | 2.43 | 0.48 |
| 13:M:197:TRP:CH2 | 14:2:171:GLY:HA2 | 2.48 | 0.48 |
| 9:I:35:PHE:CD1 | 9:I:45:ILE:HD13 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 3:Q:38:VAL:HG22 | 3:Q:39:GLY:N | 2.27 | 0.48 |
| 3:Q:57:LYS:O | 3:Q:58:LEU:HB2 | 2.13 | 0.48 |
| 6:T:56:SER:OG | 6:T:57:LYS:N | 2.44 | 0.48 |
| 14:2:174:ARG:NH1 | 14:2:18(A):ILE:HD13 | 2.28 | 0.48 |
| 4:D:185:THR:OG1 | 4:D:188:GLU:HG3 | 2.13 | 0.48 |
| 4:D:196:ILE:N | 4:D:196:ILE:HD13 | 2.27 | 0.48 |
| 5:E:210:LEU:CD2 | 5:E:233:ILE:HD11 | 2.44 | 0.48 |
| 6:T:35:THR:CG2 | 6:T:36:THR:N | 2.77 | 0.48 |
| 5:E:67:ILE:HG21 | 5:E:223:ILE:HD12 | 1.95 | 0.48 |
| 9:I:160:LEU:HD11 | 9:I:191:MET:HB3 | 1.96 | 0.48 |
| 9:I:19:ARG:HB2 | 9:I:171:TRP:HB2 | 1.95 | 0.48 |
| 10:X:161:GLU:OE2 | 10:X:161:GLU:HA | 2.12 | 0.48 |
| 14:2:54:ALA:O | 14:2:58:ILE:HG13 | 2.13 | 0.48 |
| 2:B:191:GLU:O | 2:B:195:LYS:HG2 | 2.13 | 0.48 |
| 3:C:163:GLN:HA | 3:C:163:GLN:HE21 | 1.79 | 0.48 |
| 11:K:86:LEU:HD13 | 11:K:86:LEU:C | 2.34 | 0.48 |
| 2:P:101:LYS:HZ1 | 10:X:85:GLN:NE2 | 2.09 | 0.48 |
| 5:S:175:TYR:CD2 | 5:S:196:ALA:HA | 2.48 | 0.48 |
| 5:S:52:LYS:HD2 | 5:S:63:TYR:O | 2.13 | 0.48 |
| 7:U:147:SER:O | 7:U:148:ILE:HD12 | 2.11 | 0.48 |
| 9:W:18:LEU:CD2 | 9:W:32:GLU:HG2 | 2.43 | 0.48 |
| 9:I:18:LEU:CD2 | 9:I:32:GLU:HG2 | 2.44 | 0.48 |
| 3:Q:31:VAL:HG11 | 3:Q:135:SER:HB2 | 1.96 | 0.48 |
| 3:Q:156:ILE:CD1 | 4:R:83:ALA:HB2 | 2.44 | 0.48 |
| 3:Q:235:GLN:O | 3:Q:239:GLU:HG2 | 2.14 | 0.48 |
| 8:V:37:ILE:HG21 | 8:V:63:ILE:HD12 | 1.93 | 0.48 |
| 2:B:185:LYS:CD | 2:B:187:ASP:H | 2.26 | 0.48 |
| 2:B:51:GLU:OE2 | 2:B:209:ARG:NH2 | 2.47 | 0.48 |
| 3:C:163:GLN:CA | 3:C:163:GLN:HE21 | 2.27 | 0.48 |
| 9:I:156:SER:O | 9:I:160:LEU:HB2 | 2.14 | 0.48 |
| 9:I:178:ILE:N | 9:I:178:ILE:HD12 | 2.29 | 0.48 |
| 10:J:133:TYR:OH | 10:X:24:ILE:HG13 | 2.14 | 0.48 |
| 10:J:177:ILE:CD1 | 10:J:187:VAL:CG2 | 2.86 | 0.48 |
| 3:Q:187:GLU:HG3 | 3:Q:232:TYR:OH | 2.14 | 0.48 |
| 3:Q:227:GLU:H | 3:Q:227:GLU:CD | 2.17 | 0.48 |
| 5:S:214:ILE:HD13 | 5:S:214:ILE:C | 2.33 | 0.48 |
| 1:O:97:HIS:HD2 | 8:V:61:SER:OG | 1.96 | 0.48 |
| 1:A:222:ARG:HD2 | 16:A:275:HOH:O | 2.13 | 0.48 |
| 2:B:147:GLN:CG | 3:C:62(A):ILE:HD13 | 2.43 | 0.48 |
| 4:D:121:LEU:HD23 | 4:D:123:PHE:HE1 | 1.79 | 0.48 |
| 5:E:175:TYR:CD2 | 5:E:196:ALA:HA | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:E:201:LEU:HD11 | 5:E:207:LEU:CD2 | 2.43 | 0.48 |
| 5:E:82:ALA:HB3 | 5:E:83:PRO:HD3 | 1.95 | 0.48 |
| 6:F:187:ARG:HG3 | 6:F:187:ARG:HH11 | 1.79 | 0.48 |
| 8:H:208:ARG:CZ | 9:I:149:GLU:HB2 | 2.44 | 0.48 |
| 2:P:27:ALA:O | 2:P:31:ILE:HG13 | 2.14 | 0.48 |
| 3:Q:14:ILE:C | 3:Q:21:ILE:HD13 | 2.34 | 0.48 |
| 3:Q:55:THR:C | 3:Q:56:LEU:HD22 | 2.34 | 0.48 |
| 3:Q:79:SER:HB2 | 3:Q:165:ILE:HD12 | 1.96 | 0.48 |
| 5:S:66:LYS:O | 5:S:77:SER:HA | 2.13 | 0.48 |
| 7:U:56:ASP:HB3 | 7:U:59:LEU:HG | 1.95 | 0.48 |
| 12:Z:90:LYS:HD3 | 12:Z:95:TYR:CZ | 2.48 | 0.48 |
| 2:B:69:LYS:HG3 | 2:B:221:GLN:OE1 | 2.14 | 0.48 |
| 3:C:38:VAL:HG22 | 3:C:39:GLY:N | 2.29 | 0.48 |
| 5:E:28:LEU:CA | 5:E:31:ILE:HD13 | 2.37 | 0.48 |
| 5:E:4:PHE:CG | 5:E:5:ARG:N | 2.82 | 0.48 |
| 10:J:177:ILE:N | 10:J:177:ILE:HD12 | 2.29 | 0.48 |
| 2:P:185:LYS:HD3 | 2:P:186:VAL:H | 1.79 | 0.48 |
| 2:P:51:GLU:OE2 | 2:P:202:THR:HG23 | 2.13 | 0.48 |
| 6:T:41:LYS:HA | 6:T:46:VAL:HG12 | 1.96 | 0.48 |
| 7:U:18(D):ILE:H | 7:U:18(D):ILE:CD1 | 2.24 | 0.48 |
| 7:U:78:VAL:HG11 | 7:U:85:ALA:HB2 | 1.96 | 0.48 |
| 9:W:178:ILE:N | 9:W:178:ILE:HD12 | 2.29 | 0.48 |
| 10:X:143:ARG:HG2 | 10:X:143:ARG:NH1 | 2.29 | 0.48 |
| 11:K:207:ASN:ND2 | 10:X:144:PRO:HG3 | 2.28 | 0.48 |
| 1:A:141:HIS:HA | 1:A:146:GLY:O | 2.14 | 0.47 |
| 3:C:79:SER:HB2 | 3:C:165:ILE:HD12 | 1.96 | 0.47 |
| 3:Q:134:VAL:HG12 | 3:Q:135:SER:N | 2.29 | 0.47 |
| 6:T:172:ALA:O | 6:T:176:LEU:HD23 | 2.14 | 0.47 |
| 3:C:235:GLN:O | 3:C:239:GLU:HG2 | 2.14 | 0.47 |
| 7:G:232:ARG:NE | 7:G:232:ARG:HA | 2.28 | 0.47 |
| 9:I:28:SER:CB | 10:J:120:VAL:HG21 | 2.44 | 0.47 |
| 14:N:155:ILE:HG22 | 14:N:175:MET:HE1 | 1.96 | 0.47 |
| 14:N:3:ILE:HG22 | 14:N:16:ALA:CB | 2.43 | 0.47 |
| 1:O:141:HIS:HA | 1:O:146:GLY:O | 2.14 | 0.47 |
| 1:O:62:GLU:CD | 1:O:62:GLU:H | 2.16 | 0.47 |
| 5:S:4:PHE:CG | 5:S:5:ARG:N | 2.81 | 0.47 |
| 8:V:17:ASP:CB | 8:V:163:ILE:HD11 | 2.44 | 0.47 |
| 10:X:90(B):ARG:HH11 | 10:X:90(B):ARG:HG2 | 1.78 | 0.47 |
| 12:Z:145:TYR:CD1 | 12:Z:146:LEU:N | 2.82 | 0.47 |
| 13:1:-4:ILE:HD12 | 14:2:116:GLY:HA2 | 1.96 | 0.47 |
| 1:A:40:ILE:HD12 | 1:A:193:ALA:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:97:GLN:NE2 | 16:C:244:HOH:O | 2.43 | 0.47 |
| 6:F:176:LEU:O | 6:F:180:VAL:HG23 | 2.14 | 0.47 |
| 6:F:41:LYS:HA | 6:F:46:VAL:HG12 | 1.96 | 0.47 |
| 6:F:49:ALA:HB3 | 6:F:197:ILE:HD11 | 1.96 | 0.47 |
| 6:F:67:ILE:HD13 | 6:F:77:VAL:CG2 | 2.44 | 0.47 |
| 7:G:49:ILE:HD13 | 7:G:193:ALA:HB1 | 1.95 | 0.47 |
| 7:G:8:TYR:C | 7:G:10:ARG:N | 2.68 | 0.47 |
| 12:L:76:ILE:CD1 | 12:L:101:ILE:HD13 | 2.41 | 0.47 |
| 7:U:177:GLU:O | 7:U:17(B):LYS:HG3 | 2.15 | 0.47 |
| 8:V:175:VAL:HG12 | 8:V:176:CYS:N | 2.29 | 0.47 |
| 9:W:160:LEU:HD11 | 9:W:191:MET:HB3 | 1.96 | 0.47 |
| 11:Y:4:LEU:O | 11:Y:4:LEU:HD22 | 2.14 | 0.47 |
| 14:2:3:ILE:HG22 | 14:2:16:ALA:HB2 | 1.96 | 0.47 |
| 1:A:60:MET:HE1 | 16:G:269:HOH:O | 2.13 | 0.47 |
| 5:E:74:MET:HE1 | 5:E:96:CYS:SG | 2.53 | 0.47 |
| 7:G:77:VAL:HG12 | 7:G:137:THR:HB | 1.97 | 0.47 |
| 9:I:110:ILE:HG12 | 9:I:125:ILE:HD11 | 1.96 | 0.47 |
| 5:S:69:LYS:HB3 | 16:S:237:HOH:O | 2.14 | 0.47 |
| 12:Z:9:GLU:O | 12:Z:107:LYS:HA | 2.14 | 0.47 |
| 12:Z:4:LEU:HG | 12:Z:6:ILE:CD1 | 2.45 | 0.47 |
| 13:1:8:TYR:CZ | 13:1:148:VAL:HG13 | 2.50 | 0.47 |
| 2:B:150:THR:O | 2:B:157:TYR:HA | 2.14 | 0.47 |
| 4:D:196:ILE:H | 4:D:196:ILE:CD1 | 2.27 | 0.47 |
| 6:F:127:ASN:HD22 | 6:F:128:SER:N | 2.13 | 0.47 |
| 7:G:141:VAL:HG21 | 7:G:216:THR:HA | 1.97 | 0.47 |
| 9:I:14:ILE:HG12 | 9:I:34:ILE:HD12 | 1.96 | 0.47 |
| 10:J:123:PRO:HB2 | 10:J:124:TYR:CD1 | 2.50 | 0.47 |
| 11:K:123:ASP:CB | 11:K:124:ILE:HD12 | 2.43 | 0.47 |
| 1:O:71:THR:HG1 | 1:O:74:ILE:HD13 | 1.79 | 0.47 |
| 2:P:21:LEU:O | 2:P:25:GLU:HG2 | 2.15 | 0.47 |
| 10:X:76:PRO:HD2 | 16:X:205:HOH:O | 2.15 | 0.47 |
| 12:Z:167:ILE:C | 12:Z:167:ILE:HD12 | 2.35 | 0.47 |
| 12:Z:-9:GLN:HE21 | 13:1:-8:THR:HG21 | 1.80 | 0.47 |
| 14:2:3:ILE:HD13 | 14:2:3:ILE:N | 2.29 | 0.47 |
| 7:U:82:ILE:N | 7:U:83:PRO:HD2 | 2.30 | 0.47 |
| 13:M:165:ARG:HA | 14:2:26:ILE:HB | 1.96 | 0.47 |
| 2:B:111:ILE:H | 2:B:111:ILE:HD12 | 1.80 | 0.47 |
| 3:C:31:VAL:HG11 | 3:C:135:SER:HB2 | 1.95 | 0.47 |
| 3:C:33:ARG:CB | 3:C:33:ARG:NH1 | 2.72 | 0.47 |
| 6:F:192:GLN:NE2 | 6:F:195:LYS:HE3 | 2.28 | 0.47 |
| 9:I:101:VAL:O | 9:I:110:ILE:HA | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:I:6:MET:CE | 9:I:155:ILE:HA | 2.45 | 0.47 |
| 10:J:167:PRO:CB | 10:X:168:MET:HE1 | 2.42 | 0.47 |
| 12:L:114:ASP:HB3 | 12:L:118:SER:H | 1.79 | 0.47 |
| 5:S:136:LEU:HB2 | 5:S:151:PHE:HB3 | 1.96 | 0.47 |
| 7:U:41:ARG:NH2 | 7:U:18(B):ASP:O | 2.48 | 0.47 |
| 13:1:40:ASN:ND2 | 13:1:40:ASN:N | 2.62 | 0.47 |
| 2:B:160:TRP:CD2 | 2:B:163:ILE:HD12 | 2.49 | 0.47 |
| 5:E:216:GLY:O | 5:E:219:THR:N | 2.47 | 0.47 |
| 6:F:109:ILE:HD12 | 6:F:109:ILE:N | 2.29 | 0.47 |
| 12:L:-2:ASN:HA | 12:L:21:ILE:O | 2.14 | 0.47 |
| 13:M:112:TYR:HE1 | 13:M:127:THR:HG22 | 1.79 | 0.47 |
| 2:P:108:PRO:HG2 | 2:P:111:ILE:HD12 | 1.96 | 0.47 |
| 4:R:243:ALA:O | 4:R:244:GLU:HG2 | 2.15 | 0.47 |
| 7:U:232:ARG:HA | 7:U:232:ARG:NE | 2.30 | 0.47 |
| 13:1:20:GLY:HA2 | 13:1:49:ILE:HD11 | 1.97 | 0.47 |
| 13:1:4:ILE:C | 13:1:4:ILE:HD12 | 2.34 | 0.47 |
| 3:C:134:VAL:HG12 | 3:C:135:SER:N | 2.29 | 0.47 |
| 3:C:76:LEU:HD12 | 3:C:138:ILE:HG12 | 1.96 | 0.47 |
| 5:E:194:VAL:CG1 | 5:E:207:LEU:HD11 | 2.44 | 0.47 |
| 5:E:90:ASN:O | 5:E:94:GLN:HG3 | 2.15 | 0.47 |
| 8:H:165:ASN:HD22 | 13:1:139:ARG:NH1 | 1.99 | 0.47 |
| 9:I:28:SER:HB2 | 10:J:120:VAL:HG21 | 1.96 | 0.47 |
| 14:N:84:LYS:HG3 | 14:N:119:VAL:CG2 | 2.45 | 0.47 |
| 2:P:229:ILE:O | 2:P:233:LEU:HB2 | 2.15 | 0.47 |
| 9:I:165:ARG:NH2 | 12:Z:135:MET:HE2 | 2.29 | 0.47 |
| 5:E:66:LYS:O | 5:E:77:SER:HA | 2.14 | 0.47 |
| 6:F:35:THR:CG2 | 6:F:36:THR:N | 2.77 | 0.47 |
| 7:G:78:VAL:HG11 | 7:G:85:ALA:HB2 | 1.97 | 0.47 |
| 9:I:137:MET:CE | 9:I:141:LEU:HD11 | 2.44 | 0.47 |
| 11:K:111:TYR:CE1 | 11:K:121:LYS:HB2 | 2.50 | 0.47 |
| 3:Q:163:GLN:HA | 3:Q:163:GLN:HE21 | 1.80 | 0.47 |
| 11:Y:10(A):ARG:NH1 | 11:Y:10(A):ARG:HG2 | 2.30 | 0.47 |
| 14:2:100:ILE:N | 14:2:100:ILE:HD12 | 2.29 | 0.47 |
| 1:A:138:ILE:HD12 | 1:A:138:ILE:N | 2.30 | 0.47 |
| 11:K:13:ILE:HG13 | 11:K:151:ALA:HB1 | 1.96 | 0.47 |
| 12:L:101:ILE:HD11 | 12:L:111:TYR:HB2 | 1.97 | 0.47 |
| 1:O:122:GLU:C | 1:O:124:THR:H | 2.18 | 0.47 |
| 1:O:40:ILE:HD12 | 1:O:193:ALA:HB2 | 1.95 | 0.47 |
| 2:P:185:LYS:HE2 | 2:P:187:ASP:OD1 | 2.14 | 0.47 |
| 4:R:170:GLU:HG2 | 4:R:171:GLY:N | 2.30 | 0.47 |
| 6:T:74:ILE:HG12 | 6:T:109:ILE:HD13 | 1.93 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 10:X:38:SER:HB2 | 10:X:39:PRO:HD2 | 1.97 | 0.47 |
| 1:O:92:SER:O | 1:O:95:VAL:HG12 | 2.15 | 0.46 |
| 5:S:45:HIS:HB2 | 5:S:189:LEU:HD12 | 1.97 | 0.46 |
| 10:X:90(A):ILE:HD11 | 10:X:116:LEU:HD23 | 1.96 | 0.46 |
| 14:2:19:ARG:CD | 14:2:26:ILE:CD1 | 2.92 | 0.46 |
| 3:C:97:GLN:HG3 | 10:J:65:LEU:HB2 | 1.97 | 0.46 |
| 2:P:191:GLU:O | 2:P:195:LYS:HG2 | 2.15 | 0.46 |
| 3:Q:190:VAL:O | 3:Q:194:VAL:HG23 | 2.14 | 0.46 |
| 2:P:121:GLN:CG | 3:Q:83:ALA:HB1 | 2.45 | 0.46 |
| 8:V:18:THR:HB | 8:V:30:ASN:HD22 | 1.80 | 0.46 |
| 10:J:144:PRO:HG3 | 11:Y:207:ASN:ND2 | 2.30 | 0.46 |
| 5:E:227:GLU:CD | 5:E:227:GLU:H | 2.17 | 0.46 |
| 6:F:87:HIS:HD2 | 6:F:132:PHE:CE2 | 2.33 | 0.46 |
| 2:B:144:ARG:NH1 | 10:J:72:TYR:HB2 | 2.30 | 0.46 |
| 13:M:110:LEU:HG | 13:M:125:LEU:HD12 | 1.97 | 0.46 |
| 2:P:235:LYS:N | 2:P:235:LYS:HD3 | 2.30 | 0.46 |
| 7:U:141:VAL:HG21 | 7:U:216:THR:HA | 1.97 | 0.46 |
| 13:1:46:SER:OG | 13:1:98:ALA:HB3 | 2.16 | 0.46 |
| 14:2:116:GLY:HA3 | 16:2:1408:HOH:O | 2.15 | 0.46 |
| 2:B:141:TYR:C | 2:B:141:TYR:CD1 | 2.89 | 0.46 |
| 3:C:89:ILE:CD1 | 3:C:89:ILE:N | 2.77 | 0.46 |
| 6:F:18:ASP:N | 6:F:18:ASP:OD2 | 2.42 | 0.46 |
| 8:H:2:THR:OG1 | 8:H:130:GLY:HA3 | 2.15 | 0.46 |
| 11:K:10(B):LYS:CD | 11:K:10(B):LYS:N | 2.58 | 0.46 |
| 5:S:227:GLU:CD | 5:S:227:GLU:H | 2.17 | 0.46 |
| 6:T:187:ARG:HH11 | 6:T:187:ARG:HG3 | 1.80 | 0.46 |
| 1:A:136:LEU:HB2 | 1:A:138:ILE:HD11 | 1.98 | 0.46 |
| 3:C:190:VAL:O | 3:C:194:VAL:HG23 | 2.15 | 0.46 |
| 4:D:170:GLU:HG2 | 4:D:171:GLY:N | 2.30 | 0.46 |
| 6:F:109:ILE:HG21 | 6:F:147:HIS:HB2 | 1.98 | 0.46 |
| 12:L:3:ILE:CD1 | 12:L:127:GLY:O | 2.59 | 0.46 |
| 2:P:185:LYS:CD | 2:P:187:ASP:H | 2.28 | 0.46 |
| 4:R:121:LEU:N | 16:R:853:HOH:O | 2.42 | 0.46 |
| 6:T:50:VAL:HG22 | 6:T:51:GLU:N | 2.30 | 0.46 |
| 8:V:105:ASP:HB2 | 8:V:10(A):PRO:HD2 | 1.97 | 0.46 |
| 10:X:147:THR:HG23 | 10:X:150:GLU:OE2 | 2.16 | 0.46 |
| 13:1:112:TYR:HE1 | 13:1:127:THR:HG22 | 1.80 | 0.46 |
| 2:B:196:THR:O | 2:B:200:THR:HG23 | 2.16 | 0.46 |
| 3:C:55:THR:C | 3:C:56:LEU:HD22 | 2.35 | 0.46 |
| 5:E:18(D):ILE:HG13 | 5:E:18(D):ILE:O | 2.15 | 0.46 |
| 10:J:168:MET:HE3 | 10:X:168:MET:CE | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:P:235:LYS:C | 2:P:237:GLY:H | 2.19 | 0.46 |
| 6:T:127:ASN:HD22 | 6:T:128:SER:N | 2.13 | 0.46 |
| 14:2:107:LYS:CG | 14:2:108:GLY:H | 2.28 | 0.46 |
| 14:2:41:ILE:HD13 | 14:2:103:GLY:HA3 | 1.97 | 0.46 |
| 12:Z:76:ILE:CD1 | 12:Z:101:ILE:HD13 | 2.45 | 0.46 |
| 2:B:224:PHE:N | 2:B:224:PHE:CD2 | 2.84 | 0.46 |
| 10:J:18:LYS:CD | 10:J:174:ILE:HG13 | 2.41 | 0.46 |
| 5:S:214:ILE:HD13 | 5:S:215:VAL:CA | 2.45 | 0.46 |
| 7:U:34:THR:O | 7:U:35:ILE:HG13 | 2.15 | 0.46 |
| 9:W:6:MET:CE | 9:W:155:ILE:HA | 2.45 | 0.46 |
| 11:Y:10(A):ARG:HB3 | 11:Y:10(B):LYS:CE | 2.45 | 0.46 |
| 2:B:235:LYS:HD3 | 2:B:235:LYS:N | 2.31 | 0.46 |
| 5:E:11:ASP:OD1 | 5:E:13:VAL:HG12 | 2.16 | 0.46 |
| 6:F:50:VAL:HG22 | 6:F:51:GLU:N | 2.30 | 0.46 |
| 6:F:36:THR:CG2 | 6:F:51:GLU:OE2 | 2.64 | 0.46 |
| 8:H:105:ASP:HB2 | 8:H:10(A):PRO:HD2 | 1.98 | 0.46 |
| 12:L:9:GLU:O | 12:L:107:LYS:HA | 2.16 | 0.46 |
| 13:M:186:PHE:CE1 | 13:M:188:LYS:HG3 | 2.51 | 0.46 |
| 14:N:3:ILE:HG22 | 14:N:16:ALA:HB2 | 1.98 | 0.46 |
| 1:O:206:PHE:CD1 | 1:O:210:ILE:HD11 | 2.50 | 0.46 |
| 5:S:95:GLN:HG3 | 5:S:115:LEU:HD13 | 1.97 | 0.46 |
| 13:1:186:PHE:CE1 | 13:1:188:LYS:HG3 | 2.51 | 0.46 |
| 4:D:117:CYS:HB3 | 4:D:155:GLY:O | 2.15 | 0.46 |
| 11:K:180:GLU:N | 16:K:1426:HOH:O | 2.41 | 0.46 |
| 2:P:69:LYS:HG3 | 2:P:221:GLN:OE1 | 2.16 | 0.46 |
| 3:Q:163:GLN:HE21 | 3:Q:163:GLN:CA | 2.28 | 0.46 |
| 6:T:54:ILE:HG12 | 6:T:208:PHE:CA | 2.45 | 0.46 |
| 9:W:-8:SER:O | 9:W:-6:PRO:HD3 | 2.16 | 0.46 |
| 14:2:84:LYS:HG3 | 14:2:119:VAL:CG2 | 2.46 | 0.45 |
| 1:A:62:GLU:H | 1:A:62:GLU:CD | 2.18 | 0.45 |
| 3:C:197:LEU:HD13 | 3:C:210:ILE:CD1 | 2.15 | 0.45 |
| 5:E:52:LYS:HD2 | 5:E:63:TYR:O | 2.16 | 0.45 |
| 7:G:41:ARG:NH2 | 7:G:18(B):ASP:O | 2.50 | 0.45 |
| 7:G:192:PHE:CD1 | 7:G:192:PHE:C | 2.89 | 0.45 |
| 8:H:52:THR:O | 8:H:56:THR:HB | 2.16 | 0.45 |
| 10:J:113:ILE:HA | 10:J:118:THR:O | 2.16 | 0.45 |
| 2:P:160:TRP:CD2 | 2:P:163:ILE:HD12 | 2.51 | 0.45 |
| 5:S:79:ALA:HA | 16:S:235:HOH:O | 2.16 | 0.45 |
| 6:T:87:HIS:HD2 | 6:T:132:PHE:CE2 | 2.35 | 0.45 |
| 9:W:12:VAL:HG22 | 9:W:104:ILE:CD1 | 2.46 | 0.45 |
| 10:X:88:ALA:O | 10:X:90(A):ILE:HG22 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:Z:101:ILE:HD11 | 12:Z:111:TYR:HB2 | 1.98 | 0.45 |
| 1:A:161:LYS:HE3 | 2:B:60:GLU:OE1 | 2.16 | 0.45 |
| 2:B:229:ILE:O | 2:B:233:LEU:HB2 | 2.16 | 0.45 |
| 8:H:34:LEU:HB2 | 16:H:1425:HOH:O | 2.15 | 0.45 |
| 9:I:55:LEU:HD21 | 9:I:95:TYR:CD1 | 2.51 | 0.45 |
| 11:K:10(A):ARG:NH1 | 11:K:10(A):ARG:HG2 | 2.30 | 0.45 |
| 4:R:121:LEU:HD23 | 4:R:123:PHE:HE1 | 1.81 | 0.45 |
| 5:S:111:ARG:HG2 | 5:S:111:ARG:HH11 | 1.81 | 0.45 |
| 7:U:8:TYR:C | 7:U:10:ARG:N | 2.68 | 0.45 |
| 9:W:137:MET:CE | 9:W:141:LEU:HD11 | 2.46 | 0.45 |
| 9:W:156:SER:O | 9:W:160:LEU:HB2 | 2.16 | 0.45 |
| 11:Y:4:LEU:C | 11:Y:4:LEU:HD22 | 2.36 | 0.45 |
| 12:Z:99:THR:CG2 | 16:Z:202:HOH:O | 2.59 | 0.45 |
| 13:1:201:LYS:HA | 16:1:255:HOH:O | 2.16 | 0.45 |
| 14:2:4:MET:HB3 | 14:2:126:ILE:HG22 | 1.99 | 0.45 |
| 3:C:158:SER:CB | 4:D:59:LEU:HD21 | 2.46 | 0.45 |
| 4:D:227:GLU:OE2 | 4:D:227:GLU:N | 2.42 | 0.45 |
| 5:E:39:GLY:O | 5:E:162:GLY:HA2 | 2.15 | 0.45 |
| 7:G:49:ILE:HD13 | 7:G:193:ALA:CB | 2.46 | 0.45 |
| 8:H:155:ALA:O | 8:H:159:ILE:CD1 | 2.60 | 0.45 |
| 10:J:161:GLU:HA | 10:J:161:GLU:OE2 | 2.16 | 0.45 |
| 1:O:33:GLN:CA | 1:O:33:GLN:HE21 | 2.23 | 0.45 |
| 8:V:2:THR:OG1 | 8:V:130:GLY:HA3 | 2.15 | 0.45 |
| 13:1:113:VAL:HA | 13:1:118:VAL:O | 2.17 | 0.45 |
| 1:A:205:GLU:OE2 | 1:A:205:GLU:HA | 2.17 | 0.45 |
| 6:F:54:ILE:HG12 | 6:F:208:PHE:CA | 2.46 | 0.45 |
| 7:G:96:ALA:HA | 7:G:107:MET:CE | 2.31 | 0.45 |
| 14:N:146:MET:CE | 14:N:150:GLU:HB3 | 2.43 | 0.45 |
| 4:R:117:CYS:HB3 | 4:R:155:GLY:O | 2.16 | 0.45 |
| 5:S:31:ILE:HD11 | 5:S:153:PRO:CD | 2.46 | 0.45 |
| 9:W:55:LEU:HD11 | 9:W:97:VAL:HG21 | 1.97 | 0.45 |
| 10:X:159:VAL:O | 10:X:163:GLU:HG3 | 2.17 | 0.45 |
| 12:Z:84:GLN:HG3 | 12:Z:117:GLY:O | 2.16 | 0.45 |
| 2:B:147:GLN:CB | 3:C:62(A):ILE:HD13 | 2.47 | 0.45 |
| 7:G:188:LYS:HD3 | 7:G:191:GLU:OE2 | 2.15 | 0.45 |
| 8:H:175:VAL:HG12 | 8:H:176:CYS:N | 2.31 | 0.45 |
| 1:O:205:GLU:HA | 1:O:205:GLU:OE2 | 2.15 | 0.45 |
| 2:P:122:GLY:C | 2:P:124:THR:H | 2.20 | 0.45 |
| 3:Q:89:ILE:N | 3:Q:89:ILE:CD1 | 2.80 | 0.45 |
| 6:T:109:ILE:HG21 | 6:T:147:HIS:HB2 | 1.98 | 0.45 |
| 6:T:36:THR:HG22 | 6:T:51:GLU:OE2 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:V:3:ILE:HD11 | 8:V:127:LEU:HB2 | 1.98 | 0.45 |
| 10:X:111:TYR:CE1 | 10:X:121:GLU:HG3 | 2.51 | 0.45 |
| 10:X:7:ARG:NH1 | 10:X:7:ARG:HG2 | 2.30 | 0.45 |
| 11:Y:128:GLY:O | 11:Y:131:GLN:HG2 | 2.16 | 0.45 |
| 3:C:76:LEU:HD22 | 3:C:89:ILE:HD11 | 1.99 | 0.45 |
| 2:P:150:THR:O | 2:P:157:TYR:HA | 2.16 | 0.45 |
| 2:P:224:PHE:N | 2:P:224:PHE:CD2 | 2.84 | 0.45 |
| 2:B:143:ASP:OD2 | 10:J:10(B):LYS:HE2 | 2.17 | 0.45 |
| 5:E:52:LYS:HB2 | 5:E:63:TYR:HB3 | 1.97 | 0.45 |
| 6:F:127:ASN:H | 6:F:127:ASN:ND2 | 2.15 | 0.45 |
| 7:G:82:ILE:N | 7:G:83:PRO:HD2 | 2.31 | 0.45 |
| 7:U:83:PRO:HG2 | 16:U:267:HOH:O | 2.16 | 0.45 |
| 10:J:168:MET:HE2 | 10:X:168:MET:HE2 | 1.99 | 0.45 |
| 12:Z:13:VAL:HG12 | 12:Z:177:ILE:HG13 | 1.98 | 0.45 |
| 9:I:125:ILE:N | 9:I:125:ILE:HD12 | 2.30 | 0.45 |
| 10:J:143:ARG:HA | 10:J:144:PRO:HD3 | 1.87 | 0.45 |
| 12:L:140:ASN:O | 12:L:144:PHE:HA | 2.17 | 0.45 |
| 1:O:6:ASP:OD2 | 1:O:8:TYR:HB2 | 2.17 | 0.45 |
| 3:Q:156:ILE:HD11 | 4:R:83:ALA:N | 2.31 | 0.45 |
| 11:Y:25:TRP:CH2 | 12:Z:132:SER:HA | 2.52 | 0.45 |
| 2:B:224:PHE:HD2 | 2:B:224:PHE:N | 2.14 | 0.45 |
| 3:C:232:TYR:O | 3:C:236:ILE:HG13 | 2.17 | 0.45 |
| 4:D:243:ALA:O | 4:D:244:GLU:HG2 | 2.17 | 0.45 |
| 13:M:46:SER:OG | 13:M:98:ALA:HB3 | 2.17 | 0.45 |
| 14:N:33:LYS:HE2 | 15:N:1404:BO2:H222 | 1.99 | 0.45 |
| 2:P:141:TYR:C | 2:P:141:TYR:CD1 | 2.89 | 0.45 |
| 3:Q:18(A):ASP:OD2 | 3:Q:18(C):LYS:HG2 | 2.16 | 0.45 |
| 7:U:49:ILE:HD13 | 7:U:193:ALA:CB | 2.46 | 0.45 |
| 13:1:113:VAL:HG23 | 13:1:119:THR:HG22 | 1.98 | 0.45 |
| 13:1:70:ASN:ND2 | 13:1:70(A):ALA:HA | 2.32 | 0.45 |
| 2:B:185:LYS:HD3 | 2:B:186:VAL:H | 1.81 | 0.45 |
| 4:D:91:HIS:CG | 4:D:119:LEU:HD11 | 2.52 | 0.45 |
| 5:E:67:ILE:HD13 | 5:E:77:SER:CB | 2.46 | 0.45 |
| 9:I:113:PHE:CD2 | 9:I:113:PHE:N | 2.85 | 0.45 |
| 10:J:147:THR:HG23 | 10:J:150:GLU:OE2 | 2.17 | 0.45 |
| 10:J:166:MET:HA | 10:J:167:PRO:HD3 | 1.82 | 0.45 |
| 14:N:13:ILE:HD12 | 14:N:177:VAL:CB | 2.46 | 0.45 |
| 1:O:31:VAL:HG11 | 1:O:135:SER:HB2 | 1.98 | 0.45 |
| 2:P:224:PHE:N | 2:P:224:PHE:HD2 | 2.15 | 0.45 |
| 3:Q:43:LYS:HG2 | 3:Q:43:LYS:O | 2.15 | 0.45 |
| 4:R:160:TYR:HA | 5:S:58:LEU:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:T:103:TYR:O | 6:T:104:LYS:HB3 | 2.17 | 0.45 |
| 10:X:112:GLN:HE21 | 10:X:125:GLY:HA3 | 1.83 | 0.45 |
| 12:Z:6:ILE:N | 12:Z:6:ILE:HD12 | 2.32 | 0.45 |
| 1:A:122:GLU:C | 1:A:124:THR:H | 2.19 | 0.44 |
| 2:B:194:LEU:CD1 | 2:B:232:ILE:HD13 | 2.45 | 0.44 |
| 6:F:103:TYR:O | 6:F:104:LYS:HB3 | 2.17 | 0.44 |
| 7:G:18(B):ASP:O | 7:G:18(C):HIS:HB3 | 2.17 | 0.44 |
| 9:I:104:ILE:CD1 | 9:I:179:LYS:C | 2.85 | 0.44 |
| 1:O:86:ARG:HH21 | 7:U:118:ASN:HD22 | 1.65 | 0.44 |
| 4:R:112:LEU:C | 4:R:112:LEU:HD13 | 2.38 | 0.44 |
| 6:T:36:THR:CG2 | 6:T:51:GLU:OE2 | 2.65 | 0.44 |
| 11:Y:37:ILE:HB | 11:Y:41:LEU:CB | 2.45 | 0.44 |
| 1:A:188:ASP:O | 1:A:192:ILE:HG12 | 2.18 | 0.44 |
| 2:B:235:LYS:C | 2:B:237:GLY:H | 2.20 | 0.44 |
| 2:B:94:ILE:CD1 | 2:B:94:ILE:N | 2.80 | 0.44 |
| 5:E:216:GLY:O | 5:E:217:LYS:C | 2.56 | 0.44 |
| 1:A:86:ARG:HH21 | 7:G:118:ASN:HD22 | 1.65 | 0.44 |
| 1:A:86:ARG:HH21 | 7:G:118:ASN:ND2 | 2.16 | 0.44 |
| 7:G:29:LYS:HA | 7:G:29:LYS:HD2 | 1.75 | 0.44 |
| 9:I:159:LEU:HD21 | 9:I:173:ALA:HB1 | 1.99 | 0.44 |
| 11:K:200:LYS:HG3 | 11:K:205:SER:O | 2.17 | 0.44 |
| 12:L:1:GLY:N | 16:L:218:HOH:O | 2.50 | 0.44 |
| 5:S:77:SER:OG | 5:S:137:LEU:HB2 | 2.17 | 0.44 |
| 11:Y:13:ILE:HG13 | 11:Y:151:ALA:HB1 | 1.97 | 0.44 |
| 13:1:4:ILE:HD13 | 13:1:155:ILE:HG12 | 2.00 | 0.44 |
| 1:A:15:PHE:N | 2:B:23:GLN:HE22 | 1.93 | 0.44 |
| 2:B:6:ARG:HG3 | 2:B:6:ARG:HH11 | 1.82 | 0.44 |
| 3:C:187:GLU:HG3 | 3:C:232:TYR:OH | 2.17 | 0.44 |
| 3:C:177:GLU:OE2 | 4:D:57:PRO:HD2 | 2.16 | 0.44 |
| 5:E:136:LEU:HB2 | 5:E:151:PHE:HB3 | 1.98 | 0.44 |
| 5:E:18(F):ILE:O | 5:E:18(F):ILE:HG22 | 2.17 | 0.44 |
| 5:E:222:THR:C | 5:E:223:ILE:HD13 | 2.38 | 0.44 |
| 7:G:38:LEU:HD12 | 7:G:38:LEU:C | 2.37 | 0.44 |
| 8:H:41:ILE:CD1 | 8:H:76:VAL:HG22 | 2.29 | 0.44 |
| 9:I:-6:PRO:HA | 9:I:-3:ILE:HD12 | 2.00 | 0.44 |
| 10:J:36:GLN:HG3 | 10:J:184:ILE:HD12 | 1.99 | 0.44 |
| 11:K:128:GLY:O | 11:K:131:GLN:HG2 | 2.17 | 0.44 |
| 14:N:13:ILE:CD1 | 14:N:177:VAL:HA | 2.41 | 0.44 |
| 4:R:170:GLU:OE1 | 4:R:170:GLU:N | 2.46 | 0.44 |
| 7:U:77:VAL:HG12 | 7:U:137:THR:HB | 1.99 | 0.44 |
| 9:W:104:ILE:HD12 | 9:W:104:ILE:N | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:Z:29:ARG:NH1 | 12:Z:171:ASP:OD1 | 2.45 | 0.44 |
| 14:2:21:THR:CG2 | 14:2:26:ILE:CD1 | 2.88 | 0.44 |
| 1:A:117:ALA:HB1 | 1:A:155:GLY:O | 2.17 | 0.44 |
| 1:A:58:LEU:HD12 | 7:G:173:THR:HG23 | 2.00 | 0.44 |
| 7:U:188:LYS:HD3 | 7:U:191:GLU:OE2 | 2.18 | 0.44 |
| 9:W:14:ILE:HG12 | 9:W:34:ILE:CD1 | 2.48 | 0.44 |
| 11:Y:12:ILE:HB | 11:Y:178:VAL:HB | 2.00 | 0.44 |
| 14:2:1:THR:CG2 | 14:2:3:ILE:HD12 | 2.47 | 0.44 |
| 1:A:43:THR:HG23 | 1:A:184:LEU:O | 2.16 | 0.44 |
| 2:B:126:HIS:HB3 | 3:C:129:VAL:HG12 | 1.98 | 0.44 |
| 7:G:34:THR:O | 7:G:35:ILE:HG13 | 2.17 | 0.44 |
| 9:I:176:TYR:HB3 | 9:I:178:ILE:HD11 | 2.00 | 0.44 |
| 10:J:129:TYR:O | 10:J:132:PHE:HB2 | 2.17 | 0.44 |
| 13:M:8:TYR:CZ | 13:M:148:VAL:HG13 | 2.52 | 0.44 |
| 13:M:70:ASN:ND2 | 13:M:70(A):ALA:HA | 2.33 | 0.44 |
| 14:N:20:THR:OG1 | 14:N:28:ASN:HB3 | 2.18 | 0.44 |
| 1:O:4:MET:CG | 1:O:5:THR:H | 2.31 | 0.44 |
| 7:U:119:LEU:HA | 7:U:119:LEU:HD12 | 1.82 | 0.44 |
| 7:U:38:LEU:C | 7:U:38:LEU:HD12 | 2.38 | 0.44 |
| 9:W:104:ILE:HG21 | 9:W:181:LYS:HG2 | 2.00 | 0.44 |
| 2:B:31:ILE:HD11 | 2:B:133:GLY:C | 2.38 | 0.44 |
| 3:C:163:GLN:HA | 3:C:163:GLN:NE2 | 2.33 | 0.44 |
| 13:M:13:ILE:HD12 | 13:M:151:ALA:HB1 | 2.00 | 0.44 |
| 14:N:66:TYR:CD2 | 14:N:74:PRO:HB3 | 2.53 | 0.44 |
| 2:P:196:THR:O | 2:P:200:THR:HG23 | 2.17 | 0.44 |
| 3:Q:232:TYR:O | 3:Q:236:ILE:HG13 | 2.17 | 0.44 |
| 7:U:143:GLU:HA | 7:U:217:LYS:NZ | 2.33 | 0.44 |
| 7:U:18(A):ILE:HD11 | 7:U:18(C):HIS:O | 2.16 | 0.44 |
| 9:W:176:TYR:HB3 | 9:W:178:ILE:HD11 | 2.00 | 0.44 |
| 12:Z:123:GLN:HG3 | 12:Z:145:TYR:OH | 2.18 | 0.44 |
| 13:1:1:THR:OG1 | 13:1:2:SER:N | 2.48 | 0.44 |
| 1:A:6:ASP:OD2 | 1:A:8:TYR:HB2 | 2.18 | 0.44 |
| 2:B:49:ALA:HB2 | 2:B:212:PHE:CE1 | 2.53 | 0.44 |
| 12:L:113:PHE:CD1 | 12:L:113:PHE:N | 2.85 | 0.44 |
| 14:N:105:ASP:OD2 | 14:N:106:ASN:N | 2.46 | 0.44 |
| 6:T:158:TRP:CZ3 | 7:U:64:VAL:HA | 2.52 | 0.44 |
| 6:T:53:LEU:HD11 | 6:T:205:ASN:OD1 | 2.18 | 0.44 |
| 8:V:159:ILE:O | 8:V:163:ILE:CD1 | 2.64 | 0.44 |
| 4:D:122:ARG:HG2 | 4:D:122:ARG:HH11 | 1.82 | 0.44 |
| 10:J:143:ARG:HG2 | 10:J:143:ARG:NH1 | 2.32 | 0.44 |
| 10:J:88:ALA:O | 10:J:90(A):ILE:HG22 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:V:84:LYS:HE2 | 8:V:119:THR:HG23 | 2.00 | 0.44 |
| 12:L:14(C):GLN:HG2 | 8:V:210:THR:HG21 | 2.00 | 0.44 |
| 13:1:14(C):ARG:CG | 13:1:14(C):ARG:NH1 | 2.80 | 0.44 |
| 2:B:156:ASN:ND2 | 3:C:82:ASN:HB2 | 2.33 | 0.44 |
| 3:C:43:LYS:HG2 | 3:C:43:LYS:O | 2.18 | 0.44 |
| 4:D:233:ILE:N | 4:D:233:ILE:CD1 | 2.80 | 0.44 |
| 5:E:111:ARG:HG2 | 5:E:111:ARG:HH11 | 1.82 | 0.44 |
| 6:F:187:ARG:HB2 | 16:F:262:HOH:O | 2.17 | 0.44 |
| 8:H:25:ILE:HD13 | 12:Z:165:ARG:O | 2.18 | 0.44 |
| 10:J:38:SER:HB2 | 10:J:39:PRO:HD2 | 1.99 | 0.44 |
| 11:K:137:VAL:HG21 | 11:K:161:ALA:HB2 | 2.00 | 0.44 |
| 11:K:66:HIS:CE1 | 11:K:74:ILE:HD13 | 2.52 | 0.44 |
| 12:L:123:GLN:HG3 | 12:L:145:TYR:OH | 2.18 | 0.44 |
| 2:P:70:LEU:HD21 | 2:P:89:ILE:CD1 | 2.46 | 0.44 |
| 2:P:95:HIS:CD2 | 2:P:115:ARG:HG2 | 2.52 | 0.44 |
| 3:Q:57:LYS:HZ2 | 3:Q:58:LEU:HA | 1.82 | 0.44 |
| 4:R:159:ARG:HB3 | 5:S:60:SER:CB | 2.47 | 0.44 |
| 5:S:18(F):ILE:HG22 | 5:S:18(F):ILE:O | 2.17 | 0.44 |
| 7:U:192:PHE:CD1 | 7:U:192:PHE:C | 2.89 | 0.44 |
| 9:W:113:PHE:CD2 | 9:W:113:PHE:N | 2.86 | 0.44 |
| 10:X:36:GLN:HG3 | 10:X:184:ILE:HD12 | 2.00 | 0.44 |
| 12:Z:140:ASN:O | 12:Z:144:PHE:HA | 2.17 | 0.44 |
| 3:C:151:THR:HG22 | 3:C:157:TYR:HB3 | 2.00 | 0.43 |
| 3:C:18(A):ASP:OD2 | 3:C:18(C):LYS:HG2 | 2.18 | 0.43 |
| 4:D:39:GLY:O | 4:D:162:ALA:HA | 2.18 | 0.43 |
| 7:G:70:ILE:HD12 | 7:G:92:ALA:HB3 | 2.00 | 0.43 |
| 9:I:6:MET:HG2 | 9:I:124:PHE:HB3 | 2.00 | 0.43 |
| 11:K:123:ASP:C | 11:K:124:ILE:HD12 | 2.38 | 0.43 |
| 12:L:99:THR:C | 12:L:100:ILE:HD12 | 2.38 | 0.43 |
| 4:R:160:TYR:CZ | 4:R:163:LYS:HD3 | 2.54 | 0.43 |
| 5:S:233:ILE:HG22 | 5:S:233:ILE:OXT | 2.17 | 0.43 |
| 7:U:107:MET:CE | 7:U:112:LEU:HD13 | 2.48 | 0.43 |
| 8:V:52:THR:O | 8:V:56:THR:HB | 2.18 | 0.43 |
| 9:W:93:GLY:N | 9:W:94:PRO:CD | 2.81 | 0.43 |
| 12:Z:76:ILE:HD11 | 12:Z:101:ILE:CD1 | 2.44 | 0.43 |
| 2:B:232:ILE:C | 2:B:232:ILE:HD13 | 2.38 | 0.43 |
| 2:B:147:GLN:HB3 | 3:C:62(A):ILE:CD1 | 2.47 | 0.43 |
| 4:D:160:TYR:CZ | 4:D:163:LYS:HD3 | 2.53 | 0.43 |
| 5:E:45:HIS:HB2 | 5:E:189:LEU:HD12 | 1.98 | 0.43 |
| 8:H:105:ASP:HB2 | 8:H:10(A):PRO:CD | 2.48 | 0.43 |
| 10:J:7:ARG:HG2 | 10:J:7:ARG:NH1 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:M:14(G):ILE:HB | 13:M:144:PRO:CD | 2.48 | 0.43 |
| 1:O:21(I):TYR:HE2 | 1:O:21(L):ILE:HD13 | 1.83 | 0.43 |
| 3:Q:125:GLN:NE2 | 16:Q:258:HOH:O | 2.51 | 0.43 |
| 3:Q:156:ILE:HD11 | 4:R:83:ALA:H | 1.82 | 0.43 |
| 3:Q:170:LYS:HB2 | 16:Q:255:HOH:O | 2.17 | 0.43 |
| 1:O:23:GLN:NE2 | 7:U:14:ILE:HD12 | 2.32 | 0.43 |
| 9:W:4:VAL:CG2 | 9:W:155:ILE:HD11 | 2.48 | 0.43 |
| 5:E:160:LEU:HD12 | 5:E:163:THR:HG21 | 2.00 | 0.43 |
| 8:H:3:ILE:HD11 | 8:H:127:LEU:HB2 | 1.99 | 0.43 |
| 8:H:44:ALA:HB3 | 8:H:100:ILE:HB | 2.00 | 0.43 |
| 1:A:144:PHE:CD2 | 9:I:72:ARG:HD2 | 2.53 | 0.43 |
| 13:M:14(G):ILE:N | 13:M:144:PRO:HD2 | 2.33 | 0.43 |
| 3:Q:15:PHE:HA | 3:Q:21:ILE:HD13 | 2.01 | 0.43 |
| 5:S:41:ARG:NH1 | 5:S:42:SER:O | 2.51 | 0.43 |
| 7:U:70:ILE:HD12 | 7:U:92:ALA:HB3 | 2.00 | 0.43 |
| 8:V:3:ILE:HG22 | 8:V:16:ALA:HB2 | 2.01 | 0.43 |
| 12:Z:113:PHE:N | 12:Z:113:PHE:CD1 | 2.86 | 0.43 |
| 12:Z:-2:ASN:HA | 12:Z:21:ILE:O | 2.17 | 0.43 |
| 12:Z:-7:ASN:ND2 | 12:Z:-7:ASN:C | 2.71 | 0.43 |
| 14:2:121:LYS:O | 14:2:122:LEU:HD23 | 2.18 | 0.43 |
| 1:A:97:HIS:CD2 | 8:H:61:SER:OG | 2.69 | 0.43 |
| 2:B:194:LEU:HD12 | 2:B:232:ILE:CD1 | 2.47 | 0.43 |
