



Full wwPDB X-ray Structure Validation Report i

Jul 26, 2023 – 02:55 AM EDT

PDB ID : 1AM4
Title : COMPLEX BETWEEN CDC42HS.GMPPNP AND P50 RHOGAP (H. SAPIENS)
Authors : Rittinger, K.; Walker, P.; Gamblin, S.J.; Smerdon, S.J.
Deposited on : 1997-06-22
Resolution : 2.70 Å(reported)

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

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

| | | |
|--------------------------------|---|--|
| 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) | : | 2.34 |

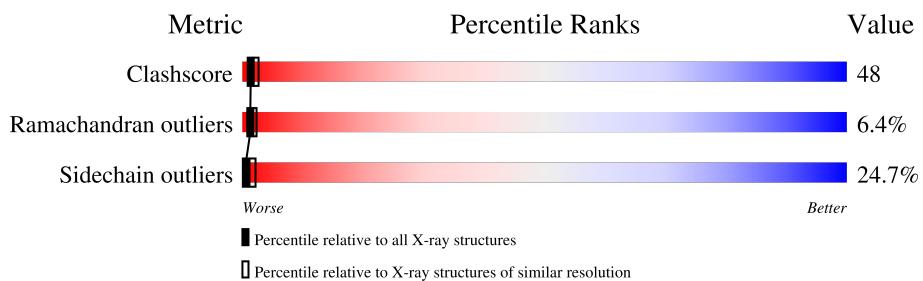
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| Clashscore | 141614 | 3122 (2.70-2.70) |
| Ramachandran outliers | 138981 | 3069 (2.70-2.70) |
| Sidechain outliers | 138945 | 3069 (2.70-2.70) |

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

Note EDS was not executed.



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

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4 | GNP | D | 678 | - | - | X | - |

2 Entry composition [\(i\)](#)

There are 5 unique types of molecules in this entry. The entry contains 9191 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 P50-RHOGAP.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1593 | 1032 | 273 | 286 | 2 | | | |
| 1 | B | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1593 | 1032 | 273 | 286 | 2 | | | |
| 1 | C | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1593 | 1032 | 273 | 286 | 2 | | | |

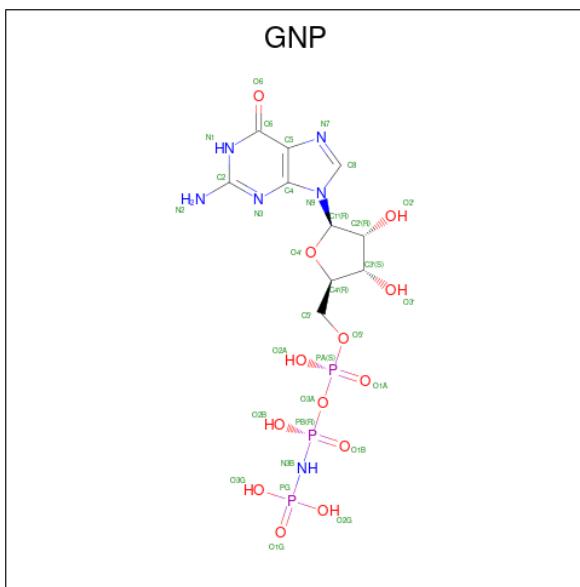
- Molecule 2 is a protein called CDC42HS.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | D | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1337 | 861 | 218 | 252 | 6 | | | |
| 2 | E | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1337 | 861 | 218 | 252 | 6 | | | |
| 2 | F | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1337 | 861 | 218 | 252 | 6 | | | |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | F | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|----|---|----|---|---------|---------|
| 4 | D | 1 | Total C N O P | | | | | 0 | 0 |
| | | | 32 | 10 | 6 | 13 | 3 | | |
| 4 | E | 1 | Total C N O P | | | | | 0 | 0 |
| | | | 32 | 10 | 6 | 13 | 3 | | |
| 4 | F | 1 | Total C N O P | | | | | 0 | 0 |
| | | | 32 | 10 | 6 | 13 | 3 | | |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------|----|---------|---------|
| 5 | A | 63 | Total O | | 0 | 0 |
| | | | 63 | 63 | | |
| 5 | D | 36 | Total O | | 0 | 0 |
| | | | 36 | 36 | | |
| 5 | B | 62 | Total O | | 0 | 0 |
| | | | 62 | 62 | | |
| 5 | E | 39 | Total O | | 0 | 0 |
| | | | 39 | 39 | | |
| 5 | C | 62 | Total O | | 0 | 0 |
| | | | 62 | 62 | | |
| 5 | F | 40 | Total O | | 0 | 0 |
| | | | 40 | 40 | | |