| 5:E:8:TYR:CE1 | 6:F:10:LEU:HD23 | 2.53 | 0.43 |
| 11:K:208:ASN:HD21 | 9:W:29:ASN:ND2 | 2.13 | 0.43 |
| 1:O:227:GLN:NE2 | 1:O:231:ASP:OD1 | 2.49 | 0.43 |
| 1:O:161:LYS:HD2 | 2:P:58:LEU:HA | 2.00 | 0.43 |
| 3:Q:168:ASN:O | 3:Q:172:VAL:HG12 | 2.19 | 0.43 |
| 3:Q:17:PRO:HA | 4:R:26:TYR:CD1 | 2.54 | 0.43 |
| 5:S:15:PHE:H | 6:T:23:GLN:NE2 | 2.08 | 0.43 |
| 9:W:104:ILE:HD11 | 9:W:178:ILE:HG22 | 1.99 | 0.43 |
| 13:1:14(G):ILE:N | 13:1:144:PRO:HD2 | 2.33 | 0.43 |
| 1:A:86:ARG:HE | 7:G:118:ASN:ND2 | 2.16 | 0.43 |
| 3:C:224:LEU:HD12 | 3:C:224:LEU:N | 2.34 | 0.43 |
| 5:E:41:ARG:NH1 | 5:E:42:SER:O | 2.51 | 0.43 |
| 5:E:58:LEU:CD1 | 5:E:58:LEU:N | 2.81 | 0.43 |
| 5:E:57:GLU:C | 5:E:58:LEU:HD12 | 2.39 | 0.43 |
| 6:F:75:GLY:O | 6:F:138:PHE:HA | 2.19 | 0.43 |
| 7:G:168:LYS:O | 7:G:172:ILE:HG12 | 2.19 | 0.43 |
| 8:H:18:THR:HB | 8:H:30:ASN:HD22 | 1.83 | 0.43 |
| 14:N:126:ILE:N | 14:N:126:ILE:CD1 | 2.81 | 0.43 |
| 5:S:15:PHE:HB2 | 6:T:23:GLN:HE22 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:S:160:LEU:HD12 | 5:S:163:THR:HG21 | 2.00 | 0.43 |
| 11:Y:180:GLU:HB2 | 16:Y:1428:HOH:O | 2.18 | 0.43 |
| 7:G:107:MET:HE3 | 7:G:112:LEU:HD13 | 1.99 | 0.43 |
| 8:H:221:ILE:HD12 | 9:I:40:HIS:HA | 2.01 | 0.43 |
| 9:I:107:LYS:HA | 9:I:108:PRO:HD3 | 1.90 | 0.43 |
| 11:K:99:THR:HG22 | 11:K:113:VAL:O | 2.18 | 0.43 |
| 2:P:194:LEU:O | 2:P:198:SER:HB2 | 2.19 | 0.43 |
| 3:Q:224:LEU:HD12 | 3:Q:224:LEU:N | 2.34 | 0.43 |
| 5:S:2(C):VAL:HG22 | 5:S:226:GLY:HA2 | 2.00 | 0.43 |
| 7:U:39:ALA:HA | 7:U:47:VAL:O | 2.19 | 0.43 |
| 9:W:137:MET:HE3 | 9:W:141:LEU:HD11 | 2.01 | 0.43 |
| 11:Y:6:PHE:HA | 11:Y:123:ASP:O | 2.18 | 0.43 |
| 13:1:83:LEU:O | 13:1:87:MET:HG2 | 2.18 | 0.43 |
| 4:D:194:LEU:HD22 | 4:D:212:LEU:HD11 | 2.01 | 0.43 |
| 4:D:79:SER:HB3 | 4:D:165:ILE:HD12 | 2.01 | 0.43 |
| 5:E:233:ILE:OXT | 5:E:233:ILE:HG22 | 2.19 | 0.43 |
| 7:G:17(C):LYS:HB2 | 7:G:17(C):LYS:HE3 | 1.78 | 0.43 |
| 4:R:21:LEU:HD21 | 5:S:130:ARG:HD2 | 2.01 | 0.43 |
| 5:S:123:ASN:N | 5:S:123:ASN:HD22 | 2.17 | 0.43 |
| 5:S:216:GLY:O | 5:S:217:LYS:C | 2.56 | 0.43 |
| 5:S:90:ASN:O | 5:S:94:GLN:HG3 | 2.17 | 0.43 |
| 3:C:227:GLU:O | 3:C:231:GLN:HG3 | 2.19 | 0.43 |
| 12:L:33:LYS:HE2 | 12:L:33:LYS:HB3 | 1.76 | 0.43 |
| 12:L:-7:ASN:ND2 | 12:L:-7:ASN:C | 2.72 | 0.43 |
| 14:N:26:ILE:HB | 13:1:165:ARG:HA | 2.00 | 0.43 |
| 2:P:113:VAL:HG22 | 2:P:138:TYR:CD2 | 2.54 | 0.43 |
| 4:R:194:LEU:HD22 | 4:R:212:LEU:HD11 | 2.00 | 0.43 |
| 4:R:79:SER:HB3 | 4:R:165:ILE:HD12 | 2.01 | 0.43 |
| 5:S:147:HIS:HA | 16:S:238:HOH:O | 2.18 | 0.43 |
| 6:T:147:HIS:HD2 | 16:T:242:HOH:O | 2.01 | 0.43 |
| 8:V:105:ASP:HB2 | 8:V:10(A):PRO:CD | 2.47 | 0.43 |
| 11:Y:123:ASP:C | 11:Y:124:ILE:HD12 | 2.39 | 0.43 |
| 1:A:227:GLN:NE2 | 1:A:231:ASP:OD1 | 2.50 | 0.43 |
| 3:C:71:ASP:OD1 | 3:C:100:ARG:NH1 | 2.51 | 0.43 |
| 4:D:195:LYS:HB3 | 4:D:196:ILE:HD13 | 2.01 | 0.43 |
| 7:G:169:GLN:HE21 | 7:G:169:GLN:HB3 | 1.67 | 0.43 |
| 9:I:104:ILE:HG21 | 9:I:181:LYS:HG2 | 2.01 | 0.43 |
| 13:M:191:GLN:HE21 | 13:M:191:GLN:HB3 | 1.55 | 0.43 |
| 14:N:171:GLY:HA2 | 13:1:197:TRP:CH2 | 2.54 | 0.43 |
| 14:N:20:THR:HG23 | 14:N:31:THR:OG1 | 2.19 | 0.43 |
| 1:O:175:PHE:O | 1:O:179:ARG:HG2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:P:121:GLN:C | 2:P:121:GLN:NE2 | 2.72 | 0.43 |
| 5:S:162:GLY:O | 5:S:163:THR:HB | 2.19 | 0.43 |
| 14:2:20:THR:HG23 | 14:2:31:THR:OG1 | 2.19 | 0.43 |
| 3:C:163:GLN:HE22 | 3:C:173:ARG:NE | 2.13 | 0.43 |
| 3:C:168:ASN:O | 3:C:172:VAL:HG12 | 2.19 | 0.43 |
| 3:C:95:GLU:OE2 | 3:C:95:GLU:HA | 2.19 | 0.43 |
| 3:Q:185:THR:HG22 | 3:Q:186:VAL:N | 2.33 | 0.43 |
| 3:Q:72:SER:O | 3:Q:221:ILE:HD13 | 2.19 | 0.43 |
| 3:Q:227:GLU:O | 3:Q:231:GLN:HG3 | 2.18 | 0.43 |
| 6:T:127:ASN:ND2 | 6:T:127:ASN:H | 2.16 | 0.43 |
| 9:W:181:LYS:HE3 | 9:W:181:LYS:HB3 | 1.90 | 0.43 |
| 14:2:15:GLY:HA2 | 14:2:174:ARG:O | 2.19 | 0.42 |
| 2:B:97:GLN:NE2 | 16:B:246:HOH:O | 2.52 | 0.42 |
| 4:D:161:ASN:HB3 | 4:D:180:TRP:CE2 | 2.54 | 0.42 |
| 8:H:144:GLN:O | 8:H:145:ASP:HB2 | 2.19 | 0.42 |
| 8:H:15:ALA:HA | 8:H:174:ASP:O | 2.18 | 0.42 |
| 9:I:93:GLY:N | 9:I:94:PRO:CD | 2.80 | 0.42 |
| 11:K:12:ILE:HB | 11:K:178:VAL:HB | 2.01 | 0.42 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:CD | 2.32 | 0.42 |
| 14:N:4:MET:HB3 | 14:N:126:ILE:HG22 | 2.01 | 0.42 |
| 14:N:85:GLU:O | 14:N:89:GLU:HB2 | 2.19 | 0.42 |
| 5:S:58:LEU:N | 5:S:58:LEU:CD1 | 2.82 | 0.42 |
| 6:T:75:GLY:O | 6:T:138:PHE:HA | 2.18 | 0.42 |
| 2:P:101:LYS:HZ1 | 10:X:85:GLN:HE22 | 1.66 | 0.42 |
| 12:Z:14:LEU:HD13 | 12:Z:34:VAL:HG13 | 1.99 | 0.42 |
| 14:2:66:TYR:CD2 | 14:2:74:PRO:HB3 | 2.53 | 0.42 |
| 4:D:215:ILE:HD13 | 4:D:216:THR:N | 2.34 | 0.42 |
| 10:J:34:THR:HG21 | 10:J:176:LYS:NZ | 2.34 | 0.42 |
| 10:J:24:ILE:O | 10:J:24:ILE:HG13 | 2.19 | 0.42 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:HG2 | 1.98 | 0.42 |
| 3:Q:163:GLN:HA | 3:Q:163:GLN:NE2 | 2.34 | 0.42 |
| 3:Q:76:LEU:HD22 | 3:Q:89:ILE:HD11 | 2.01 | 0.42 |
| 5:S:5:ARG:HG3 | 5:S:22:PHE:CE1 | 2.54 | 0.42 |
| 1:O:21(L):ILE:HD11 | 8:V:42:TRP:HH2 | 1.84 | 0.42 |
| 12:Z:170:GLY:O | 12:Z:171:ASP:HB2 | 2.20 | 0.42 |
| 4:D:24:VAL:O | 4:D:28:LEU:HD13 | 2.20 | 0.42 |
| 5:E:139:ILE:CD1 | 5:E:139:ILE:N | 2.78 | 0.42 |
| 11:K:6:PHE:HA | 11:K:123:ASP:O | 2.19 | 0.42 |
| 11:K:40:PHE:CG | 11:K:73:ARG:CZ | 3.03 | 0.42 |
| 13:M:-4:ILE:HD12 | 14:N:116:GLY:HA2 | 1.99 | 0.42 |
| 5:E:105:ARG:HB2 | 13:M:78:TYR:CD1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:44:ASP:N | 2:P:44:ASP:OD2 | 2.53 | 0.42 |
| 9:W:55:LEU:HD21 | 9:W:95:TYR:CD1 | 2.54 | 0.42 |
| 12:Z:40:ASN:ND2 | 16:Z:220:HOH:O | 2.39 | 0.42 |
| 13:1:186:PHE:HE1 | 13:1:188:LYS:HG3 | 1.85 | 0.42 |
| 13:1:40:ASN:ND2 | 13:1:40:ASN:H | 2.07 | 0.42 |
| 12:Z:-8:PHE:HB2 | 13:1:-8:THR:HG23 | 2.01 | 0.42 |
| 2:B:108:PRO:CB | 2:B:111:ILE:HD13 | 2.23 | 0.42 |
| 2:B:112:LEU:C | 2:B:112:LEU:HD23 | 2.40 | 0.42 |
| 5:E:48:LEU:CD1 | 5:E:139:ILE:CD1 | 2.92 | 0.42 |
| 10:J:168:MET:CE | 10:X:168:MET:HG2 | 2.49 | 0.42 |
| 10:J:16:SER:HB2 | 16:J:206:HOH:O | 2.18 | 0.42 |
| 2:P:45:GLY:HA3 | 2:P:216:ARG:HG2 | 2.01 | 0.42 |
| 4:R:39:GLY:O | 4:R:162:ALA:HA | 2.20 | 0.42 |
| 4:R:31:ILE:CD1 | 4:R:80:GLY:HA3 | 2.49 | 0.42 |
| 5:S:57:GLU:C | 5:S:58:LEU:HD12 | 2.40 | 0.42 |
| 13:1:150:VAL:HG21 | 16:1:233:HOH:O | 2.18 | 0.42 |
| 1:A:33:GLN:HE21 | 1:A:33:GLN:CA | 2.25 | 0.42 |
| 2:B:20:ARG:NH2 | 3:C:33:ARG:HE | 2.16 | 0.42 |
| 6:F:127:ASN:HD22 | 6:F:127:ASN:H | 1.66 | 0.42 |
| 6:F:49:ALA:HA | 6:F:211:GLU:O | 2.18 | 0.42 |
| 7:G:8:TYR:O | 7:G:12:ILE:CD1 | 2.65 | 0.42 |
| 13:M:5:SER:HB3 | 13:M:14:ILE:HG13 | 2.01 | 0.42 |
| 13:M:83:LEU:O | 13:M:87:MET:HG2 | 2.20 | 0.42 |
| 4:R:121:LEU:HA | 4:R:123:PHE:CE1 | 2.55 | 0.42 |
| 6:T:70:VAL:HG11 | 6:T:112:PHE:CE1 | 2.55 | 0.42 |
| 9:W:6:MET:HG2 | 9:W:124:PHE:HB3 | 2.01 | 0.42 |
| 11:K:207:ASN:HD21 | 10:X:144:PRO:CG | 2.32 | 0.42 |
| 12:Z:99:THR:C | 12:Z:100:ILE:HD12 | 2.40 | 0.42 |
| 13:1:152:GLU:O | 13:1:156:VAL:HG23 | 2.19 | 0.42 |
| 14:2:105:ASP:OD2 | 14:2:106:ASN:N | 2.45 | 0.42 |
| 14:2:159:LEU:CB | 14:2:173:ILE:HD12 | 2.50 | 0.42 |
| 3:C:185:THR:HG22 | 3:C:186:VAL:N | 2.33 | 0.42 |
| 4:D:40:ILE:HD12 | 4:D:193:VAL:HG23 | 2.00 | 0.42 |
| 5:E:104:ASN:HB2 | 13:M:81:GLU:HG2 | 2.00 | 0.42 |
| 5:E:227:GLU:OE2 | 5:E:227:GLU:N | 2.52 | 0.42 |
| 6:F:43:ASN:N | 6:F:43:ASN:ND2 | 2.67 | 0.42 |
| 9:I:55:LEU:HD11 | 9:I:97:VAL:HG21 | 2.01 | 0.42 |
| 10:J:143:ARG:HB2 | 10:J:146:MET:HG3 | 2.01 | 0.42 |
| 11:K:74:ILE:HD11 | 11:K:78:ALA:HB3 | 2.02 | 0.42 |
| 13:M:8:TYR:CE2 | 13:M:148:VAL:HG22 | 2.54 | 0.42 |
| 2:P:136:PHE:O | 2:P:150:THR:HA | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:O:86:ARG:NE | 7:U:118:ASN:HD21 | 2.13 | 0.42 |
| 8:V:15:ALA:HA | 8:V:174:ASP:O | 2.20 | 0.42 |
| 10:X:129:TYR:O | 10:X:132:PHE:HB2 | 2.18 | 0.42 |
| 14:2:20:THR:OG1 | 14:2:28:ASN:HB3 | 2.19 | 0.42 |
| 14:2:85:GLU:O | 14:2:89:GLU:HB2 | 2.20 | 0.42 |
| 1:A:175:PHE:O | 1:A:179:ARG:HG2 | 2.19 | 0.42 |
| 1:A:198:LYS:HE3 | 1:A:236:LEU:HD11 | 2.02 | 0.42 |
| 5:E:123:ASN:HD22 | 5:E:123:ASN:N | 2.18 | 0.42 |
| 5:E:5:ARG:HG3 | 5:E:22:PHE:CE1 | 2.55 | 0.42 |
| 6:F:53:LEU:HD11 | 6:F:205:ASN:OD1 | 2.20 | 0.42 |
| 7:G:101:TYR:OH | 14:N:58:ILE:HD11 | 2.20 | 0.42 |
| 8:H:84:LYS:HE2 | 8:H:119:THR:HG23 | 2.02 | 0.42 |
| 12:L:21:ILE:HD12 | 12:L:21:ILE:C | 2.39 | 0.42 |
| 13:M:113:VAL:HG23 | 13:M:119:THR:HG22 | 2.01 | 0.42 |
| 14:N:114:PRO:HD2 | 14:N:118:SER:O | 2.20 | 0.42 |
| 3:Q:38:VAL:CG2 | 3:Q:39:GLY:N | 2.83 | 0.42 |
| 9:W:28:SER:HB2 | 10:X:120:VAL:HG21 | 2.01 | 0.42 |
| 10:X:166:MET:HA | 10:X:167:PRO:HD3 | 1.81 | 0.42 |
| 8:H:167:LEU:HD13 | 12:Z:167:ILE:HD13 | 2.00 | 0.42 |
| 1:A:92:SER:O | 1:A:95:VAL:HG12 | 2.20 | 0.42 |
| 2:B:113:VAL:HG22 | 2:B:138:TYR:CD2 | 2.54 | 0.42 |
| 2:B:45:GLY:HA3 | 2:B:216:ARG:HG2 | 2.01 | 0.42 |
| 3:C:14:ILE:CD1 | 3:C:14:ILE:N | 2.83 | 0.42 |
| 6:F:172:ALA:O | 6:F:176:LEU:HD23 | 2.19 | 0.42 |
| 8:H:3:ILE:HG22 | 8:H:16:ALA:HB2 | 2.02 | 0.42 |
| 11:K:4:LEU:C | 11:K:4:LEU:HD22 | 2.40 | 0.42 |
| 4:R:161:ASN:HB3 | 4:R:180:TRP:CE2 | 2.55 | 0.42 |
| 4:R:46:VAL:HG11 | 4:R:139:ALA:HB1 | 2.01 | 0.42 |
| 5:S:37:THR:HG22 | 5:S:165:ILE:HG13 | 2.02 | 0.42 |
| 4:R:173:GLN:HG2 | 5:S:56:ASP:OD2 | 2.19 | 0.42 |
| 11:Y:180:GLU:CB | 16:Y:1428:HOH:O | 2.68 | 0.42 |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:CD | 2.32 | 0.42 |
| 1:A:31:VAL:HG11 | 1:A:135:SER:HB2 | 2.01 | 0.42 |
| 2:B:87:ILE:CD1 | 2:B:87:ILE:N | 2.83 | 0.42 |
| 7:G:172:ILE:HD12 | 7:G:197:MET:CE | 2.50 | 0.42 |
| 10:J:193:GLN:OXT | 10:J:193:GLN:HG2 | 2.19 | 0.42 |
| 13:M:115:LEU:HD23 | 13:M:115:LEU:N | 2.35 | 0.42 |
| 13:M:123:PRO:HB3 | 13:M:14(G):ILE:HD11 | 2.02 | 0.42 |
| 1:O:74:ILE:HD12 | 1:O:74:ILE:N | 2.34 | 0.42 |
| 3:Q:18(A):ASP:OD1 | 3:Q:18(C):LYS:HB2 | 2.19 | 0.42 |
| 3:Q:33:ARG:HH11 | 3:Q:33:ARG:HB3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:Q:95:GLU:OE2 | 3:Q:95:GLU:HA | 2.19 | 0.42 |
| 5:S:104:ASN:HB2 | 13:1:81:GLU:HG2 | 2.01 | 0.42 |
| 5:S:136:LEU:HD12 | 5:S:151:PHE:CD2 | 2.55 | 0.42 |
| 5:S:227:GLU:OE2 | 5:S:227:GLU:N | 2.53 | 0.42 |
| 6:T:136:THR:O | 6:T:150:MET:HA | 2.20 | 0.42 |
| 6:T:43:ASN:ND2 | 6:T:185:SER:HA | 2.34 | 0.42 |
| 1:O:86:ARG:HH21 | 7:U:118:ASN:ND2 | 2.18 | 0.42 |
| 11:Y:200:LYS:HG3 | 11:Y:205:SER:O | 2.20 | 0.42 |
| 9:I:29:ASN:ND2 | 11:Y:208:ASN:HD21 | 2.16 | 0.42 |
| 13:1:-3:VAL:HA | 13:1:21:SER:O | 2.20 | 0.42 |
| 14:2:13:ILE:HD12 | 14:2:151:THR:HG22 | 2.02 | 0.42 |
| 1:A:26:TYR:CD1 | 1:A:26:TYR:N | 2.87 | 0.42 |
| 2:B:116:LEU:HA | 2:B:119:ILE:HD12 | 2.01 | 0.42 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:HG2 | 1.99 | 0.42 |
| 4:D:121:LEU:HA | 4:D:123:PHE:CE1 | 2.55 | 0.42 |
| 7:G:18(D):ILE:HD12 | 7:G:192:PHE:CE2 | 2.55 | 0.42 |
| 14:N:21:THR:O | 15:N:1404:BO2:H3 | 2.19 | 0.42 |
| 14:N:163:ILE:N | 14:N:163:ILE:CD1 | 2.82 | 0.42 |
| 4:R:70:ILE:HD13 | 4:R:112:LEU:HD11 | 2.02 | 0.42 |
| 6:T:127:ASN:H | 6:T:127:ASN:HD22 | 1.67 | 0.42 |
| 8:V:24:PRO:HG2 | 8:V:25:ILE:HD12 | 2.02 | 0.42 |
| 9:W:29:ASN:C | 9:W:29:ASN:HD22 | 2.22 | 0.42 |
| 10:X:185:ARG:HG2 | 10:X:185:ARG:HH11 | 1.85 | 0.42 |
| 14:2:163:ILE:HD12 | 14:2:173:ILE:HD11 | 2.02 | 0.41 |
| 4:D:192:LEU:HD12 | 4:D:196:ILE:HD11 | 2.02 | 0.41 |
| 6:F:136:THR:O | 6:F:150:MET:HA | 2.20 | 0.41 |
| 6:F:216:SER:HB3 | 6:F:21(A):GLU:HB2 | 2.01 | 0.41 |
| 11:K:74:ILE:HD11 | 11:K:78:ALA:CB | 2.50 | 0.41 |
| 13:M:-3:VAL:HA | 13:M:21:SER:O | 2.20 | 0.41 |
| 2:P:202:THR:HG22 | 2:P:203:ASP:N | 2.35 | 0.41 |
| 6:T:95:GLU:HG3 | 6:T:115:ARG:HD2 | 2.02 | 0.41 |
| 10:J:144:PRO:HG2 | 11:Y:207:ASN:HD21 | 1.85 | 0.41 |
| 14:2:126:ILE:N | 14:2:126:ILE:CD1 | 2.81 | 0.41 |
| 4:D:177:LEU:HD22 | 5:E:58:LEU:HD13 | 2.01 | 0.41 |
| 4:D:229:THR:HG22 | 4:D:233:ILE:HD13 | 2.01 | 0.41 |
| 6:F:203:GLU:HA | 6:F:203:GLU:OE1 | 2.20 | 0.41 |
| 7:G:143:GLU:HA | 7:G:217:LYS:NZ | 2.35 | 0.41 |
| 8:H:114:HIS:CE1 | 15:N:1404:BO2:H5 | 2.55 | 0.41 |
| 9:I:90:ARG:HH11 | 9:I:90:ARG:HA | 1.85 | 0.41 |
| 10:J:112:GLN:HE21 | 10:J:125:GLY:HA3 | 1.84 | 0.41 |
| 10:J:143:ARG:O | 10:J:146:MET:HG3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:O:177:GLU:HG2 | 2:P:58:LEU:CD2 | 2.48 | 0.41 |
| 1:O:43:THR:HG23 | 1:O:184:LEU:O | 2.20 | 0.41 |
| 2:P:15:PHE:H | 3:Q:23:GLN:NE2 | 2.15 | 0.41 |
| 1:O:17:PRO:HA | 2:P:26:TYR:CD1 | 2.55 | 0.41 |
| 2:P:6:ARG:HG3 | 2:P:6:ARG:HH11 | 1.85 | 0.41 |
| 7:U:105:TYR:OH | 8:V:66:HIS:HE1 | 2.04 | 0.41 |
| 8:V:114:HIS:ND1 | 15:2:1405:BO2:H5 | 2.35 | 0.41 |
| 8:V:72:ARG:HH11 | 8:V:72:ARG:HG3 | 1.85 | 0.41 |
| 10:X:143:ARG:HB2 | 10:X:146:MET:HG3 | 2.02 | 0.41 |
| 10:X:24:ILE:HG13 | 10:X:24:ILE:O | 2.20 | 0.41 |
| 12:Z:80:ALA:HA | 12:Z:113:PHE:HZ | 1.84 | 0.41 |
| 13:1:14(G):ILE:HB | 13:1:144:PRO:CD | 2.50 | 0.41 |
| 1:A:46:VAL:HB | 1:A:215:ILE:HD13 | 2.02 | 0.41 |
| 7:G:107:MET:CE | 7:G:112:LEU:HD13 | 2.50 | 0.41 |
| 8:H:210:THR:HG21 | 12:Z:14(C):GLN:HG2 | 2.01 | 0.41 |
| 9:I:110:ILE:CG1 | 9:I:125:ILE:HD13 | 2.50 | 0.41 |
| 11:K:10(A):ARG:HB3 | 11:K:10(B):LYS:CE | 2.43 | 0.41 |
| 11:K:14:VAL:HB | 11:K:176:TYR:HB2 | 2.03 | 0.41 |
| 12:L:27:ASN:HB3 | 13:M:120:TYR:CE1 | 2.55 | 0.41 |
| 13:M:14(C):ARG:CG | 13:M:14(C):ARG:NH1 | 2.78 | 0.41 |
| 1:O:26:TYR:CD1 | 1:O:26:TYR:N | 2.87 | 0.41 |
| 3:Q:163:GLN:HE22 | 3:Q:173:ARG:NE | 2.13 | 0.41 |
| 3:Q:190:VAL:HG13 | 3:Q:212:ILE:HG21 | 2.02 | 0.41 |
| 6:T:100:LYS:O | 6:T:104:LYS:N | 2.51 | 0.41 |
| 6:T:157:TYR:CD1 | 6:T:157:TYR:C | 2.93 | 0.41 |
| 6:T:45:GLY:HA3 | 6:T:215:CYS:O | 2.20 | 0.41 |
| 8:V:44:ALA:HB3 | 8:V:100:ILE:HB | 2.02 | 0.41 |
| 10:X:16:SER:HB2 | 16:X:227:HOH:O | 2.20 | 0.41 |
| 8:H:197:ARG:HG3 | 12:Z:164:GLU:CD | 2.41 | 0.41 |
| 5:E:77:SER:OG | 5:E:137:LEU:HB2 | 2.21 | 0.41 |
| 7:G:152:ASP:HB2 | 7:G:153:PRO:HD2 | 2.03 | 0.41 |
| 12:L:19:ARG:NE | 12:L:171:ASP:OD2 | 2.43 | 0.41 |
| 13:M:113:VAL:HA | 13:M:118:VAL:O | 2.19 | 0.41 |
| 5:S:216:GLY:O | 5:S:219:THR:N | 2.47 | 0.41 |
| 7:U:110:ASP:HB3 | 7:U:149:TYR:CZ | 2.55 | 0.41 |
| 10:X:53:VAL:HB | 16:Y:1427:HOH:O | 2.19 | 0.41 |
| 5:S:105:ARG:HB2 | 13:1:78:TYR:CE1 | 2.56 | 0.41 |
| 3:C:75:VAL:HG13 | 3:C:221:ILE:HD13 | 2.01 | 0.41 |
| 2:B:160:TRP:HA | 3:C:59:GLN:HA | 2.01 | 0.41 |
| 5:E:2(C):VAL:HG22 | 5:E:226:GLY:HA2 | 2.01 | 0.41 |
| 9:I:29:ASN:HD22 | 9:I:29:ASN:C | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:114:ASP:OD1 | 11:K:114:ASP:C | 2.58 | 0.41 |
| 7:G:101:TYR:CE1 | 14:N:58:ILE:HD13 | 2.55 | 0.41 |
| 2:P:112:LEU:HD23 | 2:P:112:LEU:C | 2.40 | 0.41 |
| 4:R:40:ILE:HG12 | 4:R:193:VAL:CG2 | 2.51 | 0.41 |
| 5:S:171:GLY:HA3 | 5:S:199:GLN:O | 2.21 | 0.41 |
| 6:T:127:ASN:ND2 | 6:T:127:ASN:N | 2.69 | 0.41 |
| 7:U:55:PRO:HG2 | 7:U:56:ASP:H | 1.85 | 0.41 |
| 10:X:193:GLN:HG2 | 10:X:193:GLN:OXT | 2.20 | 0.41 |
| 11:Y:111:TYR:CE1 | 11:Y:121:LYS:HB2 | 2.56 | 0.41 |
| 2:B:40:ILE:HD12 | 2:B:193:ALA:HB2 | 2.01 | 0.41 |
| 2:B:95:HIS:CD2 | 2:B:115:ARG:HG2 | 2.56 | 0.41 |
| 3:C:35:THR:HB | 3:C:51:GLU:CG | 2.50 | 0.41 |
| 5:E:162:GLY:O | 5:E:163:THR:HB | 2.20 | 0.41 |
| 7:G:17(D):SER:O | 7:G:17(E):LYS:HB2 | 2.21 | 0.41 |
| 10:J:162:LEU:O | 10:J:166:MET:HB2 | 2.20 | 0.41 |
| 11:K:40:PHE:CE2 | 11:K:73:ARG:HD2 | 2.56 | 0.41 |
| 3:Q:71:ASP:OD1 | 3:Q:100:ARG:NH1 | 2.53 | 0.41 |
| 4:R:120:ALA:CB | 4:R:155:GLY:HA2 | 2.50 | 0.41 |
| 4:R:215:ILE:HD13 | 4:R:216:THR:N | 2.35 | 0.41 |
| 4:R:91:HIS:CG | 4:R:119:LEU:HD11 | 2.56 | 0.41 |
| 9:W:104:ILE:N | 9:W:104:ILE:HD13 | 2.36 | 0.41 |
| 11:Y:137:VAL:HG21 | 11:Y:161:ALA:HB2 | 2.03 | 0.41 |
| 11:Y:40:PHE:CG | 11:Y:73:ARG:CZ | 3.04 | 0.41 |
| 13:1:9:ASP:OD1 | 13:1:10:ASN:N | 2.53 | 0.41 |
| 14:2:48:SER:O | 14:2:52:THR:HG23 | 2.20 | 0.41 |
| 1:A:161:LYS:HD3 | 1:A:180:TRP:CZ3 | 2.55 | 0.41 |
| 3:C:201:VAL:HG11 | 3:C:210:ILE:HG12 | 2.02 | 0.41 |
| 10:J:168:MET:HG2 | 10:X:168:MET:CE | 2.51 | 0.41 |
| 3:Q:219:SER:C | 3:Q:221:ILE:HD12 | 2.41 | 0.41 |
| 3:Q:39:GLY:HA2 | 3:Q:47:VAL:O | 2.20 | 0.41 |
| 6:T:107:ILE:HA | 6:T:108:PRO:HD3 | 1.84 | 0.41 |
| 10:X:143:ARG:O | 10:X:146:MET:HG3 | 2.20 | 0.41 |
| 11:Y:195:LEU:O | 11:Y:199:VAL:HG23 | 2.20 | 0.41 |
| 11:Y:99:THR:HG22 | 11:Y:113:VAL:O | 2.20 | 0.41 |
| 14:2:184:VAL:HG21 | 16:2:1412:HOH:O | 2.20 | 0.41 |
| 2:B:122:GLY:C | 2:B:124:THR:H | 2.23 | 0.41 |
| 2:B:130:ARG:HA | 2:B:131:PRO:HD3 | 1.89 | 0.41 |
| 2:B:38:ILE:CD1 | 2:B:164:SER:HB3 | 2.39 | 0.41 |
| 3:C:224:LEU:N | 3:C:224:LEU:CD1 | 2.84 | 0.41 |
| 11:K:4:LEU:O | 11:K:4:LEU:HD22 | 2.21 | 0.41 |
| 13:M:42:VAL:HG23 | 13:M:178:ILE:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:Q:161:SER:HB3 | 3:Q:180:TYR:CE1 | 2.56 | 0.41 |
| 3:Q:224:LEU:CD1 | 3:Q:224:LEU:N | 2.84 | 0.41 |
| 4:R:227:GLU:OE2 | 4:R:227:GLU:N | 2.44 | 0.41 |
| 4:R:24:VAL:O | 4:R:28:LEU:HD13 | 2.21 | 0.41 |
| 6:T:203:GLU:OE1 | 6:T:203:GLU:HA | 2.21 | 0.41 |
| 7:U:110:ASP:HB3 | 7:U:149:TYR:CE2 | 2.56 | 0.41 |
| 2:B:209:ARG:HH11 | 2:B:209:ARG:HG2 | 1.85 | 0.41 |
| 4:D:46:VAL:HG11 | 4:D:139:ALA:HB1 | 2.03 | 0.41 |
| 4:D:205:GLU:HA | 4:D:205:GLU:OE2 | 2.21 | 0.41 |
| 6:F:175:GLU:OE2 | 6:F:175:GLU:HA | 2.21 | 0.41 |
| 7:G:119:LEU:HA | 7:G:119:LEU:HD12 | 1.83 | 0.41 |
| 6:F:176:LEU:HB3 | 7:G:58:LEU:HD21 | 2.02 | 0.41 |
| 10:J:10(B):LYS:HB2 | 10:J:10(B):LYS:HZ2 | 1.82 | 0.41 |
| 10:J:52:THR:HG22 | 10:J:53:VAL:H | 1.86 | 0.41 |
| 12:L:-7:ASN:HD22 | 12:L:-5:TYR:H | 1.67 | 0.41 |
| 12:L:90:LYS:HD3 | 12:L:95:TYR:CE1 | 2.56 | 0.41 |
| 13:M:-3:VAL:HG12 | 13:M:49:ILE:HG13 | 2.03 | 0.41 |
| 2:P:89:ILE:O | 2:P:92:ALA:HB3 | 2.21 | 0.41 |
| 4:R:67:ILE:HG22 | 4:R:221:PHE:HZ | 1.86 | 0.41 |
| 5:S:134:VAL:O | 5:S:153:PRO:HG3 | 2.21 | 0.41 |
| 5:S:52:LYS:HB3 | 5:S:63:TYR:O | 2.21 | 0.41 |
| 10:X:3:ILE:HD13 | 10:X:46:ALA:HB2 | 2.02 | 0.41 |
| 11:Y:22:ALA:HB2 | 15:Y:1403:BO2:H6 | 2.02 | 0.41 |
| 11:Y:4:LEU:C | 11:Y:4:LEU:CD2 | 2.89 | 0.41 |
| 14:2:33:LYS:HE2 | 15:2:1405:BO2:H222 | 2.03 | 0.41 |
| 2:B:111:ILE:H | 2:B:111:ILE:CD1 | 2.34 | 0.41 |
| 5:E:37:THR:HG22 | 5:E:165:ILE:HG13 | 2.03 | 0.41 |
| 7:G:121:GLN:C | 7:G:121:GLN:NE2 | 2.74 | 0.41 |
| 11:K:37:ILE:HB | 11:K:41:LEU:CB | 2.44 | 0.41 |
| 12:L:80:ALA:HA | 12:L:113:PHE:HZ | 1.86 | 0.41 |
| 2:P:21(A):LYS:O | 2:P:21(B):GLY:C | 2.60 | 0.41 |
| 3:Q:105:ASP:OD2 | 3:Q:106:PRO:HD2 | 2.21 | 0.41 |
| 3:Q:201:VAL:HG11 | 3:Q:210:ILE:HG12 | 2.02 | 0.41 |
| 3:Q:241:GLN:C | 3:Q:243:GLN:N | 2.74 | 0.41 |
| 6:T:32:GLU:HB3 | 6:T:169:ARG:NH2 | 2.36 | 0.41 |
| 6:T:43:ASN:ND2 | 6:T:43:ASN:N | 2.68 | 0.41 |
| 7:U:17(D):SER:O | 7:U:17(E):LYS:HB2 | 2.21 | 0.41 |
| 13:M:208:THR:HG22 | 8:V:77:VAL:HB | 2.02 | 0.41 |
| 10:X:162:LEU:O | 10:X:166:MET:HB2 | 2.21 | 0.41 |
| 11:Y:65:LEU:HD12 | 11:Y:65:LEU:HA | 1.93 | 0.41 |
| 12:Z:3:ILE:CD1 | 12:Z:46:ASN:CB | 2.90 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:225:LYS:O | 2:B:226:PRO:C | 2.60 | 0.41 |
| 3:C:18(A):ASP:OD1 | 3:C:18(C):LYS:HB2 | 2.21 | 0.41 |
| 3:C:39:GLY:HA2 | 3:C:47:VAL:O | 2.21 | 0.41 |
| 4:D:192:LEU:HD12 | 4:D:196:ILE:CD1 | 2.50 | 0.41 |
| 7:G:224:LEU:HD12 | 7:G:229:ILE:CD1 | 2.51 | 0.41 |
| 9:I:14:ILE:HG12 | 9:I:34:ILE:CD1 | 2.50 | 0.41 |
| 1:O:117:ALA:HB1 | 1:O:155:GLY:O | 2.20 | 0.41 |
| 2:P:5:SER:O | 2:P:6:ARG:C | 2.59 | 0.41 |
| 4:R:122:ARG:HH11 | 4:R:122:ARG:HG2 | 1.86 | 0.41 |
| 3:Q:158:SER:HB2 | 4:R:59:LEU:HD21 | 2.03 | 0.41 |
| 5:S:97:ASN:HD21 | 12:Z:61:ASN:ND2 | 2.18 | 0.41 |
| 6:T:38:ILE:HD12 | 6:T:38:ILE:C | 2.42 | 0.41 |
| 8:V:144:GLN:O | 8:V:145:ASP:HB2 | 2.21 | 0.41 |
| 14:2:114:PRO:HD2 | 14:2:118:SER:O | 2.20 | 0.40 |
| 4:D:177:LEU:HD22 | 5:E:58:LEU:HD11 | 2.04 | 0.40 |
| 9:I:165:ARG:NH2 | 12:Z:135:MET:HE3 | 2.37 | 0.40 |
| 12:L:48:PHE:CZ | 12:L:50:ALA:HB3 | 2.56 | 0.40 |
| 12:L:27:ASN:HB3 | 13:M:120:TYR:CZ | 2.55 | 0.40 |
| 3:Q:182:PRO:O | 3:Q:183:PRO:C | 2.59 | 0.40 |
| 5:S:75:GLY:HA3 | 5:S:221:PHE:CZ | 2.56 | 0.40 |
| 6:T:175:GLU:OE2 | 6:T:175:GLU:HA | 2.21 | 0.40 |
| 6:T:49:ALA:CB | 6:T:212:ILE:HD13 | 2.51 | 0.40 |
| 9:W:159:LEU:HD21 | 9:W:173:ALA:HB1 | 2.03 | 0.40 |
| 9:W:29:ASN:H | 9:W:29:ASN:ND2 | 2.19 | 0.40 |
| 10:X:35:ARG:HD3 | 10:X:35:ARG:HA | 1.91 | 0.40 |
| 1:A:232:ARG:NH1 | 1:A:232:ARG:HG3 | 2.35 | 0.40 |
| 2:B:202:THR:HG22 | 2:B:203:ASP:N | 2.36 | 0.40 |
| 3:C:182:PRO:O | 3:C:183:PRO:C | 2.59 | 0.40 |
| 3:C:33:ARG:HH11 | 3:C:33:ARG:HB3 | 1.84 | 0.40 |
| 6:F:127:ASN:N | 6:F:127:ASN:ND2 | 2.68 | 0.40 |
| 6:F:93:ARG:HD3 | 13:M:68:TYR:CD2 | 2.56 | 0.40 |
| 13:M:186:PHE:HE1 | 13:M:188:LYS:HG3 | 1.85 | 0.40 |
| 15:N:1404:BO2:H21 | 16:N:1440:HOH:O | 2.20 | 0.40 |
| 1:O:100:TYR:HD1 | 1:O:105:GLU:O | 2.02 | 0.40 |
| 4:R:90:GLU:OE2 | 11:Y:69:ARG:NH1 | 2.54 | 0.40 |
| 7:U:18(B):ASP:O | 7:U:18(C):HIS:HB3 | 2.21 | 0.40 |
| 10:X:143:ARG:HA | 10:X:144:PRO:HD3 | 1.87 | 0.40 |
| 12:Z:176:LEU:HG | 12:Z:186:LYS:HG2 | 2.03 | 0.40 |
| 14:2:104:TYR:OH | 14:2:180:ALA:HB2 | 2.21 | 0.40 |
| 1:A:39:GLY:HA2 | 1:A:47:VAL:O | 2.22 | 0.40 |
| 2:B:14:ILE:HD13 | 16:B:268:HOH:O | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:161:SER:HB3 | 3:C:180:TYR:CE1 | 2.56 | 0.40 |
| 4:D:17:PRO:HD2 | 16:D:266:HOH:O | 2.21 | 0.40 |
| 8:H:3:ILE:CD1 | 8:H:100:ILE:HG12 | 2.44 | 0.40 |
| 11:K:4:LEU:HD11 | 11:K:15:ALA:HB3 | 2.02 | 0.40 |
| 12:L:34:VAL:HB | 16:L:227:HOH:O | 2.19 | 0.40 |
| 13:M:150:VAL:HG21 | 16:M:259:HOH:O | 2.22 | 0.40 |
| 2:P:49:ALA:HB2 | 2:P:212:PHE:CE1 | 2.56 | 0.40 |
| 4:R:205:GLU:OE2 | 4:R:205:GLU:HA | 2.21 | 0.40 |
| 4:R:59:LEU:HD13 | 4:R:59:LEU:C | 2.42 | 0.40 |
| 6:T:49:ALA:HA | 6:T:211:GLU:O | 2.22 | 0.40 |
| 6:T:216:SER:HB3 | 6:T:21(A):GLU:HB2 | 2.02 | 0.40 |
| 7:U:139:VAL:O | 7:U:140:SER:HB3 | 2.20 | 0.40 |
| 7:U:168:LYS:O | 7:U:172:ILE:HG13 | 2.21 | 0.40 |
| 7:U:188:LYS:HA | 7:U:188:LYS:HD3 | 1.91 | 0.40 |
| 7:U:82:ILE:HG22 | 7:U:83:PRO:HD3 | 2.03 | 0.40 |
| 8:V:3:ILE:HG22 | 8:V:16:ALA:CB | 2.51 | 0.40 |
| 11:Y:114:ASP:C | 11:Y:114:ASP:OD1 | 2.59 | 0.40 |
| 13:I:115:LEU:N | 13:I:115:LEU:HD23 | 2.36 | 0.40 |
| 2:B:41:MET:HE1 | 3:C:62:ARG:NH2 | 2.36 | 0.40 |
| 6:F:67:ILE:CD1 | 6:F:77:VAL:HB | 2.47 | 0.40 |
| 7:G:39:ALA:HA | 7:G:47:VAL:O | 2.20 | 0.40 |
| 10:J:18:LYS:CG | 10:J:174:ILE:HG13 | 2.52 | 0.40 |
| 2:P:85:ALA:O | 2:P:89:ILE:HG12 | 2.21 | 0.40 |
| 3:Q:55:THR:O | 3:Q:56:LEU:HD13 | 2.22 | 0.40 |
| 5:S:185:ASN:HA | 5:S:186:PRO:HD2 | 1.96 | 0.40 |
| 8:V:10:ASN:O | 8:V:180:ILE:HG12 | 2.21 | 0.40 |
| 10:X:52:THR:HG22 | 10:X:53:VAL:H | 1.86 | 0.40 |
| 5:E:136:LEU:HD12 | 5:E:151:PHE:CD2 | 2.57 | 0.40 |
| 6:F:87:HIS:HD2 | 6:F:132:PHE:HE2 | 1.69 | 0.40 |
| 6:F:197:ILE:HG21 | 6:F:210:LEU:HD13 | 2.02 | 0.40 |
| 6:F:43:ASN:ND2 | 6:F:185:SER:HA | 2.36 | 0.40 |
| 9:I:29:ASN:ND2 | 9:I:29:ASN:H | 2.20 | 0.40 |
| 10:J:133:TYR:C | 16:J:198:HOH:O | 2.59 | 0.40 |
| 11:K:5:ALA:HA | 11:K:13:ILE:O | 2.21 | 0.40 |
| 13:M:152:GLU:O | 13:M:156:VAL:HG23 | 2.21 | 0.40 |
| 1:O:198:LYS:HE3 | 1:O:236:LEU:HD11 | 2.02 | 0.40 |
| 2:P:169:THR:O | 2:P:173:GLN:HB2 | 2.22 | 0.40 |
| 3:Q:11:ALA:CB | 4:R:12:VAL:HG11 | 2.51 | 0.40 |
| 4:R:17:PRO:HA | 5:S:26:TYR:CD2 | 2.56 | 0.40 |
| 4:R:238:LYS:HE2 | 4:R:238:LYS:HB3 | 1.90 | 0.40 |
| 4:R:32:LYS:O | 4:R:167:SER:HA | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:S:105:ARG:HB2 | 13:1:78:TYR:CD1 | 2.57 | 0.40 |
| 10:X:104:TYR:CD1 | 10:X:180:LYS:HA | 2.57 | 0.40 |
| 11:Y:131:GLN:HG3 | 11:Y:132:THR:N | 2.37 | 0.40 |
| 11:Y:5:ALA:HA | 11:Y:13:ILE:O | 2.22 | 0.40 |
| 11:Y:83:LEU:HD23 | 11:Y:99:THR:HG21 | 2.03 | 0.40 |
| 12:Z:21:ILE:CD1 | 12:Z:168:GLN:HG2 | 2.51 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1 | A | 248/250 (99%) | 236 (95%) | 10 (4%) | 2 (1%) | 19 | 49 |
| 1 | O | 248/250 (99%) | 235 (95%) | 11 (4%) | 2 (1%) | 19 | 49 |
| 2 | B | 242/244 (99%) | 221 (91%) | 16 (7%) | 5 (2%) | 7 | 23 |
| 2 | P | 242/244 (99%) | 220 (91%) | 17 (7%) | 5 (2%) | 7 | 23 |
| 3 | C | 239/241 (99%) | 219 (92%) | 16 (7%) | 4 (2%) | 9 | 29 |
| 3 | Q | 239/241 (99%) | 218 (91%) | 17 (7%) | 4 (2%) | 9 | 29 |
| 4 | D | 240/242 (99%) | 225 (94%) | 11 (5%) | 4 (2%) | 9 | 29 |
| 4 | R | 240/242 (99%) | 223 (93%) | 12 (5%) | 5 (2%) | 7 | 23 |
| 5 | E | 231/233 (99%) | 210 (91%) | 15 (6%) | 6 (3%) | 5 | 18 |
| 5 | S | 231/233 (99%) | 210 (91%) | 15 (6%) | 6 (3%) | 5 | 18 |
| 6 | F | 242/244 (99%) | 222 (92%) | 17 (7%) | 3 (1%) | 13 | 39 |
| 6 | T | 242/244 (99%) | 222 (92%) | 17 (7%) | 3 (1%) | 13 | 39 |
| 7 | G | 241/243 (99%) | 226 (94%) | 12 (5%) | 3 (1%) | 13 | 39 |
| 7 | U | 241/243 (99%) | 224 (93%) | 15 (6%) | 2 (1%) | 19 | 49 |
| 8 | H | 220/222 (99%) | 208 (94%) | 11 (5%) | 1 (0%) | 29 | 61 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 8 | V | 220/222 (99%) | 211 (96%) | 8 (4%) | 1 (0%) | 29 | 61 |
| 9 | I | 202/204 (99%) | 195 (96%) | 6 (3%) | 1 (0%) | 29 | 61 |
| 9 | W | 202/204 (99%) | 195 (96%) | 6 (3%) | 1 (0%) | 29 | 61 |
| 10 | J | 196/198 (99%) | 184 (94%) | 11 (6%) | 1 (0%) | 29 | 61 |
| 10 | X | 196/198 (99%) | 186 (95%) | 9 (5%) | 1 (0%) | 29 | 61 |
| 11 | K | 210/212 (99%) | 201 (96%) | 9 (4%) | 0 | 100 | 100 |
| 11 | Y | 210/212 (99%) | 202 (96%) | 8 (4%) | 0 | 100 | 100 |
| 12 | L | 220/222 (99%) | 205 (93%) | 14 (6%) | 1 (0%) | 29 | 61 |
| 12 | Z | 220/222 (99%) | 206 (94%) | 12 (6%) | 2 (1%) | 17 | 46 |
| 13 | 1 | 231/233 (99%) | 218 (94%) | 13 (6%) | 0 | 100 | 100 |
| 13 | M | 231/233 (99%) | 218 (94%) | 11 (5%) | 2 (1%) | 17 | 46 |
| 14 | 2 | 194/196 (99%) | 184 (95%) | 10 (5%) | 0 | 100 | 100 |
| 14 | N | 194/196 (99%) | 185 (95%) | 9 (5%) | 0 | 100 | 100 |
| All | All | 6312/6368 (99%) | 5909 (94%) | 338 (5%) | 65 (1%) | 15 | 44 |

All (65) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 2 | B | 20(A) | SER |
| 3 | C | 58 | LEU |
| 4 | D | 12(G) | GLU |
| 5 | E | 217 | LYS |
| 2 | P | 20(A) | SER |
| 3 | Q | 58 | LEU |
| 4 | R | 12(G) | GLU |
| 5 | S | 217 | LYS |
| 1 | A | 5 | THR |
| 2 | B | 6 | ARG |
| 2 | B | 54 | VAL |
| 2 | B | 21(B) | GLY |
| 2 | B | 21(C) | ASP |
| 3 | C | 183 | PRO |
| 5 | E | 5 | ARG |
| 5 | E | 202 | ARG |
| 6 | F | 64 | ASN |
| 6 | F | 205 | ASN |
| 9 | I | 145 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | O | 5 | THR |
| 2 | P | 6 | ARG |
| 2 | P | 54 | VAL |
| 2 | P | 21(B) | GLY |
| 2 | P | 21(C) | ASP |
| 3 | Q | 183 | PRO |
| 5 | S | 5 | ARG |
| 5 | S | 202 | ARG |
| 6 | T | 64 | ASN |
| 6 | T | 205 | ASN |
| 9 | W | 145 | ASN |
| 3 | C | 203 | THR |
| 4 | D | 12(F) | GLY |
| 5 | E | 64 | GLN |
| 5 | E | 18(A) | ASP |
| 8 | H | 91 | GLN |
| 12 | L | 71 | ASP |
| 3 | Q | 203 | THR |
| 4 | R | 12(F) | GLY |
| 5 | S | 64 | GLN |
| 5 | S | 18(A) | ASP |
| 6 | T | 206 | LYS |
| 8 | V | 91 | GLN |
| 4 | D | 18(D) | SER |
| 5 | E | 180 | LEU |
| 6 | F | 206 | LYS |
| 10 | J | 192 | ALA |
| 1 | O | 167 | LYS |
| 4 | R | 18(D) | SER |
| 5 | S | 180 | LEU |
| 10 | X | 192 | ALA |
| 12 | Z | 71 | ASP |
| 1 | A | 167 | LYS |
| 3 | C | 242 | GLU |
| 4 | D | 12(C) | GLY |
| 7 | G | 239 | GLN |
| 13 | M | 2 | SER |
| 13 | M | 96 | TRP |
| 4 | R | 120 | ALA |
| 4 | R | 12(C) | GLY |
| 7 | G | 55 | PRO |
| 3 | Q | 242 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | U | 55 | PRO |
| 7 | U | 239 | GLN |
| 12 | Z | 93 | PHE |
| 7 | G | 7 | GLY |