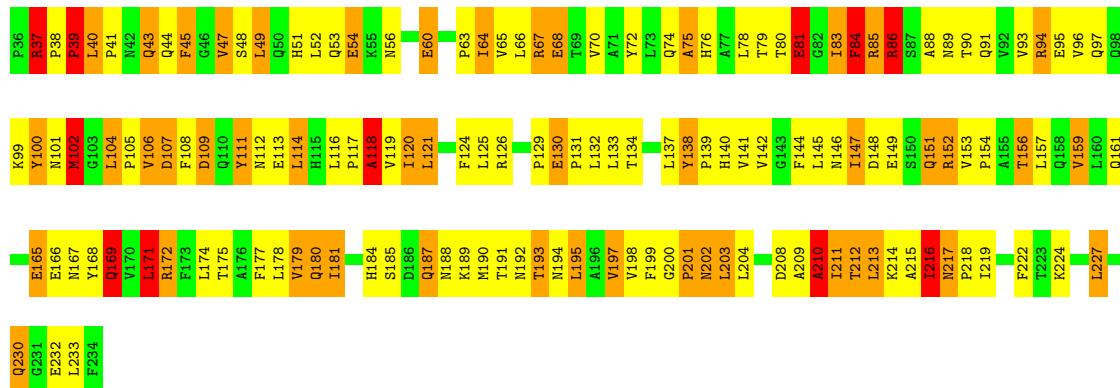
3 Residue-property plots

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

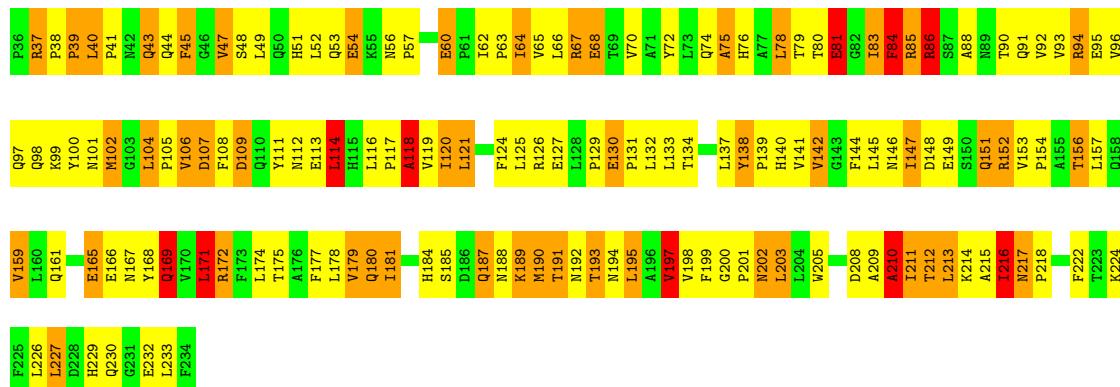
- Molecule 1: P50-RHOGAP

Chain A: 27% 43% 24% 6%



- Molecule 1: P50-RHOGAP

Chain B: 25% 46% 25% 5%



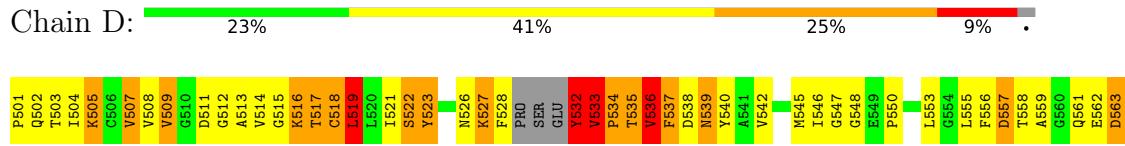
- Molecule 1: P50-RHOGAP

Chain C: 25% 45% 25% 6%

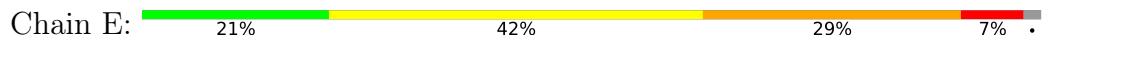




- Molecule 2: CDC42HS



- Molecule 2: CDC42HS



4 Data and refinement statistics [\(i\)](#)

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

| Property | Value | | | Source |
|--|------------------------|------------------|------------------|-----------|
| Space group | P 1 | | | Depositor |
| Cell constants a, b, c, α , β , γ | 78.11Å 90.01° | 78.12Å 90.00° | 78.10Å 90.05° | Depositor |
| Resolution (Å) | 12.00 – 2.70 | | | Depositor |
| % Data completeness (in resolution range) | 96.0 (12.00-2.70) | | | Depositor |
| R_{merge} | 0.06 | | | Depositor |
| R_{sym} | (Not available) | | | Depositor |
| Refinement program | CCP4 | | | Depositor |
| R , R_{free} | 0.230 , 0.280 | | | Depositor |
| Estimated twinning fraction | No twinning to report. | | | Xtriage |
| Total number of atoms | 9191 | | | wwPDB-VP |
| Average B, all atoms (Å ²) | 18.0 | | | 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: GNP, MG

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 | 0.92 | 0/1633 | 2.14 | 68/2231 (3.0%) |
| 1 | B | 0.92 | 0/1633 | 2.16 | 61/2231 (2.7%) |
| 1 | C | 0.94 | 0/1633 | 2.16 | 65/2231 (2.9%) |
| 2 | D | 0.97 | 0/1366 | 2.18 | 53/1860 (2.8%) |
| 2 | E | 0.96 | 0/1366 | 2.18 | 52/1860 (2.8%) |
| 2 | F | 0.95 | 0/1366 | 2.17 | 53/1860 (2.8%) |
| All | All | 0.94 | 0/8997 | 2.16 | 352/12273 (2.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 4 |
| 1 | B | 0 | 4 |
| 1 | C | 0 | 4 |
| 2 | D | 0 | 5 |
| 2 | E | 0 | 2 |
| 2 | F | 0 | 2 |
| All | All | 0 | 21 |

There are no bond length outliers.