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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 209/209 (100%) | 201 (96%) | 8 (4%) | 33 | 67 |
| 1 | O | 209/209 (100%) | 202 (97%) | 7 (3%) | 38 | 72 |
| 2 | B | 203/203 (100%) | 190 (94%) | 13 (6%) | 17 | 45 |
| 2 | P | 203/203 (100%) | 193 (95%) | 10 (5%) | 25 | 57 |
| 3 | C | 213/213 (100%) | 200 (94%) | 13 (6%) | 18 | 48 |
| 3 | Q | 213/213 (100%) | 201 (94%) | 12 (6%) | 21 | 51 |
| 4 | D | 198/198 (100%) | 188 (95%) | 10 (5%) | 24 | 55 |
| 4 | R | 198/198 (100%) | 189 (96%) | 9 (4%) | 27 | 60 |
| 5 | E | 192/192 (100%) | 178 (93%) | 14 (7%) | 14 | 38 |
| 5 | S | 192/192 (100%) | 177 (92%) | 15 (8%) | 12 | 35 |
| 6 | F | 201/201 (100%) | 187 (93%) | 14 (7%) | 15 | 40 |
| 6 | T | 201/201 (100%) | 188 (94%) | 13 (6%) | 17 | 44 |
| 7 | G | 207/207 (100%) | 194 (94%) | 13 (6%) | 18 | 46 |
| 7 | U | 207/207 (100%) | 194 (94%) | 13 (6%) | 18 | 46 |
| 8 | H | 181/181 (100%) | 175 (97%) | 6 (3%) | 38 | 72 |
| 8 | V | 181/181 (100%) | 175 (97%) | 6 (3%) | 38 | 72 |
| 9 | I | 172/172 (100%) | 165 (96%) | 7 (4%) | 30 | 64 |
| 9 | W | 172/172 (100%) | 164 (95%) | 8 (5%) | 26 | 59 |
| 10 | J | 175/175 (100%) | 169 (97%) | 6 (3%) | 37 | 71 |
| 10 | X | 175/175 (100%) | 170 (97%) | 5 (3%) | 42 | 76 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 11 | K | 169/169 (100%) | 161 (95%) | 8 (5%) | 26 | 59 |
| 11 | Y | 169/169 (100%) | 161 (95%) | 8 (5%) | 26 | 59 |
| 12 | L | 185/185 (100%) | 172 (93%) | 13 (7%) | 15 | 40 |
| 12 | Z | 185/185 (100%) | 173 (94%) | 12 (6%) | 17 | 44 |
| 13 | 1 | 199/199 (100%) | 190 (96%) | 9 (4%) | 27 | 60 |
| 13 | M | 199/199 (100%) | 191 (96%) | 8 (4%) | 31 | 65 |
| 14 | 2 | 162/162 (100%) | 155 (96%) | 7 (4%) | 29 | 62 |
| 14 | N | 162/162 (100%) | 154 (95%) | 8 (5%) | 25 | 57 |
| All | All | 5332/5332 (100%) | 5057 (95%) | 275 (5%) | 23 | 55 |