All (352) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|-----------|-------|------------------------|---------------------|
| 2 | F | 647 | ARG | CD-NE-CZ | 19.40 | 150.76 | 123.60 |
| 2 | E | 647 | ARG | CD-NE-CZ | 19.30 | 150.61 | 123.60 |
| 2 | D | 647 | ARG | CD-NE-CZ | 19.27 | 150.58 | 123.60 |
| 1 | C | 85 | ARG | NE-CZ-NH1 | 18.11 | 129.35 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | B | 85 | ARG | NE-CZ-NH1 | 16.45 | 128.53 | 120.30 |
| 1 | A | 85 | ARG | NE-CZ-NH1 | 15.60 | 128.10 | 120.30 |
| 1 | C | 67 | ARG | NE-CZ-NH1 | 14.61 | 127.61 | 120.30 |
| 1 | B | 67 | ARG | NE-CZ-NH1 | 12.75 | 126.67 | 120.30 |
| 1 | B | 172 | ARG | NE-CZ-NH1 | 12.12 | 126.36 | 120.30 |
| 2 | F | 519 | LEU | CA-CB-CG | 11.96 | 142.81 | 115.30 |
| 2 | E | 519 | LEU | CA-CB-CG | 11.92 | 142.72 | 115.30 |
| 2 | D | 519 | LEU | CA-CB-CG | 11.40 | 141.53 | 115.30 |
| 1 | C | 172 | ARG | CD-NE-CZ | 10.96 | 138.95 | 123.60 |
| 2 | D | 557 | ASP | CB-CG-OD2 | 10.91 | 128.12 | 118.30 |
| 2 | E | 557 | ASP | CB-CG-OD2 | 10.71 | 127.94 | 118.30 |
| 1 | C | 172 | ARG | NE-CZ-NH1 | 10.55 | 125.57 | 120.30 |
| 1 | A | 172 | ARG | NE-CZ-NH1 | 10.46 | 125.53 | 120.30 |
| 1 | C | 203 | LEU | CA-CB-CG | 10.36 | 139.12 | 115.30 |
| 1 | B | 203 | LEU | CA-CB-CG | 10.12 | 138.59 | 115.30 |
| 1 | B | 86 | ARG | NE-CZ-NH1 | 10.12 | 125.36 | 120.30 |
| 1 | A | 203 | LEU | CA-CB-CG | 10.08 | 138.49 | 115.30 |
| 1 | A | 86 | ARG | NE-CZ-NH1 | 10.03 | 125.31 | 120.30 |
| 2 | D | 535 | THR | CA-CB-OG1 | -10.00 | 88.00 | 109.00 |
| 1 | A | 67 | ARG | CD-NE-CZ | 9.99 | 137.59 | 123.60 |
| 2 | F | 579 | LEU | CA-CB-CG | 9.95 | 138.18 | 115.30 |
| 2 | E | 647 | ARG | NE-CZ-NH1 | 9.95 | 125.27 | 120.30 |
| 1 | B | 138 | TYR | CB-CG-CD2 | -9.94 | 115.03 | 121.00 |
| 2 | F | 535 | THR | CA-CB-OG1 | -9.87 | 88.27 | 109.00 |
| 2 | D | 579 | LEU | CA-CB-CG | 9.84 | 137.94 | 115.30 |
| 1 | B | 81 | GLU | CA-CB-CG | 9.82 | 135.00 | 113.40 |
| 2 | D | 535 | THR | CA-CB-CG2 | 9.78 | 126.10 | 112.40 |
| 1 | A | 138 | TYR | CB-CG-CD2 | -9.78 | 115.13 | 121.00 |
| 2 | F | 535 | THR | CA-CB-CG2 | 9.74 | 126.04 | 112.40 |
| 2 | E | 535 | THR | CA-CB-OG1 | -9.66 | 88.71 | 109.00 |
| 1 | C | 148 | ASP | CB-CG-OD2 | -9.56 | 109.70 | 118.30 |
| 1 | B | 67 | ARG | CD-NE-CZ | 9.53 | 136.94 | 123.60 |
| 2 | F | 557 | ASP | CB-CG-OD2 | 9.46 | 126.82 | 118.30 |
| 2 | E | 535 | THR | CA-CB-CG2 | 9.45 | 125.63 | 112.40 |
| 2 | E | 579 | LEU | CA-CB-CG | 9.43 | 136.98 | 115.30 |
| 1 | B | 138 | TYR | CB-CG-CD1 | 9.36 | 126.62 | 121.00 |
| 1 | A | 172 | ARG | CD-NE-CZ | 9.34 | 136.68 | 123.60 |
| 1 | C | 81 | GLU | CA-CB-CG | 9.27 | 133.79 | 113.40 |
| 2 | E | 532 | TYR | CA-CB-CG | -9.26 | 95.80 | 113.40 |
| 1 | A | 138 | TYR | CB-CG-CD1 | 9.23 | 126.54 | 121.00 |
| 1 | A | 81 | GLU | CA-CB-CG | 9.21 | 133.65 | 113.40 |
| 1 | A | 67 | ARG | NE-CZ-NH1 | 9.12 | 124.86 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | F | 532 | TYR | CA-CB-CG | -9.05 | 96.20 | 113.40 |
| 2 | D | 532 | TYR | CA-CB-CG | -9.05 | 96.21 | 113.40 |
| 1 | B | 60 | GLU | CA-CB-CG | 8.93 | 133.04 | 113.40 |
| 1 | B | 165 | GLU | C-N-CA | 8.91 | 143.99 | 121.70 |
| 2 | E | 532 | TYR | CB-CG-CD1 | -8.77 | 115.74 | 121.00 |
| 1 | A | 60 | GLU | CA-CB-CG | 8.69 | 132.51 | 113.40 |
| 1 | C | 67 | ARG | CD-NE-CZ | 8.37 | 135.32 | 123.60 |
| 1 | C | 60 | GLU | CA-CB-CG | 8.35 | 131.76 | 113.40 |
| 1 | A | 165 | GLU | C-N-CA | 8.35 | 142.57 | 121.70 |
| 2 | D | 647 | ARG | NE-CZ-NH1 | 8.31 | 124.45 | 120.30 |
| 1 | B | 148 | ASP | CB-CG-OD2 | -8.28 | 110.85 | 118.30 |
| 1 | C | 165 | GLU | C-N-CA | 8.26 | 142.34 | 121.70 |
| 1 | A | 148 | ASP | CB-CG-OD2 | -8.23 | 110.89 | 118.30 |
| 1 | B | 172 | ARG | CD-NE-CZ | 8.18 | 135.05 | 123.60 |
| 2 | F | 647 | ARG | NE-CZ-NH1 | 8.16 | 124.38 | 120.30 |
| 1 | A | 152 | ARG | NE-CZ-NH2 | 8.11 | 124.35 | 120.30 |
| 1 | C | 152 | ARG | NE-CZ-NH2 | 8.04 | 124.32 | 120.30 |
| 1 | C | 166 | GLU | CA-CB-CG | 7.88 | 130.73 | 113.40 |
| 1 | B | 64 | ILE | CB-CG1-CD1 | 7.87 | 135.92 | 113.90 |
| 1 | A | 64 | ILE | CB-CG1-CD1 | 7.83 | 135.82 | 113.90 |
| 2 | E | 647 | ARG | CG-CD-NE | 7.57 | 127.70 | 111.80 |
| 2 | F | 647 | ARG | CG-CD-NE | 7.55 | 127.66 | 111.80 |
| 1 | C | 109 | ASP | CB-CA-C | 7.54 | 125.49 | 110.40 |
| 2 | D | 647 | ARG | CG-CD-NE | 7.53 | 127.61 | 111.80 |
| 1 | A | 168 | TYR | CB-CG-CD2 | 7.49 | 125.49 | 121.00 |