All (275) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 32 | LYS |
| 1 | A | 33 | GLN |
| 1 | A | 64 | LEU |
| 1 | A | 124 | THR |
| 1 | A | 135 | SER |
| 1 | A | 158 | PHE |
| 1 | A | 179 | ARG |
| 1 | A | 210 | ILE |
| 2 | B | 14 | ILE |
| 2 | B | 71 | ASN |
| 2 | B | 87 | ILE |
| 2 | B | 94 | ILE |
| 2 | B | 121 | GLN |
| 2 | B | 135 | SER |
| 2 | B | 150 | THR |
| 2 | B | 156 | ASN |
| 2 | B | 185 | LYS |
| 2 | B | 192 | LEU |
| 2 | B | 212 | PHE |
| 2 | B | 218 | ASN |
| 2 | B | 232 | ILE |
| 3 | C | 10 | ARG |
| 3 | C | 14 | ILE |
| 3 | C | 25 | GLU |
| 3 | C | 57 | LYS |
| 3 | C | 89 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 3 | C | 121 | GLN |
| 3 | C | 135 | SER |
| 3 | C | 150 | GLN |
| 3 | C | 163 | GLN |
| 3 | C | 174 | GLU |
| 3 | C | 178 | LYS |
| 3 | C | 208 | LYS |
| 3 | C | 227 | GLU |
| 4 | D | 76 | CYS |
| 4 | D | 110 | GLU |
| 4 | D | 126 | ARG |
| 4 | D | 177 | LEU |
| 4 | D | 18(E) | SER |
| 4 | D | 191 | LEU |
| 4 | D | 194 | LEU |
| 4 | D | 196 | ILE |
| 4 | D | 215 | ILE |
| 4 | D | 237 | LEU |
| 5 | E | 11 | ASP |
| 5 | E | 12 | THR |
| 5 | E | 32 | LYS |
| 5 | E | 57 | GLU |
| 5 | E | 68 | ILE |
| 5 | E | 76 | LEU |
| 5 | E | 121 | GLN |
| 5 | E | 139 | ILE |
| 5 | E | 185 | ASN |
| 5 | E | 189 | LEU |
| 5 | E | 199 | GLN |
| 5 | E | 207 | LEU |
| 5 | E | 227 | GLU |
| 5 | E | 231 | LYS |
| 6 | F | 11 | SER |
| 6 | F | 35 | THR |
| 6 | F | 36 | THR |
| 6 | F | 43 | ASN |
| 6 | F | 121 | GLN |
| 6 | F | 127 | ASN |
| 6 | F | 144 | ASN |
| 6 | F | 18(E) | GLU |
| 6 | F | 187 | ARG |
| 6 | F | 203 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 6 | F | 204 | ASP |
| 6 | F | 205 | ASN |
| 6 | F | 214 | TRP |
| 6 | F | 21(C) | ASN |
| 7 | G | 12 | ILE |
| 7 | G | 14 | ILE |
| 7 | G | 72 | ARG |
| 7 | G | 87 | ASN |
| 7 | G | 119 | LEU |
| 7 | G | 121 | GLN |
| 7 | G | 124 | THR |
| 7 | G | 169 | GLN |
| 7 | G | 174 | THR |
| 7 | G | 184 | ASN |
| 7 | G | 197 | MET |
| 7 | G | 232 | ARG |
| 7 | G | 233 | LEU |
| 8 | H | 30 | ASN |
| 8 | H | 34 | LEU |
| 8 | H | 56 | THR |
| 8 | H | 68 | LEU |
| 8 | H | 144 | GLN |
| 8 | H | 197 | ARG |
| 9 | I | 29 | ASN |
| 9 | I | 45 | ILE |
| 9 | I | 110 | ILE |
| 9 | I | 113 | PHE |
| 9 | I | 159 | LEU |
| 9 | I | 160 | LEU |
| 9 | I | 171 | TRP |
| 10 | J | 52 | THR |
| 10 | J | 70 | GLU |
| 10 | J | 77 | GLN |
| 10 | J | 90(A) | ILE |
| 10 | J | 121 | GLU |
| 10 | J | 166 | MET |
| 11 | K | 4 | LEU |
| 11 | K | 8 | PHE |
| 11 | K | 9 | GLN |
| 11 | K | 65 | LEU |
| 11 | K | 99 | THR |
| 11 | K | 100 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 11 | K | 104 | TYR |
| 11 | K | 10(B) | LYS |
| 12 | L | -9 | GLN |
| 12 | L | -7 | ASN |
| 12 | L | 3 | ILE |
| 12 | L | 14 | LEU |
| 12 | L | 25 | SER |
| 12 | L | 40 | ASN |
| 12 | L | 58 | ARG |
| 12 | L | 70(A) | ASN |
| 12 | L | 82 | ASN |
| 12 | L | 98 | HIS |
| 12 | L | 99 | THR |
| 12 | L | 115 | PRO |
| 12 | L | 138 | LEU |
| 13 | M | 40 | ASN |
| 13 | M | 62 | LEU |
| 13 | M | 91 | ARG |
| 13 | M | 129 | PHE |
| 13 | M | 14(C) | ARG |
| 13 | M | 148 | VAL |
| 13 | M | 149 | GLN |
| 13 | M | 204 | LYS |
| 14 | N | 36 | ARG |
| 14 | N | 84 | LYS |
| 14 | N | 89 | GLU |
| 14 | N | 10(B) | LYS |
| 14 | N | 126 | ILE |
| 14 | N | 134 | ILE |
| 14 | N | 163 | ILE |
| 14 | N | 18(I) | GLN |
| 1 | O | 32 | LYS |
| 1 | O | 33 | GLN |
| 1 | O | 64 | LEU |
| 1 | O | 124 | THR |
| 1 | O | 135 | SER |
| 1 | O | 158 | PHE |
| 1 | O | 179 | ARG |
| 2 | P | 71 | ASN |
| 2 | P | 121 | GLN |
| 2 | P | 135 | SER |
| 2 | P | 150 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 2 | P | 156 | ASN |
| 2 | P | 185 | LYS |
| 2 | P | 187 | ASP |
| 2 | P | 192 | LEU |
| 2 | P | 212 | PHE |
| 2 | P | 218 | ASN |
| 3 | Q | 10 | ARG |
| 3 | Q | 25 | GLU |
| 3 | Q | 57 | LYS |
| 3 | Q | 89 | ILE |
| 3 | Q | 121 | GLN |
| 3 | Q | 135 | SER |
| 3 | Q | 150 | GLN |
| 3 | Q | 163 | GLN |
| 3 | Q | 174 | GLU |
| 3 | Q | 178 | LYS |
| 3 | Q | 208 | LYS |
| 3 | Q | 227 | GLU |
| 4 | R | 76 | CYS |
| 4 | R | 110 | GLU |
| 4 | R | 126 | ARG |
| 4 | R | 177 | LEU |
| 4 | R | 18(E) | SER |
| 4 | R | 191 | LEU |
| 4 | R | 194 | LEU |
| 4 | R | 215 | ILE |
| 4 | R | 237 | LEU |
| 5 | S | 11 | ASP |
| 5 | S | 12 | THR |
| 5 | S | 32 | LYS |
| 5 | S | 57 | GLU |
| 5 | S | 76 | LEU |
| 5 | S | 104 | ASN |
| 5 | S | 121 | GLN |
| 5 | S | 18(D) | ILE |
| 5 | S | 185 | ASN |
| 5 | S | 189 | LEU |
| 5 | S | 199 | GLN |
| 5 | S | 207 | LEU |
| 5 | S | 214 | ILE |
| 5 | S | 227 | GLU |
| 5 | S | 231 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 6 | T | 11 | SER |
| 6 | T | 36 | THR |
| 6 | T | 43 | ASN |
| 6 | T | 121 | GLN |
| 6 | T | 127 | ASN |
| 6 | T | 144 | ASN |
| 6 | T | 18(E) | GLU |
| 6 | T | 187 | ARG |
| 6 | T | 203 | GLU |
| 6 | T | 204 | ASP |
| 6 | T | 205 | ASN |
| 6 | T | 214 | TRP |
| 6 | T | 21(C) | ASN |
| 7 | U | 72 | ARG |
| 7 | U | 87 | ASN |
| 7 | U | 119 | LEU |
| 7 | U | 121 | GLN |
| 7 | U | 124 | THR |
| 7 | U | 148 | ILE |
| 7 | U | 169 | GLN |
| 7 | U | 174 | THR |
| 7 | U | 184 | ASN |
| 7 | U | 197 | MET |
| 7 | U | 217 | LYS |
| 7 | U | 232 | ARG |
| 7 | U | 233 | LEU |
| 8 | V | 30 | ASN |
| 8 | V | 34 | LEU |
| 8 | V | 56 | THR |
| 8 | V | 68 | LEU |
| 8 | V | 144 | GLN |
| 8 | V | 197 | ARG |
| 9 | W | 29 | ASN |
| 9 | W | 61 | TYR |
| 9 | W | 104 | ILE |
| 9 | W | 113 | PHE |
| 9 | W | 155 | ILE |
| 9 | W | 159 | LEU |
| 9 | W | 160 | LEU |
| 9 | W | 171 | TRP |
| 10 | X | 52 | THR |
| 10 | X | 70 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 10 | X | 77 | GLN |
| 10 | X | 121 | GLU |
| 10 | X | 166 | MET |
| 11 | Y | 4 | LEU |
| 11 | Y | 8 | PHE |
| 11 | Y | 9 | GLN |
| 11 | Y | 65 | LEU |
| 11 | Y | 99 | THR |
| 11 | Y | 100 | MET |
| 11 | Y | 104 | TYR |
| 11 | Y | 10(B) | LYS |
| 12 | Z | -9 | GLN |
| 12 | Z | -7 | ASN |
| 12 | Z | 3 | ILE |
| 12 | Z | 14 | LEU |
| 12 | Z | 25 | SER |
| 12 | Z | 40 | ASN |
| 12 | Z | 58 | ARG |
| 12 | Z | 70(A) | ASN |
| 12 | Z | 82 | ASN |
| 12 | Z | 98 | HIS |
| 12 | Z | 99 | THR |
| 12 | Z | 138 | LEU |
| 13 | 1 | 40 | ASN |
| 13 | 1 | 62 | LEU |
| 13 | 1 | 91 | ARG |
| 13 | 1 | 96 | TRP |
| 13 | 1 | 129 | PHE |
| 13 | 1 | 14(C) | ARG |
| 13 | 1 | 148 | VAL |
| 13 | 1 | 149 | GLN |
| 13 | 1 | 204 | LYS |
| 14 | 2 | 3 | ILE |
| 14 | 2 | 36 | ARG |
| 14 | 2 | 84 | LYS |
| 14 | 2 | 89 | GLU |
| 14 | 2 | 10(B) | LYS |
| 14 | 2 | 126 | ILE |
| 14 | 2 | 18(I) | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 1 | A | 33 | GLN |
| 1 | A | 97 | HIS |
| 2 | B | 23 | GLN |
| 2 | B | 71 | ASN |
| 2 | B | 95 | HIS |
| 2 | B | 97 | GLN |
| 2 | B | 121 | GLN |
| 2 | B | 125 | GLN |
| 2 | B | 156 | ASN |
| 2 | B | 177 | GLN |
| 2 | B | 218 | ASN |
| 3 | C | 23 | GLN |
| 3 | C | 82 | ASN |
| 3 | C | 97 | GLN |
| 3 | C | 121 | GLN |
| 3 | C | 125 | GLN |
| 3 | C | 150 | GLN |
| 3 | C | 163 | GLN |
| 3 | C | 238 | GLN |
| 3 | C | 243 | GLN |
| 4 | D | 23 | GLN |
| 4 | D | 108 | ASN |
| 4 | D | 147 | GLN |
| 4 | D | 211 | GLN |
| 4 | D | 226 | ASN |
| 5 | E | 33 | GLN |
| 5 | E | 73 | HIS |
| 5 | E | 104 | ASN |
| 5 | E | 121 | GLN |
| 5 | E | 123 | ASN |
| 5 | E | 125 | GLN |
| 5 | E | 156 | ASN |
| 5 | E | 185 | ASN |
| 5 | E | 199 | GLN |
| 5 | E | 2(E) | ASN |
| 6 | F | 23 | GLN |
| 6 | F | 43 | ASN |
| 6 | F | 90 | ASN |
| 6 | F | 121 | GLN |
| 6 | F | 127 | ASN |
| 6 | F | 192 | GLN |
| 7 | G | 34(A) | ASN |
| 7 | G | 87 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 7 | G | 118 | ASN |
| 7 | G | 121 | GLN |
| 7 | G | 125 | GLN |
| 7 | G | 169 | GLN |
| 7 | G | 170 | GLN |
| 7 | G | 178 | ASN |
| 7 | G | 184 | ASN |
| 7 | G | 228 | ASN |
| 8 | H | 30 | ASN |
| 8 | H | 66 | HIS |
| 8 | H | 144 | GLN |
| 8 | H | 165 | ASN |
| 8 | H | 172 | ASN |
| 8 | H | 190 | ASN |
| 9 | I | 29 | ASN |
| 9 | I | 81 | GLN |
| 9 | I | 145 | ASN |
| 10 | J | 54 | GLN |
| 10 | J | 77 | GLN |
| 10 | J | 85 | GLN |
| 10 | J | 112 | GLN |
| 10 | J | 141 | HIS |
| 10 | J | 186 | GLN |
| 11 | K | 9 | GLN |
| 11 | K | 85 | ASN |
| 11 | K | 131 | GLN |
| 11 | K | 174 | ASN |
| 11 | K | 207 | ASN |
| 11 | K | 208 | ASN |
| 12 | L | -9 | GLN |
| 12 | L | -7 | ASN |
| 12 | L | 40 | ASN |
| 12 | L | 61 | ASN |
| 12 | L | 70(A) | ASN |
| 12 | L | 82 | ASN |
| 12 | L | 85 | HIS |
| 12 | L | 98 | HIS |
| 12 | L | 14(B) | ASN |
| 12 | L | 1(I) | ASN |
| 13 | M | -7 | GLN |
| 13 | M | 10 | ASN |
| 13 | M | 40 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 13 | M | 89 | GLN |
| 13 | M | 93 | ASN |
| 13 | M | 149 | GLN |
| 13 | M | 157 | ASN |
| 13 | M | 172 | ASN |
| 13 | M | 191 | GLN |
| 14 | N | 69 | GLN |
| 14 | N | 145 | ASN |
| 14 | N | 157 | HIS |
| 14 | N | 161 | GLN |
| 1 | O | 33 | GLN |
| 1 | O | 97 | HIS |
| 2 | P | 23 | GLN |
| 2 | P | 71 | ASN |
| 2 | P | 95 | HIS |
| 2 | P | 97 | GLN |
| 2 | P | 121 | GLN |
| 2 | P | 125 | GLN |
| 2 | P | 156 | ASN |
| 2 | P | 177 | GLN |
| 2 | P | 218 | ASN |
| 3 | Q | 23 | GLN |
| 3 | Q | 82 | ASN |
| 3 | Q | 121 | GLN |
| 3 | Q | 125 | GLN |
| 3 | Q | 150 | GLN |
| 3 | Q | 163 | GLN |
| 3 | Q | 238 | GLN |
| 3 | Q | 243 | GLN |
| 4 | R | 23 | GLN |
| 4 | R | 108 | ASN |
| 4 | R | 114 | GLN |
| 4 | R | 147 | GLN |
| 4 | R | 211 | GLN |
| 4 | R | 226 | ASN |
| 5 | S | 73 | HIS |
| 5 | S | 104 | ASN |
| 5 | S | 121 | GLN |
| 5 | S | 123 | ASN |
| 5 | S | 125 | GLN |
| 5 | S | 156 | ASN |
| 5 | S | 185 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 5 | S | 199 | GLN |
| 5 | S | 2(E) | ASN |
| 6 | T | 23 | GLN |
| 6 | T | 43 | ASN |
| 6 | T | 90 | ASN |
| 6 | T | 121 | GLN |
| 6 | T | 127 | ASN |
| 6 | T | 147 | HIS |
| 6 | T | 192 | GLN |
| 7 | U | 34(A) | ASN |
| 7 | U | 87 | ASN |
| 7 | U | 118 | ASN |
| 7 | U | 121 | GLN |
| 7 | U | 125 | GLN |
| 7 | U | 169 | GLN |
| 7 | U | 170 | GLN |
| 7 | U | 178 | ASN |
| 7 | U | 184 | ASN |
| 7 | U | 228 | ASN |
| 8 | V | 10 | ASN |
| 8 | V | 30 | ASN |
| 8 | V | 66 | HIS |
| 8 | V | 144 | GLN |
| 8 | V | 165 | ASN |
| 8 | V | 172 | ASN |
| 8 | V | 190 | ASN |
| 9 | W | 29 | ASN |
| 9 | W | 81 | GLN |
| 9 | W | 145 | ASN |
| 10 | X | 54 | GLN |
| 10 | X | 77 | GLN |
| 10 | X | 85 | GLN |
| 10 | X | 112 | GLN |
| 10 | X | 141 | HIS |
| 10 | X | 186 | GLN |
| 11 | Y | 85 | ASN |
| 11 | Y | 131 | GLN |
| 11 | Y | 174 | ASN |
| 11 | Y | 207 | ASN |
| 11 | Y | 208 | ASN |
| 12 | Z | -9 | GLN |
| 12 | Z | -7 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 12 | Z | 40 | ASN |
| 12 | Z | 61 | ASN |
| 12 | Z | 70(A) | ASN |
| 12 | Z | 82 | ASN |
| 12 | Z | 85 | HIS |
| 12 | Z | 14(B) | ASN |
| 12 | Z | 1(I) | ASN |
| 12 | Z | 166 | HIS |
| 12 | Z | 168 | GLN |
| 13 | 1 | 10 | ASN |
| 13 | 1 | 40 | ASN |
| 13 | 1 | 89 | GLN |
| 13 | 1 | 93 | ASN |
| 13 | 1 | 149 | GLN |
| 13 | 1 | 157 | ASN |
| 13 | 1 | 172 | ASN |
| 13 | 1 | 191 | GLN |
| 14 | 2 | 69 | GLN |
| 14 | 2 | 145 | ASN |
| 14 | 2 | 157 | HIS |
| 14 | 2 | 161 | GLN |