| 2 | D | 615 | THR | O-C-N | 7.43 | 134.59 | 122.70 |
| 2 | D | 595 | GLU | CG-CD-OE1 | 7.42 | 133.14 | 118.30 |
| 1 | C | 86 | ARG | NE-CZ-NH1 | 7.40 | 124.00 | 120.30 |
| 2 | E | 532 | TYR | CB-CG-CD2 | 7.36 | 125.42 | 121.00 |
| 2 | F | 648 | ASP | CB-CG-OD1 | 7.34 | 124.91 | 118.30 |
| 1 | C | 91 | GLN | CB-CG-CD | 7.33 | 130.65 | 111.60 |
| 1 | B | 166 | GLU | CA-CB-CG | 7.29 | 129.45 | 113.40 |
| 1 | A | 149 | GLU | CG-CD-OE2 | 7.26 | 132.83 | 118.30 |
| 1 | B | 195 | LEU | CA-CB-CG | 7.23 | 131.94 | 115.30 |
| 1 | B | 91 | GLN | CB-CG-CD | 7.23 | 130.39 | 111.60 |
| 1 | A | 106 | VAL | CA-CB-CG2 | 7.21 | 121.72 | 110.90 |
| 2 | E | 648 | ASP | CB-CG-OD1 | 7.21 | 124.79 | 118.30 |
| 1 | A | 91 | GLN | CB-CG-CD | 7.21 | 130.34 | 111.60 |
| 2 | F | 669 | PHE | CB-CA-C | 7.19 | 124.77 | 110.40 |
| 2 | D | 648 | ASP | CB-CG-OD1 | 7.18 | 124.76 | 118.30 |
| 1 | A | 109 | ASP | CB-CA-C | 7.18 | 124.76 | 110.40 |
| 1 | B | 149 | GLU | CG-CD-OE2 | 7.14 | 132.58 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | F | 595 | GLU | CG-CD-OE1 | 7.10 | 132.50 | 118.30 |
| 1 | A | 195 | LEU | CA-CB-CG | 7.09 | 131.61 | 115.30 |
| 2 | E | 669 | PHE | CB-CA-C | 7.08 | 124.56 | 110.40 |
| 2 | E | 595 | GLU | CG-CD-OE1 | 7.07 | 132.44 | 118.30 |
| 2 | F | 665 | LEU | CA-CB-CG | 7.05 | 131.52 | 115.30 |
| 1 | B | 106 | VAL | CA-CB-CG2 | 7.05 | 121.47 | 110.90 |
| 1 | A | 166 | GLU | CA-CB-CG | 7.04 | 128.90 | 113.40 |
| 1 | C | 138 | TYR | CB-CG-CD2 | -7.04 | 116.78 | 121.00 |
| 2 | D | 656 | GLU | OE1-CD-OE2 | 7.03 | 131.73 | 123.30 |
| 1 | C | 64 | ILE | CB-CG1-CD1 | 7.00 | 133.51 | 113.90 |
| 1 | C | 121 | LEU | CA-CB-CG | 6.99 | 131.37 | 115.30 |
| 1 | B | 109 | ASP | CB-CA-C | 6.98 | 124.36 | 110.40 |
| 2 | D | 649 | LEU | CB-CA-C | 6.96 | 123.43 | 110.20 |
| 2 | F | 615 | THR | O-C-N | 6.94 | 133.80 | 122.70 |
| 1 | C | 195 | LEU | CA-CB-CG | 6.93 | 131.25 | 115.30 |
| 1 | B | 49 | LEU | O-C-N | 6.90 | 133.75 | 122.70 |
| 2 | F | 649 | LEU | CB-CA-C | 6.88 | 123.27 | 110.20 |
| 2 | E | 649 | LEU | CB-CA-C | 6.87 | 123.25 | 110.20 |
| 2 | E | 557 | ASP | CB-CG-OD1 | -6.85 | 112.14 | 118.30 |
| 2 | E | 615 | THR | O-C-N | 6.83 | 133.63 | 122.70 |
| 1 | B | 54 | GLU | CA-CB-CG | 6.82 | 128.41 | 113.40 |
| 2 | D | 665 | LEU | CA-CB-CG | 6.80 | 130.93 | 115.30 |
| 1 | C | 168 | TYR | CB-CG-CD2 | 6.77 | 125.06 | 121.00 |
| 1 | C | 68 | GLU | CA-C-O | -6.75 | 105.92 | 120.10 |
| 2 | D | 517 | THR | CA-CB-OG1 | -6.73 | 94.86 | 109.00 |
| 2 | D | 563 | ASP | CB-CG-OD2 | 6.72 | 124.35 | 118.30 |
| 2 | E | 572 | TYR | CB-CG-CD1 | 6.71 | 125.03 | 121.00 |
| 1 | C | 54 | GLU | CA-CB-CG | 6.71 | 128.16 | 113.40 |
| 2 | D | 562 | GLU | CG-CD-OE1 | 6.67 | 131.64 | 118.30 |
| 2 | D | 570 | LEU | C-N-CA | 6.67 | 138.37 | 121.70 |
| 2 | F | 576 | ASP | CB-CG-OD2 | -6.66 | 112.31 | 118.30 |
| 1 | B | 168 | TYR | CB-CG-CD2 | 6.64 | 124.98 | 121.00 |
| 2 | E | 536 | VAL | CA-CB-CG1 | -6.63 | 100.95 | 110.90 |
| 2 | F | 517 | THR | CA-CB-OG1 | -6.63 | 95.07 | 109.00 |
| 1 | C | 191 | THR | CA-CB-CG2 | 6.63 | 121.68 | 112.40 |
| 2 | E | 665 | LEU | CA-CB-CG | 6.63 | 130.54 | 115.30 |
| 1 | C | 85 | ARG | NE-CZ-NH2 | -6.62 | 116.99 | 120.30 |
| 2 | D | 669 | PHE | CB-CA-C | 6.62 | 123.64 | 110.40 |
| 1 | A | 54 | GLU | CA-CB-CG | 6.61 | 127.94 | 113.40 |
| 2 | F | 557 | ASP | CB-CG-OD1 | -6.60 | 112.36 | 118.30 |
| 2 | D | 536 | VAL | CA-CB-CG1 | -6.58 | 101.02 | 110.90 |
| 2 | D | 572 | TYR | CB-CG-CD2 | -6.54 | 117.08 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 152 | ARG | CG-CD-NE | 6.52 | 125.50 | 111.80 |
| 1 | B | 121 | LEU | CA-CB-CG | 6.52 | 130.29 | 115.30 |
| 1 | B | 152 | ARG | NE-CZ-NH1 | -6.51 | 117.04 | 120.30 |
| 1 | C | 67 | ARG | NE-CZ-NH2 | -6.51 | 117.05 | 120.30 |
| 1 | A | 85 | ARG | NE-CZ-NH2 | -6.50 | 117.05 | 120.30 |
| 2 | D | 536 | VAL | CB-CA-C | 6.49 | 123.72 | 111.40 |
| 1 | C | 106 | VAL | CA-CB-CG2 | 6.48 | 120.62 | 110.90 |
| 1 | A | 49 | LEU | O-C-N | 6.47 | 133.06 | 122.70 |
| 1 | B | 67 | ARG | NE-CZ-NH2 | -6.45 | 117.07 | 120.30 |
| 2 | D | 597 | TRP | CA-CB-CG | -6.41 | 101.52 | 113.70 |
| 2 | F | 562 | GLU | CG-CD-OE1 | 6.41 | 131.11 | 118.30 |
| 2 | E | 536 | VAL | CB-CA-C | 6.39 | 123.55 | 111.40 |
| 2 | F | 677 | LEU | CB-CA-C | 6.39 | 122.35 | 110.20 |
| 1 | C | 152 | ARG | NE-CZ-NH1 | -6.39 | 117.11 | 120.30 |