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](#)

6 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 |
| 15 | BO2 | V | 1401 | 8 | 25,29,29 | 1.42 | 3 (12%) | 32,38,38 | 2.07 | 9 (28%) |
| 15 | BO2 | H | 1400 | 8 | 25,29,29 | 1.45 | 4 (16%) | 32,38,38 | 2.00 | 8 (25%) |
| 15 | BO2 | N | 1404 | 14 | 25,29,29 | 1.60 | 8 (32%) | 32,38,38 | 2.32 | 12 (37%) |
| 15 | BO2 | K | 1402 | 11 | 25,29,29 | 1.23 | 0 | 32,38,38 | 2.15 | 11 (34%) |
| 15 | BO2 | Y | 1403 | 11 | 25,29,29 | 1.28 | 2 (8%) | 32,38,38 | 2.09 | 11 (34%) |
| 15 | BO2 | 2 | 1405 | 14 | 25,29,29 | 1.53 | 7 (28%) | 32,38,38 | 2.31 | 12 (37%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 15 | BO2 | V | 1401 | 8 | - | 5/22/28/28 | 0/2/2/2 |
| 15 | BO2 | H | 1400 | 8 | - | 5/22/28/28 | 0/2/2/2 |
| 15 | BO2 | N | 1404 | 14 | - | 8/22/28/28 | 0/2/2/2 |
| 15 | BO2 | K | 1402 | 11 | - | 4/22/28/28 | 0/2/2/2 |
| 15 | BO2 | Y | 1403 | 11 | - | 4/22/28/28 | 0/2/2/2 |
| 15 | BO2 | 2 | 1405 | 14 | - | 8/22/28/28 | 0/2/2/2 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | 2 | 1405 | BO2 | C17-C12 | 2.89 | 1.45 | 1.38 |
| 15 | N | 1404 | BO2 | C17-C12 | 2.88 | 1.45 | 1.38 |
| 15 | N | 1404 | BO2 | C13-C12 | 2.73 | 1.44 | 1.38 |
| 15 | N | 1404 | BO2 | C14-C13 | 2.65 | 1.44 | 1.38 |
| 15 | 2 | 1405 | BO2 | C13-C12 | 2.60 | 1.44 | 1.38 |
| 15 | H | 1400 | BO2 | C16-C17 | 2.47 | 1.44 | 1.38 |
| 15 | N | 1404 | BO2 | C15-C14 | 2.45 | 1.44 | 1.38 |
| 15 | 2 | 1405 | BO2 | C11-C12 | 2.41 | 1.57 | 1.51 |
| 15 | Y | 1403 | BO2 | C13-C12 | 2.40 | 1.44 | 1.38 |
| 15 | N | 1404 | BO2 | C11-C12 | 2.38 | 1.57 | 1.51 |
| 15 | H | 1400 | BO2 | C13-C12 | 2.37 | 1.43 | 1.38 |
| 15 | 2 | 1405 | BO2 | C15-C14 | 2.32 | 1.44 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | H | 1400 | BO2 | C14-C13 | 2.31 | 1.43 | 1.38 |
| 15 | H | 1400 | BO2 | C17-C12 | 2.31 | 1.43 | 1.38 |
| 15 | N | 1404 | BO2 | C11-C10 | 2.25 | 1.59 | 1.54 |
| 15 | V | 1401 | BO2 | C14-C13 | 2.24 | 1.43 | 1.38 |
| 15 | N | 1404 | BO2 | C16-C17 | 2.21 | 1.43 | 1.38 |
| 15 | N | 1404 | BO2 | C16-C15 | 2.18 | 1.43 | 1.38 |
| 15 | V | 1401 | BO2 | C16-C17 | 2.17 | 1.43 | 1.38 |
| 15 | 2 | 1405 | BO2 | C14-C13 | 2.12 | 1.43 | 1.38 |
| 15 | V | 1401 | BO2 | C13-C12 | 2.11 | 1.43 | 1.38 |
| 15 | 2 | 1405 | BO2 | C16-C17 | 2.04 | 1.43 | 1.38 |
| 15 | Y | 1403 | BO2 | C17-C12 | 2.01 | 1.43 | 1.38 |
| 15 | 2 | 1405 | BO2 | C16-C15 | 2.00 | 1.43 | 1.38 |