| 1 | A | 208 | ASP | CB-CG-OD1 | 6.38 | 124.04 | 118.30 |
| 2 | F | 536 | VAL | CB-CA-C | 6.37 | 123.51 | 111.40 |
| 2 | F | 566 | ARG | NE-CZ-NH2 | -6.37 | 117.11 | 120.30 |
| 2 | E | 644 | LYS | CA-C-O | 6.36 | 133.46 | 120.10 |
| 1 | B | 227 | LEU | CB-CA-C | 6.32 | 122.21 | 110.20 |
| 2 | F | 568 | ARG | NE-CZ-NH2 | -6.32 | 117.14 | 120.30 |
| 1 | C | 169 | GLN | CA-CB-CG | 6.32 | 127.30 | 113.40 |
| 1 | B | 104 | LEU | CB-CA-C | 6.31 | 122.19 | 110.20 |
| 2 | E | 562 | GLU | CG-CD-OE1 | 6.30 | 130.90 | 118.30 |
| 1 | B | 68 | GLU | CA-C-O | -6.29 | 106.89 | 120.10 |
| 2 | E | 537 | PHE | CA-CB-CG | 6.29 | 129.00 | 113.90 |
| 2 | F | 537 | PHE | CA-CB-CG | 6.29 | 129.00 | 113.90 |
| 2 | E | 670 | ASP | CB-CG-OD2 | 6.27 | 123.95 | 118.30 |
| 2 | D | 537 | PHE | CA-CB-CG | 6.25 | 128.90 | 113.90 |
| 1 | A | 68 | GLU | CA-C-O | -6.25 | 106.98 | 120.10 |
| 1 | C | 49 | LEU | O-C-N | 6.25 | 132.69 | 122.70 |
| 2 | D | 532 | TYR | CB-CG-CD1 | -6.24 | 117.25 | 121.00 |
| 2 | D | 656 | GLU | CG-CD-OE2 | -6.24 | 105.83 | 118.30 |
| 2 | D | 518 | CYS | CB-CA-C | 6.23 | 122.87 | 110.40 |
| 1 | B | 127 | GLU | OE1-CD-OE2 | -6.20 | 115.86 | 123.30 |
| 1 | C | 149 | GLU | CG-CD-OE2 | 6.20 | 130.70 | 118.30 |
| 1 | B | 86 | ARG | NE-CZ-NH2 | -6.18 | 117.21 | 120.30 |
| 2 | F | 518 | CYS | CB-CA-C | 6.18 | 122.75 | 110.40 |
| 1 | C | 227 | LEU | CB-CA-C | 6.17 | 121.93 | 110.20 |
| 2 | F | 536 | VAL | CA-CB-CG1 | -6.16 | 101.67 | 110.90 |
| 1 | A | 152 | ARG | NE-CZ-NH1 | -6.15 | 117.23 | 120.30 |
| 2 | F | 663 | ARG | CD-NE-CZ | 6.13 | 132.19 | 123.60 |
| 2 | D | 532 | TYR | CB-CG-CD2 | 6.13 | 124.68 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | F | 597 | TRP | CA-CB-CG | -6.11 | 102.09 | 113.70 |
| 2 | E | 518 | CYS | CB-CA-C | 6.09 | 122.59 | 110.40 |
| 1 | C | 169 | GLN | CB-CG-CD | 6.09 | 127.43 | 111.60 |
| 2 | E | 677 | LEU | CB-CA-C | 6.08 | 121.76 | 110.20 |
| 2 | D | 557 | ASP | CB-CG-OD1 | -6.08 | 112.83 | 118.30 |
| 1 | C | 104 | LEU | CB-CA-C | 6.08 | 121.75 | 110.20 |
| 2 | E | 656 | GLU | OE1-CD-OE2 | 6.07 | 130.59 | 123.30 |
| 2 | E | 534 | PRO | CA-C-O | 6.06 | 134.73 | 120.20 |
| 1 | A | 37 | ARG | NE-CZ-NH1 | -6.05 | 117.27 | 120.30 |
| 2 | E | 671 | GLU | CG-CD-OE1 | 6.05 | 130.39 | 118.30 |
| 1 | B | 88 | ALA | C-N-CA | 6.04 | 136.79 | 121.70 |
| 1 | A | 107 | ASP | CB-CA-C | 6.03 | 122.46 | 110.40 |
| 2 | E | 597 | TRP | CA-CB-CG | -6.02 | 102.26 | 113.70 |
| 1 | C | 68 | GLU | N-CA-CB | 6.02 | 121.43 | 110.60 |
| 1 | B | 202 | ASN | CB-CG-OD1 | -6.02 | 109.57 | 121.60 |
| 1 | B | 152 | ARG | NE-CZ-NH2 | 6.01 | 123.31 | 120.30 |
| 1 | A | 169 | GLN | CA-CB-CG | 5.99 | 126.58 | 113.40 |
| 2 | F | 671 | GLU | CG-CD-OE1 | 5.99 | 130.28 | 118.30 |
| 1 | C | 208 | ASP | CB-CG-OD1 | 5.98 | 123.68 | 118.30 |
| 2 | E | 538 | ASP | CB-CG-OD1 | 5.98 | 123.68 | 118.30 |
| 2 | D | 656 | GLU | CA-CB-CG | 5.97 | 126.53 | 113.40 |
| 1 | A | 171 | LEU | CA-CB-CG | 5.96 | 129.02 | 115.30 |
| 1 | B | 179 | VAL | C-N-CA | 5.96 | 136.61 | 121.70 |
| 1 | B | 169 | GLN | CA-CB-CG | 5.96 | 126.51 | 113.40 |
| 2 | D | 523 | TYR | CB-CG-CD1 | 5.95 | 124.57 | 121.00 |
| 1 | C | 107 | ASP | CB-CA-C | 5.95 | 122.29 | 110.40 |
| 2 | F | 534 | PRO | CA-C-O | 5.94 | 134.46 | 120.20 |
| 2 | E | 644 | LYS | C-N-CA | 5.94 | 136.54 | 121.70 |
| 2 | D | 568 | ARG | CD-NE-CZ | -5.93 | 115.29 | 123.60 |
| 2 | F | 568 | ARG | CD-NE-CZ | -5.92 | 115.31 | 123.60 |
| 1 | C | 202 | ASN | CB-CG-OD1 | -5.92 | 109.77 | 121.60 |
| 2 | F | 656 | GLU | CA-CB-CG | 5.91 | 126.41 | 113.40 |
| 2 | D | 576 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 2 | E | 572 | TYR | CB-CG-CD2 | -5.90 | 117.46 | 121.00 |
| 2 | E | 656 | GLU | CA-CB-CG | 5.88 | 126.34 | 113.40 |
| 2 | D | 677 | LEU | CB-CA-C | 5.88 | 121.38 | 110.20 |
| 1 | A | 202 | ASN | CB-CG-OD1 | -5.88 | 109.84 | 121.60 |
| 1 | A | 68 | GLU | N-CA-CB | 5.88 | 121.18 | 110.60 |
| 1 | C | 88 | ALA | C-N-CA | 5.87 | 136.38 | 121.70 |
| 1 | A | 169 | GLN | CB-CG-CD | 5.85 | 126.81 | 111.60 |
| 1 | B | 171 | LEU | CA-CB-CG | 5.85 | 128.75 | 115.30 |
| 1 | A | 88 | ALA | C-N-CA | 5.84 | 136.29 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 104 | LEU | CB-CA-C | 5.83 | 121.28 | 110.20 |
| 1 | B | 169 | GLN | CB-CG-CD | 5.83 | 126.75 | 111.60 |
| 1 | B | 152 | ARG | CG-CD-NE | 5.82 | 124.02 | 111.80 |