All (63) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | N | 1404 | BO2 | C21-C22-C23 | 6.46 | 123.51 | 115.39 |
| 15 | K | 1402 | BO2 | C21-C22-C23 | 5.97 | 122.90 | 115.39 |
| 15 | 2 | 1405 | BO2 | C21-C22-C23 | 5.96 | 122.89 | 115.39 |
| 15 | Y | 1403 | BO2 | C21-C22-C23 | 5.81 | 122.70 | 115.39 |
| 15 | V | 1401 | BO2 | C21-C22-C23 | 5.18 | 121.91 | 115.39 |
| 15 | H | 1400 | BO2 | C21-C22-C23 | 5.18 | 121.91 | 115.39 |
| 15 | 2 | 1405 | BO2 | C6-N1-C2 | 4.94 | 123.35 | 116.93 |
| 15 | N | 1404 | BO2 | C6-N1-C2 | 4.89 | 123.27 | 116.93 |
| 15 | 2 | 1405 | BO2 | C3-C2-C7 | 4.52 | 124.43 | 119.62 |
| 15 | V | 1401 | BO2 | C6-N1-C2 | 4.42 | 122.67 | 116.93 |
| 15 | N | 1404 | BO2 | C3-C2-C7 | 4.27 | 124.17 | 119.62 |
| 15 | K | 1402 | BO2 | C6-N1-C2 | 4.25 | 122.45 | 116.93 |
| 15 | K | 1402 | BO2 | C3-C2-C7 | 4.25 | 124.14 | 119.62 |
| 15 | Y | 1403 | BO2 | C6-N1-C2 | 4.19 | 122.37 | 116.93 |
| 15 | V | 1401 | BO2 | C2-C7-N9 | 4.14 | 122.90 | 115.20 |
| 15 | N | 1404 | BO2 | C2-C7-N9 | 4.08 | 122.78 | 115.20 |
| 15 | H | 1400 | BO2 | C6-N1-C2 | 4.08 | 122.22 | 116.93 |
| 15 | 2 | 1405 | BO2 | C2-C7-N9 | 4.07 | 122.75 | 115.20 |
| 15 | Y | 1403 | BO2 | C3-C2-C7 | 4.03 | 123.92 | 119.62 |
| 15 | H | 1400 | BO2 | C2-C7-N9 | 3.96 | 122.56 | 115.20 |
| 15 | V | 1401 | BO2 | C3-C2-C7 | 3.60 | 123.46 | 119.62 |
| 15 | H | 1400 | BO2 | C3-C2-C7 | 3.55 | 123.41 | 119.62 |
| 15 | V | 1401 | BO2 | C3-C2-N1 | -3.51 | 117.44 | 121.61 |
| 15 | H | 1400 | BO2 | C3-C2-N1 | -3.40 | 117.57 | 121.61 |
| 15 | N | 1404 | BO2 | C5-N4-C3 | 3.39 | 122.72 | 116.85 |
| 15 | 2 | 1405 | BO2 | C5-N4-C3 | 3.31 | 122.57 | 116.85 |

Continued on next page...

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 15 | K | 1402 | BO2 | C5-N4-C3 | 3.28 | 122.52 | 116.85 |
| 15 | V | 1401 | BO2 | C5-N4-C3 | 3.12 | 122.24 | 116.85 |
| 15 | Y | 1403 | BO2 | C5-N4-C3 | 3.04 | 122.12 | 116.85 |
| 15 | H | 1400 | BO2 | C5-N4-C3 | 2.96 | 121.97 | 116.85 |
| 15 | 2 | 1405 | BO2 | C3-C2-N1 | -2.92 | 118.14 | 121.61 |
| 15 | N | 1404 | BO2 | C3-C2-N1 | -2.87 | 118.19 | 121.61 |
| 15 | K | 1402 | BO2 | C2-C7-N9 | 2.83 | 120.46 | 115.20 |
| 15 | H | 1400 | BO2 | C6-C5-N4 | -2.83 | 118.41 | 121.95 |
| 15 | K | 1402 | BO2 | C18-C10-N9 | -2.79 | 103.55 | 111.16 |
| 15 | Y | 1403 | BO2 | C18-C10-N9 | -2.77 | 103.62 | 111.16 |
| 15 | Y | 1403 | BO2 | C2-C7-N9 | 2.74 | 120.29 | 115.20 |
| 15 | Y | 1403 | BO2 | C11-C10-N9 | -2.72 | 105.07 | 110.79 |
| 15 | 2 | 1405 | BO2 | C2-C3-N4 | -2.69 | 118.71 | 122.05 |
| 15 | N | 1404 | BO2 | C5-C6-N1 | -2.68 | 118.32 | 122.17 |
| 15 | 2 | 1405 | BO2 | C5-C6-N1 | -2.67 | 118.32 | 122.17 |
| 15 | 2 | 1405 | BO2 | C11-C10-N9 | -2.67 | 105.17 | 110.79 |
| 15 | K | 1402 | BO2 | C11-C10-N9 | -2.66 | 105.18 | 110.79 |
| 15 | V | 1401 | BO2 | C6-C5-N4 | -2.65 | 118.64 | 121.95 |
| 15 | N | 1404 | BO2 | C2-C3-N4 | -2.62 | 118.80 | 122.05 |
| 15 | N | 1404 | BO2 | C6-C5-N4 | -2.60 | 118.70 | 121.95 |
| 15 | 2 | 1405 | BO2 | O8-C7-C2 | -2.58 | 115.46 | 121.08 |
| 15 | Y | 1403 | BO2 | C6-C5-N4 | -2.58 | 118.73 | 121.95 |
| 15 | K | 1402 | BO2 | C2-C3-N4 | -2.52 | 118.91 | 122.05 |
| 15 | N | 1404 | BO2 | O8-C7-C2 | -2.51 | 115.62 | 121.08 |
| 15 | K | 1402 | BO2 | C6-C5-N4 | -2.50 | 118.83 | 121.95 |
| 15 | K | 1402 | BO2 | C3-C2-N1 | -2.48 | 118.65 | 121.61 |
| 15 | N | 1404 | BO2 | C11-C10-N9 | -2.47 | 105.59 | 110.79 |
| 15 | K | 1402 | BO2 | C5-C6-N1 | -2.46 | 118.64 | 122.17 |
| 15 | 2 | 1405 | BO2 | C6-C5-N4 | -2.43 | 118.91 | 121.95 |
| 15 | 2 | 1405 | BO2 | C18-C10-N9 | -2.42 | 104.56 | 111.16 |
| 15 | Y | 1403 | BO2 | C3-C2-N1 | -2.40 | 118.75 | 121.61 |
| 15 | N | 1404 | BO2 | C18-C10-N9 | -2.35 | 104.78 | 111.16 |
| 15 | Y | 1403 | BO2 | C2-C3-N4 | -2.34 | 119.14 | 122.05 |
| 15 | V | 1401 | BO2 | O8-C7-C2 | -2.28 | 116.12 | 121.08 |
| 15 | Y | 1403 | BO2 | C5-C6-N1 | -2.27 | 118.90 | 122.17 |
| 15 | V | 1401 | BO2 | C5-C6-N1 | -2.13 | 119.10 | 122.17 |
| 15 | H | 1400 | BO2 | O8-C7-C2 | -2.06 | 116.60 | 121.08 |

There are no chirality outliers.

All (34) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 15 | V | 1401 | BO2 | N20-C21-C22-C23 |
| 15 | H | 1400 | BO2 | N20-C21-C22-C23 |
| 15 | K | 1402 | BO2 | N20-C21-C22-C23 |
| 15 | Y | 1403 | BO2 | N20-C21-C22-C23 |
| 15 | N | 1404 | BO2 | N1-C2-C7-O8 |
| 15 | 2 | 1405 | BO2 | N1-C2-C7-O8 |
| 15 | N | 1404 | BO2 | N1-C2-C7-N9 |
| 15 | 2 | 1405 | BO2 | N1-C2-C7-N9 |
| 15 | 2 | 1405 | BO2 | N20-C21-C22-C23 |
| 15 | N | 1404 | BO2 | C3-C2-C7-O8 |
| 15 | 2 | 1405 | BO2 | C3-C2-C7-O8 |
| 15 | N | 1404 | BO2 | N20-C21-C22-C23 |
| 15 | N | 1404 | BO2 | C3-C2-C7-N9 |
| 15 | 2 | 1405 | BO2 | C3-C2-C7-N9 |
| 15 | V | 1401 | BO2 | C22-C21-N20-C18 |
| 15 | H | 1400 | BO2 | C22-C21-N20-C18 |
| 15 | N | 1404 | BO2 | C22-C21-N20-C18 |
| 15 | K | 1402 | BO2 | C22-C21-N20-C18 |
| 15 | Y | 1403 | BO2 | C22-C21-N20-C18 |
| 15 | 2 | 1405 | BO2 | C22-C21-N20-C18 |
| 15 | V | 1401 | BO2 | N9-C10-C18-O19 |
| 15 | H | 1400 | BO2 | N9-C10-C18-O19 |
| 15 | V | 1401 | BO2 | N9-C10-C18-N20 |
| 15 | H | 1400 | BO2 | N9-C10-C18-N20 |
| 15 | K | 1402 | BO2 | N9-C10-C18-N20 |
| 15 | 2 | 1405 | BO2 | N9-C10-C18-N20 |
| 15 | K | 1402 | BO2 | N9-C10-C18-O19 |
| 15 | N | 1404 | BO2 | N9-C10-C18-N20 |
| 15 | Y | 1403 | BO2 | N9-C10-C18-O19 |
| 15 | 2 | 1405 | BO2 | N9-C10-C18-O19 |
| 15 | Y | 1403 | BO2 | N9-C10-C18-N20 |
| 15 | N | 1404 | BO2 | N9-C10-C18-O19 |
| 15 | V | 1401 | BO2 | C11-C10-C18-O19 |
| 15 | H | 1400 | BO2 | C11-C10-C18-O19 |

There are no ring outliers.

5 monomers are involved in 18 short contacts:

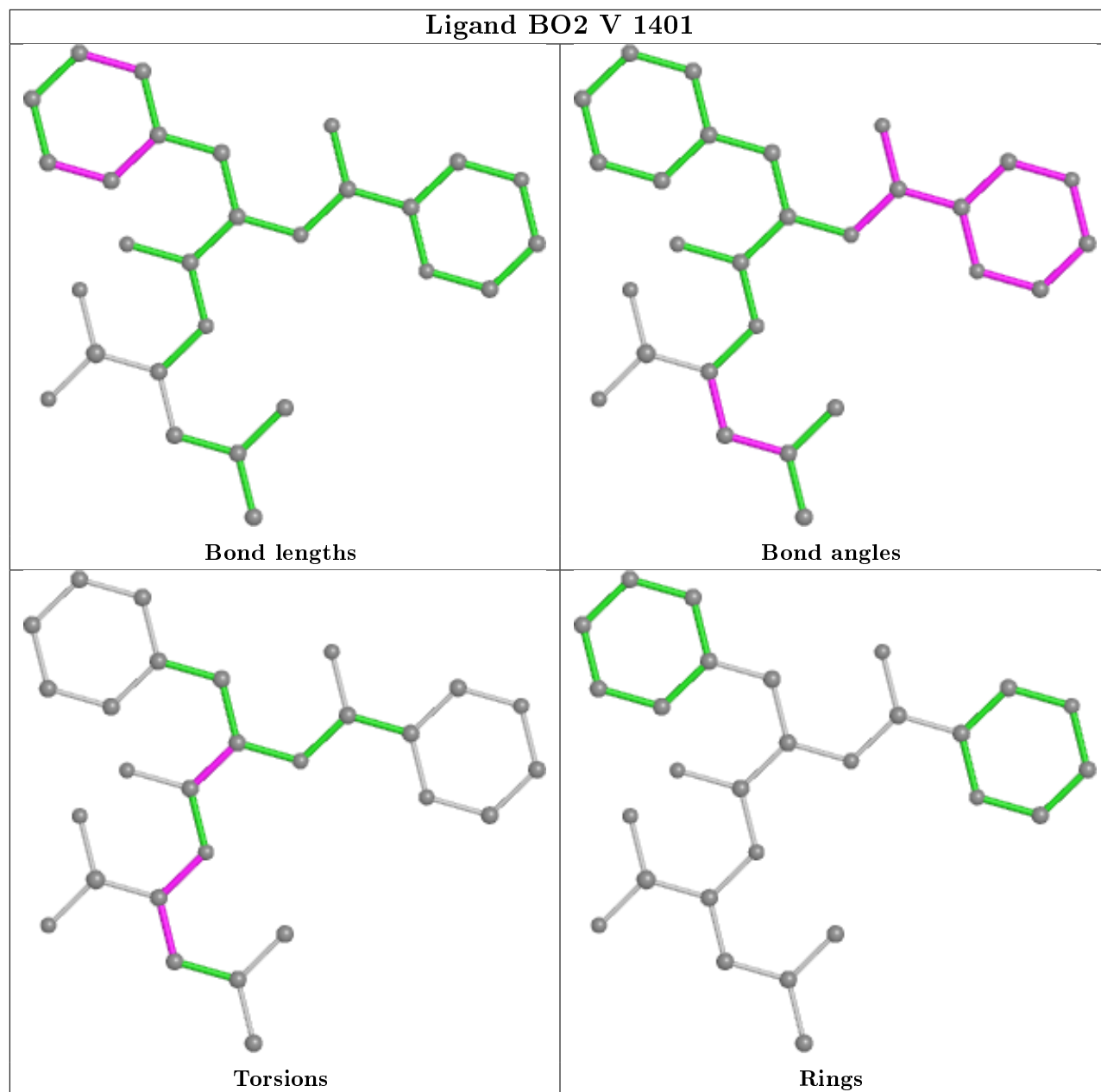
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15 | V | 1401 | BO2 | 2 | 0 |
| 15 | H | 1400 | BO2 | 2 | 0 |
| 15 | N | 1404 | BO2 | 5 | 0 |
| 15 | Y | 1403 | BO2 | 1 | 0 |