| 1 | C | 76 | HIS | CA-CB-CG | -5.81 | 103.72 | 113.60 |
| 1 | A | 227 | LEU | CB-CA-C | 5.81 | 121.24 | 110.20 |
| 1 | B | 68 | GLU | N-CA-CB | 5.81 | 121.06 | 110.60 |
| 1 | B | 130 | GLU | CG-CD-OE2 | -5.80 | 106.71 | 118.30 |
| 2 | D | 534 | PRO | CA-C-O | 5.79 | 134.09 | 120.20 |
| 1 | A | 159 | VAL | O-C-N | 5.78 | 131.95 | 122.70 |
| 1 | A | 145 | LEU | CA-CB-CG | 5.77 | 128.58 | 115.30 |
| 1 | A | 120 | ILE | CB-CA-C | 5.76 | 123.11 | 111.60 |
| 1 | C | 190 | MET | CA-CB-CG | 5.75 | 123.07 | 113.30 |
| 1 | C | 100 | TYR | CB-CG-CD2 | -5.74 | 117.56 | 121.00 |
| 1 | C | 201 | PRO | C-N-CA | 5.70 | 135.95 | 121.70 |
| 1 | A | 152 | ARG | CG-CD-NE | 5.69 | 123.76 | 111.80 |
| 2 | D | 671 | GLU | CG-CD-OE1 | 5.69 | 129.67 | 118.30 |
| 1 | B | 107 | ASP | CB-CA-C | 5.68 | 121.77 | 110.40 |
| 2 | E | 570 | LEU | C-N-CA | 5.68 | 135.89 | 121.70 |
| 2 | F | 572 | TYR | CB-CG-CD2 | -5.68 | 117.59 | 121.00 |
| 2 | D | 568 | ARG | NE-CZ-NH2 | -5.67 | 117.46 | 120.30 |
| 2 | D | 644 | LYS | C-N-CA | 5.67 | 135.88 | 121.70 |
| 2 | F | 570 | LEU | C-N-CA | 5.67 | 135.88 | 121.70 |
| 2 | D | 564 | TYR | CB-CG-CD2 | 5.67 | 124.40 | 121.00 |
| 1 | B | 145 | LEU | CA-CB-CG | 5.66 | 128.31 | 115.30 |
| 1 | B | 102 | MET | CA-CB-CG | 5.64 | 122.90 | 113.30 |
| 1 | A | 121 | LEU | CA-CB-CG | 5.64 | 128.28 | 115.30 |
| 1 | B | 76 | HIS | CA-CB-CG | -5.64 | 104.01 | 113.60 |
| 1 | B | 114 | LEU | CA-CB-CG | 5.64 | 128.27 | 115.30 |
| 1 | C | 89 | ASN | CA-CB-CG | 5.62 | 125.77 | 113.40 |
| 1 | A | 89 | ASN | CA-CB-CG | 5.62 | 125.77 | 113.40 |
| 2 | E | 562 | GLU | CA-CB-CG | 5.62 | 125.77 | 113.40 |
| 1 | B | 159 | VAL | O-C-N | 5.62 | 131.69 | 122.70 |
| 1 | A | 111 | TYR | CB-CG-CD2 | 5.62 | 124.37 | 121.00 |
| 1 | A | 76 | HIS | CA-CB-CG | -5.61 | 104.06 | 113.60 |
| 1 | C | 171 | LEU | CA-CB-CG | 5.60 | 128.17 | 115.30 |
| 1 | C | 159 | VAL | O-C-N | 5.58 | 131.63 | 122.70 |
| 1 | A | 49 | LEU | CA-CB-CG | 5.57 | 128.11 | 115.30 |
| 2 | F | 670 | ASP | CB-CG-OD2 | 5.56 | 123.30 | 118.30 |
| 2 | F | 582 | PHE | O-C-N | 5.55 | 131.59 | 122.70 |
| 1 | C | 120 | ILE | CB-CA-C | 5.55 | 122.69 | 111.60 |
| 2 | E | 595 | GLU | CG-CD-OE2 | -5.54 | 107.22 | 118.30 |
| 2 | F | 644 | LYS | CA-C-O | 5.54 | 131.72 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | D | 595 | GLU | CG-CD-OE2 | -5.53 | 107.24 | 118.30 |
| 2 | D | 538 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | C | 84 | PHE | N-CA-CB | -5.50 | 100.70 | 110.60 |
| 2 | F | 514 | VAL | C-N-CA | 5.49 | 133.84 | 122.30 |
| 1 | B | 118 | ALA | CB-CA-C | 5.49 | 118.33 | 110.10 |
| 2 | E | 517 | THR | CA-CB-OG1 | -5.47 | 97.50 | 109.00 |
| 1 | A | 210 | ALA | N-CA-CB | 5.45 | 117.72 | 110.10 |
| 1 | A | 130 | GLU | CG-CD-OE2 | -5.44 | 107.42 | 118.30 |
| 1 | B | 85 | ARG | NH1-CZ-NH2 | -5.43 | 113.43 | 119.40 |
| 1 | B | 45 | PHE | CB-CA-C | 5.42 | 121.24 | 110.40 |
| 1 | B | 191 | THR | CA-CB-CG2 | 5.42 | 119.98 | 112.40 |
| 1 | B | 84 | PHE | N-CA-CB | -5.42 | 100.85 | 110.60 |
| 1 | C | 145 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 1 | A | 100 | TYR | CB-CG-CD2 | -5.40 | 117.76 | 121.00 |
| 1 | A | 102 | MET | CA-CB-CG | 5.40 | 122.48 | 113.30 |
| 2 | F | 563 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 2 | F | 621 | ASP | CB-CG-OD2 | 5.38 | 123.14 | 118.30 |
| 1 | A | 208 | ASP | CB-CA-C | 5.38 | 121.16 | 110.40 |
| 1 | A | 130 | GLU | OE1-CD-OE2 | 5.37 | 129.74 | 123.30 |
| 1 | A | 216 | ILE | C-N-CA | 5.37 | 135.12 | 121.70 |
| 2 | F | 595 | GLU | CG-CD-OE2 | -5.36 | 107.58 | 118.30 |
| 1 | B | 216 | ILE | C-N-CA | 5.34 | 135.06 | 121.70 |
| 2 | E | 568 | ARG | CD-NE-CZ | -5.34 | 116.13 | 123.60 |
| 2 | E | 621 | ASP | CB-CA-C | 5.33 | 121.07 | 110.40 |
| 2 | F | 621 | ASP | CB-CA-C | 5.33 | 121.07 | 110.40 |
| 2 | F | 547 | GLY | C-N-CA | 5.33 | 133.50 | 122.30 |
| 2 | F | 655 | VAL | CA-C-O | 5.33 | 131.29 | 120.10 |
| 2 | E | 514 | VAL | C-N-CA | 5.33 | 133.49 | 122.30 |
| 2 | D | 655 | VAL | CA-CB-CG2 | 5.32 | 118.88 | 110.90 |
| 1 | B | 120 | ILE | CB-CA-C | 5.31 | 122.21 | 111.60 |
| 1 | C | 210 | ALA | N-CA-CB | 5.30 | 117.52 | 110.10 |
| 2 | E | 615 | THR | CA-C-O | -5.29 | 108.99 | 120.10 |
| 2 | F | 532 | TYR | CA-C-O | -5.29 | 109.00 | 120.10 |
| 2 | D | 615 | THR | CA-C-O | -5.29 | 109.00 | 120.10 |
| 2 | D | 655 | VAL | CA-C-O | 5.29 | 131.20 | 120.10 |
| 2 | D | 582 | PHE | O-C-N | 5.26 | 131.12 | 122.70 |
| 2 | D | 663 | ARG | CD-NE-CZ | 5.26 | 130.97 | 123.60 |
| 1 | A | 168 | TYR | CB-CG-CD1 | -5.26 | 117.84 | 121.00 |
| 2 | F | 644 | LYS | C-N-CA | 5.26 | 134.84 | 121.70 |
| 1 | B | 208 | ASP | CB-CA-C | 5.25 | 120.90 | 110.40 |
| 1 | C | 114 | LEU | CA-CB-CG | 5.24 | 127.34 | 115.30 |
| 2 | D | 665 | LEU | CA-C-O | -5.23 | 109.12 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 208 | ASP | OD1-CG-OD2 | -5.23 | 113.37 | 123.30 |
| 2 | F | 538 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | B | 118 | ALA | CA-C-O | -5.22 | 109.14 | 120.10 |
| 1 | C | 85 | ARG | NH1-CZ-NH2 | -5.22 | 113.66 | 119.40 |
| 1 | A | 45 | PHE | CB-CA-C | 5.22 | 120.84 | 110.40 |
| 2 | D | 621 | ASP | CB-CA-C | 5.21 | 120.83 | 110.40 |
| 1 | C | 118 | ALA | CA-C-O | -5.21 | 109.15 | 120.10 |
| 2 | E | 563 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 2 | E | 655 | VAL | CA-C-O | 5.21 | 131.03 | 120.10 |
| 2 | F | 559 | ALA | CB-CA-C | 5.21 | 117.91 | 110.10 |
| 1 | A | 84 | PHE | N-CA-CB | -5.20 | 101.23 | 110.60 |
| 1 | B | 197 | VAL | CA-CB-CG2 | 5.20 | 118.70 | 110.90 |
| 1 | A | 179 | VAL | C-N-CA | 5.19 | 134.69 | 121.70 |
| 2 | F | 562 | GLU | CG-CD-OE2 | -5.18 | 107.94 | 118.30 |
| 2 | F | 615 | THR | CA-C-O | -5.18 | 109.22 | 120.10 |
| 1 | A | 201 | PRO | C-N-CA | 5.17 | 134.64 | 121.70 |
| 2 | E | 564 | TYR | CB-CG-CD2 | 5.17 | 124.10 | 121.00 |
| 1 | B | 98 | GLN | CA-CB-CG | 5.17 | 124.78 | 113.40 |
| 2 | E | 582 | PHE | O-C-N | 5.17 | 130.97 | 122.70 |
| 2 | E | 656 | GLU | CG-CD-OE2 | -5.17 | 107.96 | 118.30 |
| 2 | D | 623 | PRO | C-N-CA | 5.16 | 134.60 | 121.70 |
| 2 | D | 670 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 1 | B | 190 | MET | CA-CB-CG | 5.16 | 122.07 | 113.30 |
| 1 | C | 192 | ASN | CB-CA-C | 5.14 | 120.69 | 110.40 |
| 2 | F | 654 | TYR | CB-CG-CD2 | -5.13 | 117.92 | 121.00 |
| 1 | C | 109 | ASP | N-CA-CB | -5.12 | 101.38 | 110.60 |
| 2 | E | 663 | ARG | CD-NE-CZ | 5.11 | 130.76 | 123.60 |
| 2 | F | 623 | PRO | C-N-CA | 5.11 | 134.48 | 121.70 |
| 1 | A | 230 | GLN | O-C-N | 5.11 | 131.88 | 123.20 |
| 2 | E | 623 | PRO | C-N-CA | 5.09 | 134.44 | 121.70 |
| 2 | D | 514 | VAL | C-N-CA | 5.09 | 133.00 | 122.30 |
| 2 | E | 621 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 1 | A | 219 | ILE | CB-CA-C | 5.09 | 121.78 | 111.60 |
| 1 | B | 210 | ALA | N-CA-CB | 5.09 | 117.22 | 110.10 |
| 2 | D | 671 | GLU | CG-CD-OE2 | -5.08 | 108.13 | 118.30 |
| 1 | A | 118 | ALA | CA-C-O | -5.08 | 109.44 | 120.10 |
| 1 | A | 204 | LEU | CB-CG-CD1 | -5.07 | 102.38 | 111.00 |
| 2 | E | 654 | TYR | O-C-N | 5.07 | 130.81 | 122.70 |
| 1 | C | 136 | ASP | CB-CG-OD2 | -5.06 | 113.74 | 118.30 |
| 1 | C | 126 | ARG | N-CA-CB | 5.06 | 119.71 | 110.60 |
| 1 | A | 171 | LEU | CB-CG-CD1 | 5.06 | 119.60 | 111.00 |
| 1 | C | 216 | ILE | C-N-CA | 5.05 | 134.34 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | C | 49 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 1 | C | 179 | VAL | C-N-CA | 5.05 | 134.32 | 121.70 |
| 1 | A | 126 | ARG | CB-CG-CD | 5.05 | 124.72 | 111.60 |
| 1 | B | 127 | GLU | CG-CD-OE1 | 5.04 | 128.38 | 118.30 |
| 1 | C | 102 | MET | CA-CB-CG | 5.04 | 121.87 | 113.30 |
| 1 | C | 78 | LEU | O-C-N | 5.04 | 130.76 | 122.70 |
| 1 | C | 208 | ASP | CB-CA-C | 5.04 | 120.47 | 110.40 |
| 1 | C | 138 | TYR | CB-CG-CD1 | 5.03 | 124.02 | 121.00 |
| 2 | F | 552 | THR | N-CA-CB | 5.02 | 119.84 | 110.30 |
| 1 | C | 197 | VAL | CA-CB-CG2 | 5.01 | 118.42 | 110.90 |
| 1 | A | 126 | ARG | NE-CZ-NH2 | 5.01 | 122.80 | 120.30 |
| 1 | A | 39 | PRO | N-CA-C | 5.00 | 125.11 | 112.10 |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 118 | ALA | Mainchain |
| 1 | A | 156 | THR | Mainchain |
| 1 | A | 193 | THR | Mainchain |
| 1 | A | 216 | ILE | Mainchain |
| 1 | B | 118 | ALA | Mainchain |
| 1 | B | 156 | THR | Mainchain |
| 1 | B | 193 | THR | Mainchain |
| 1 | B | 216 | ILE | Mainchain |
| 1 | C | 118 | ALA | Mainchain |
| 1 | C | 156 | THR | Mainchain |
| 1 | C | 193 | THR | Mainchain |
| 1 | C | 216 | ILE | Mainchain |
| 2 | D | 532 | TYR | Mainchain |
| 2 | D | 533 | VAL | Mainchain |
| 2 | D | 545 | MET | Mainchain |
| 2 | D | 593 | VAL | Mainchain |
| 2 | D | 666 | LYS | Mainchain |
| 2 | E | 545 | MET | Mainchain |
| 2 | E | 666 | LYS | Mainchain |
| 2 | F | 593 | VAL | Mainchain |
| 2 | F | 666 | LYS | Mainchain |