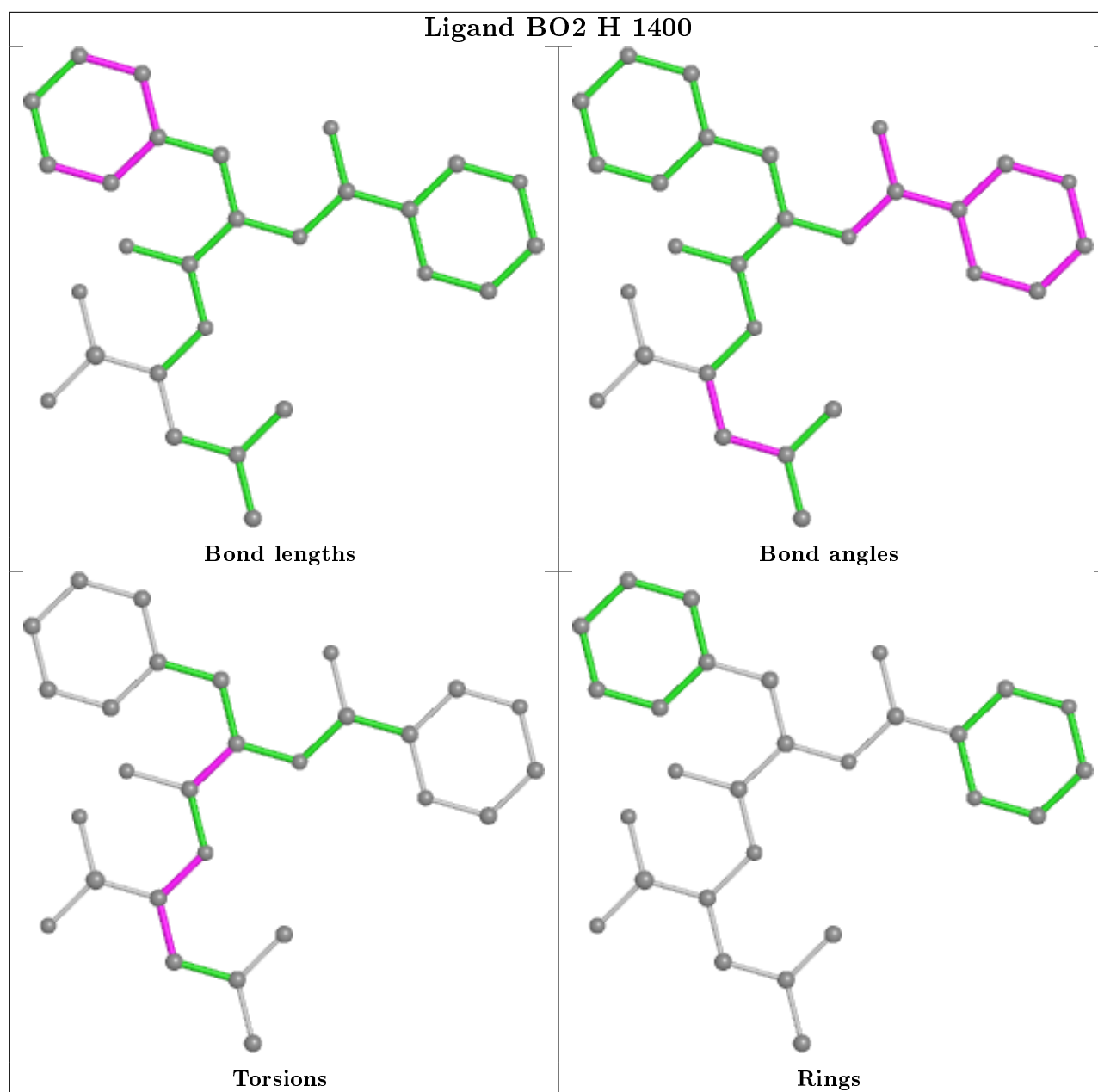
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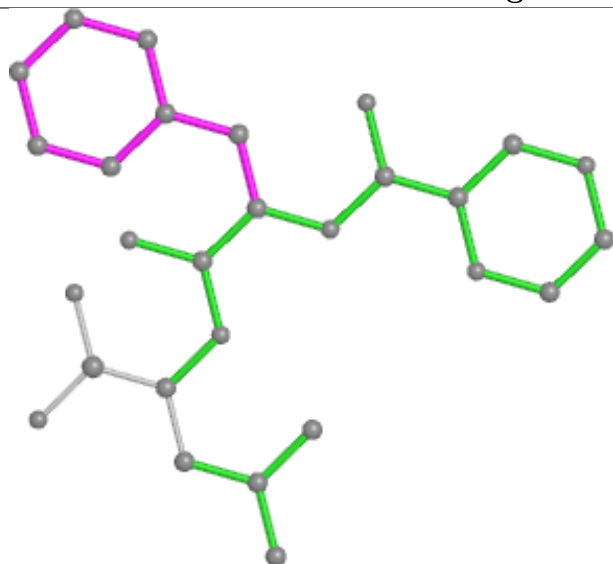
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15 | 2 | 1405 | BO2 | 8 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

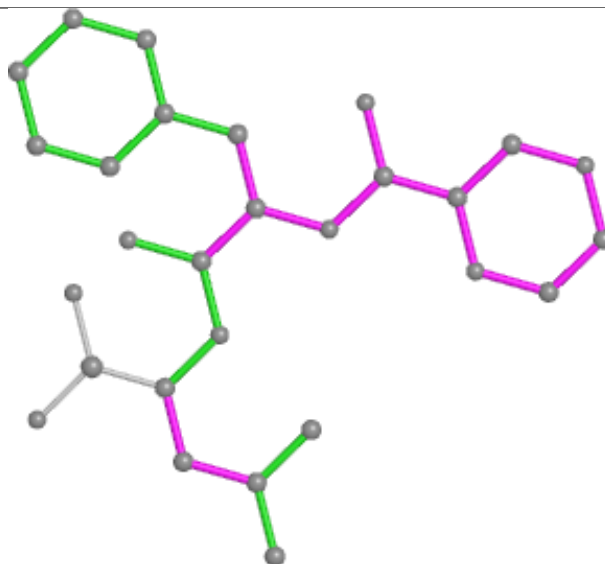




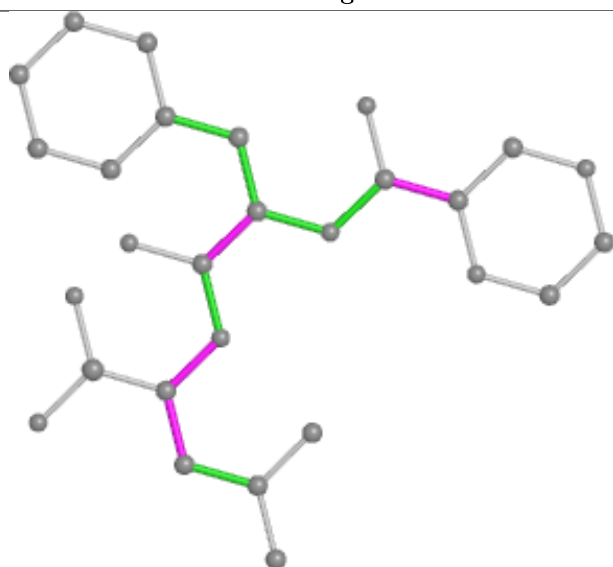
Ligand BO2 N 1404



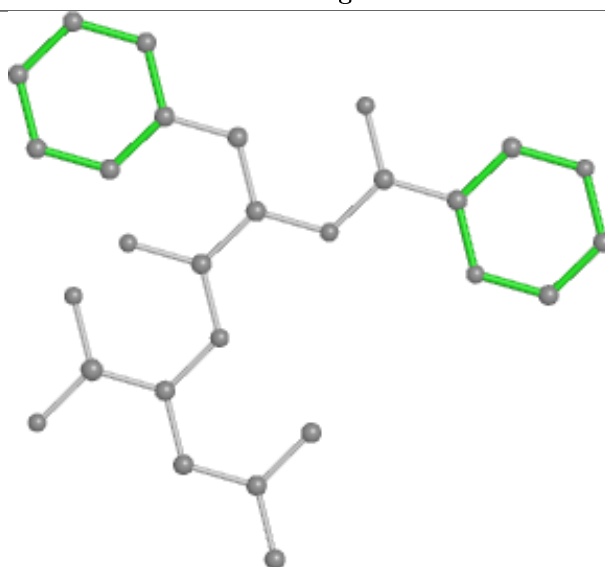
Bond lengths



Bond angles

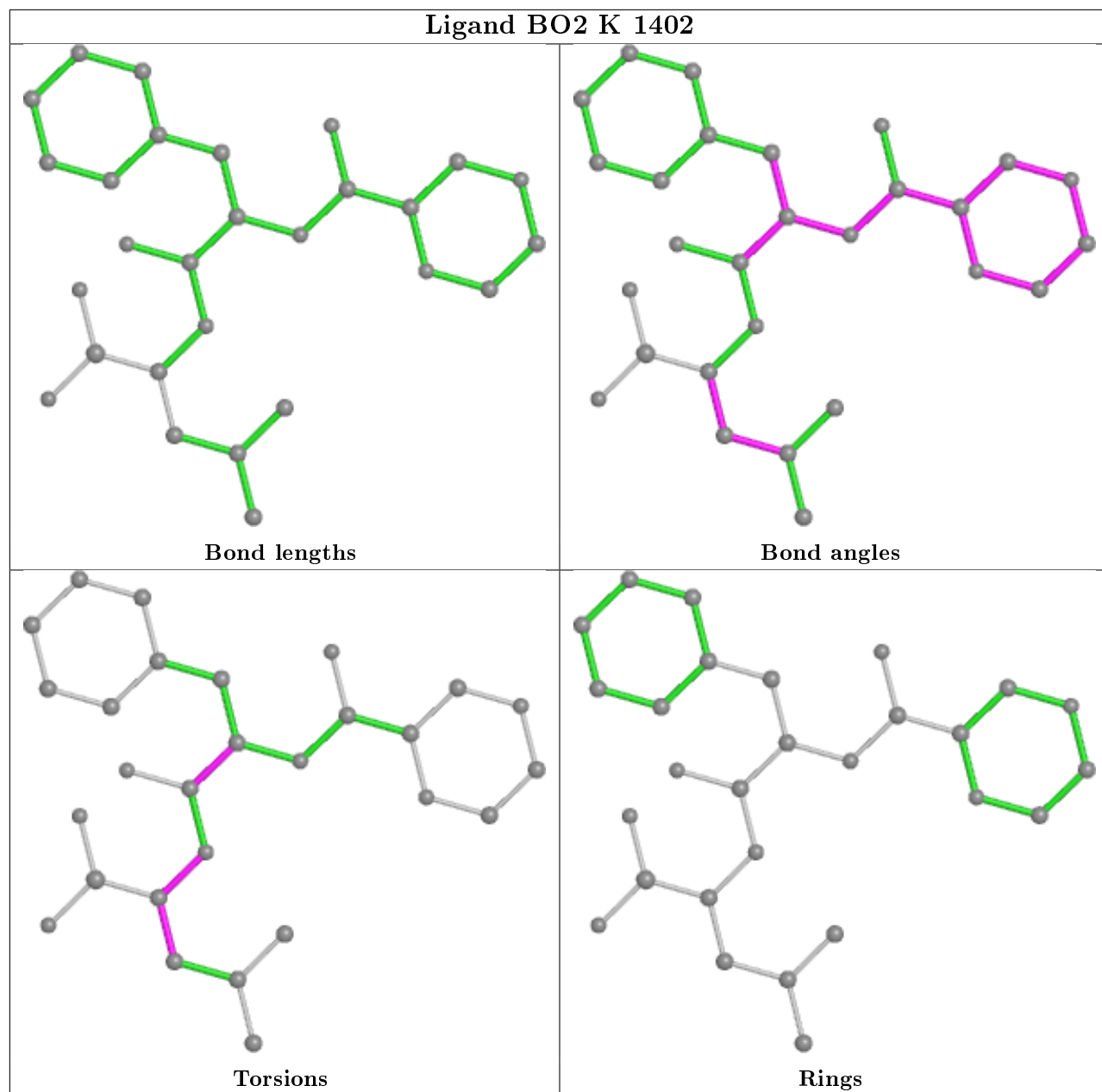


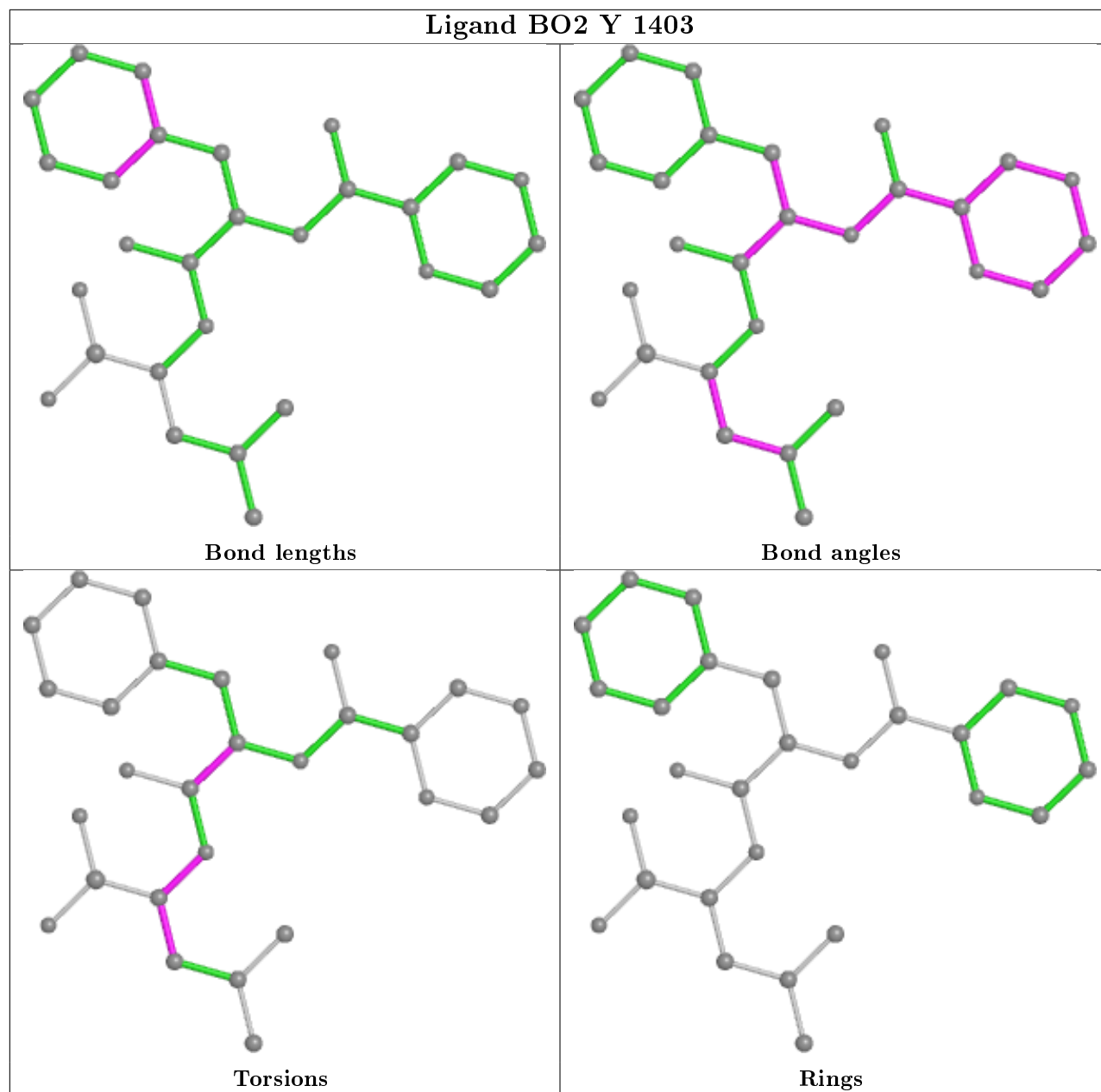
Torsions

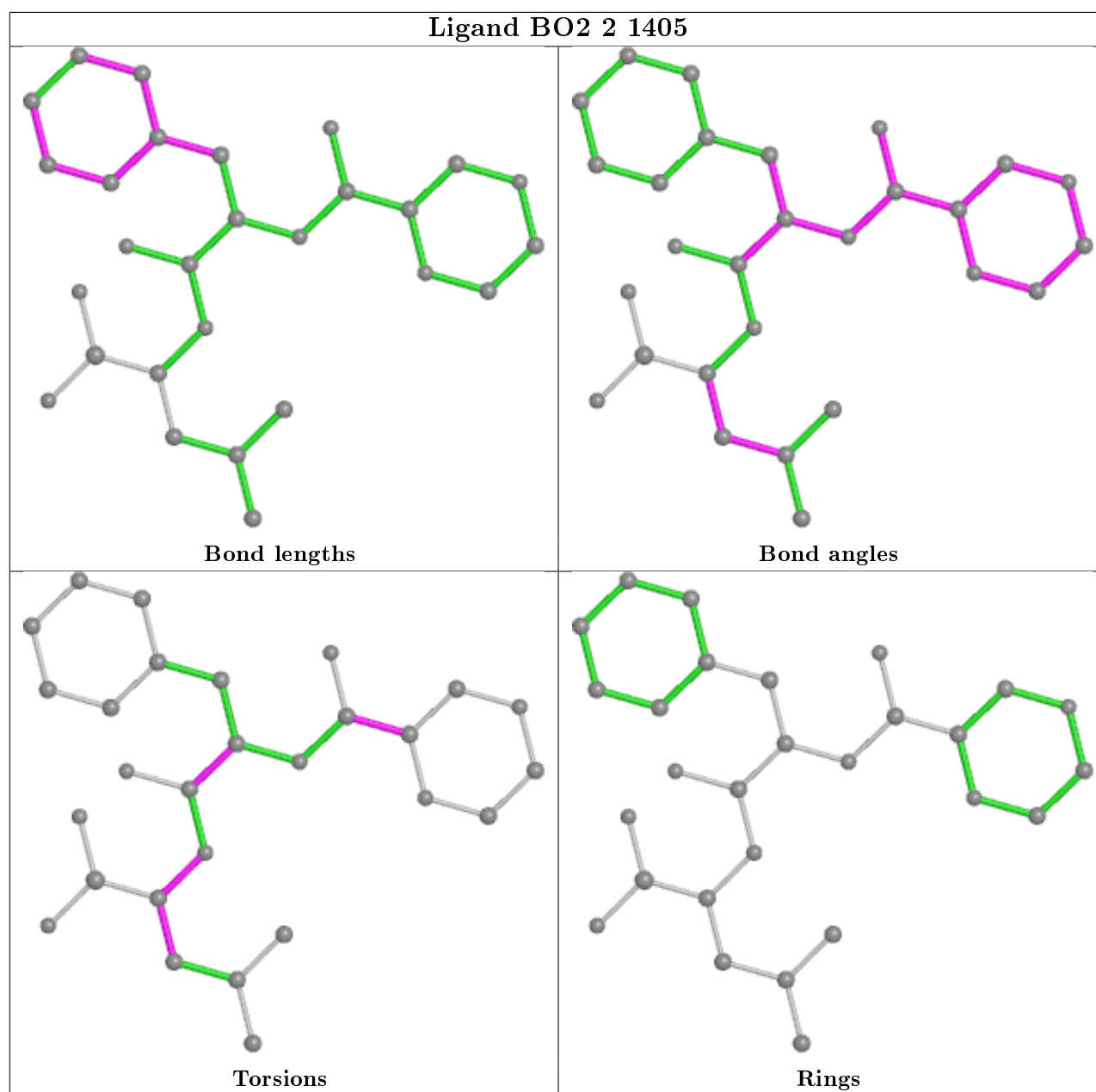


Rings

Ligand BO2 K 1402







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.