5.2 Too-close contacts [\(i\)](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1593 | 0 | 1595 | 152 | 0 |
| 1 | B | 1593 | 0 | 1595 | 160 | 0 |
| 1 | C | 1593 | 0 | 1595 | 154 | 0 |
| 2 | D | 1337 | 0 | 1328 | 155 | 0 |
| 2 | E | 1337 | 0 | 1329 | 156 | 0 |
| 2 | F | 1337 | 0 | 1329 | 153 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 32 | 0 | 13 | 9 | 0 |
| 4 | E | 32 | 0 | 13 | 7 | 0 |
| 4 | F | 32 | 0 | 13 | 7 | 0 |
| 5 | A | 63 | 0 | 0 | 7 | 0 |
| 5 | B | 62 | 0 | 0 | 14 | 0 |
| 5 | C | 62 | 0 | 0 | 10 | 0 |
| 5 | D | 36 | 0 | 0 | 9 | 0 |
| 5 | E | 39 | 0 | 0 | 8 | 0 |
| 5 | F | 40 | 0 | 0 | 10 | 0 |
| All | All | 9191 | 0 | 8810 | 857 | 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 48.

All (857) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------|--------------------------|-------------------|
| 1:A:40:LEU:HB3 | 1:A:41:PRO:HD2 | 1.47 | 0.97 |
| 1:C:211:ILE:HG13 | 1:C:212:THR:H | 1.28 | 0.97 |
| 1:A:211:ILE:HG13 | 1:A:212:THR:H | 1.30 | 0.96 |
| 1:B:211:ILE:HG13 | 1:B:212:THR:H | 1.27 | 0.96 |
| 1:B:40:LEU:HB3 | 1:B:41:PRO:HD2 | 1.48 | 0.94 |
| 1:C:40:LEU:HB3 | 1:C:41:PRO:HD2 | 1.47 | 0.93 |
| 2:E:535:THR:HG22 | 2:E:536:VAL:O | 1.69 | 0.92 |
| 2:D:535:THR:HG22 | 2:D:536:VAL:O | 1.69 | 0.91 |
| 2:F:535:THR:HG22 | 2:F:536:VAL:O | 1.72 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:655:VAL:HG23 | 2:D:668:VAL:HG22 | 1.52 | 0.88 |
| 2:F:655:VAL:HG23 | 2:F:668:VAL:HG22 | 1.55 | 0.88 |
| 1:C:84:PHE:HB3 | 1:C:198:VAL:HG11 | 1.53 | 0.88 |
| 2:D:532:TYR:N | 4:D:678:GNP:H3' | 1.89 | 0.88 |
| 1:C:216:ILE:HG22 | 1:C:217:ASN:H | 1.38 | 0.87 |
| 1:C:212:THR:HG22 | 1:C:213:LEU:HG | 1.57 | 0.87 |
| 1:B:84:PHE:HB3 | 1:B:198:VAL:HG11 | 1.56 | 0.86 |
| 1:B:216:ILE:HG22 | 1:B:217:ASN:H | 1.41 | 0.86 |
| 1:C:212:THR:HB | 1:C:214:LYS:H | 1.40 | 0.86 |
| 1:A:84:PHE:HB3 | 1:A:198:VAL:HG11 | 1.57 | 0.86 |
| 1:A:212:THR:HG22 | 1:A:213:LEU:HG | 1.58 | 0.86 |
| 1:A:212:THR:HB | 1:A:214:LYS:H | 1.41 | 0.85 |
| 2:E:655:VAL:HG23 | 2:E:668:VAL:HG22 | 1.57 | 0.85 |
| 2:D:508:VAL:HG22 | 2:D:579:LEU:HD12 | 1.59 | 0.85 |
| 1:A:216:ILE:HG22 | 1:A:217:ASN:H | 1.42 | 0.84 |
| 1:B:212:THR:HB | 1:B:214:LYS:H | 1.41 | 0.84 |
| 2:E:508:VAL:HG22 | 2:E:579:LEU:HD12 | 1.58 | 0.83 |
| 2:F:508:VAL:HG22 | 2:F:579:LEU:HD12 | 1.59 | 0.83 |
| 2:E:532:TYR:N | 4:E:678:GNP:H3' | 1.94 | 0.83 |
| 2:E:576:ASP:O | 2:E:577:VAL:HB | 1.76 | 0.82 |
| 1:B:212:THR:HG22 | 1:B:213:LEU:HG | 1.60 | 0.82 |
| 2:E:620:ARG:O | 2:E:626:ILE:HD11 | 1.79 | 0.82 |
| 1:B:126:ARG:HA | 5:B:277:HOH:O | 1.80 | 0.81 |
| 2:F:576:ASP:O | 2:F:577:VAL:HB | 1.79 | 0.81 |
| 1:A:210:ALA:O | 1:A:214:LYS:HD2 | 1.81 | 0.81 |
| 2:D:576:ASP:O | 2:D:577:VAL:HB | 1.79 | 0.81 |
| 2:F:620:ARG:O | 2:F:626:ILE:HD11 | 1.81 | 0.81 |
| 2:D:620:ARG:O | 2:D:626:ILE:HD11 | 1.82 | 0.79 |
| 1:B:210:ALA:O | 1:B:214:LYS:HD2 | 1.82 | 0.79 |
| 2:F:532:TYR:N | 4:F:678:GNP:H3' | 1.98 | 0.79 |
| 2:F:532:TYR:O | 2:F:533:VAL:HG13 | 1.83 | 0.77 |
| 1:C:81:GLU:HA | 1:C:188:ASN:HA | 1.66 | 0.77 |
| 1:A:147:ILE:O | 1:A:152:ARG:NH1 | 2.18 | 0.76 |
| 2:D:532:TYR:O | 2:D:533:VAL:HG13 | 1.84 | 0.76 |
| 1:A:199:PHE:HB3 | 5:A:281:HOH:O | 1.85 | 0.76 |
| 1:A:81:GLU:HA | 1:A:188:ASN:HA | 1.66 | 0.76 |
| 1:A:37:ARG:N | 1:A:38:PRO:HD3 | 1.99 | 0.76 |
| 1:B:37:ARG:N | 1:B:38:PRO:HD3 | 2.00 | 0.76 |
| 1:B:147:ILE:O | 1:B:152:ARG:NH1 | 2.18 | 0.75 |
| 1:B:197:VAL:HG21 | 2:E:534:PRO:HG2 | 1.68 | 0.75 |
| 1:A:212:THR:HG22 | 1:A:213:LEU:H | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:147:ILE:O | 1:C:152:ARG:NH1 | 2.19 | 0.75 |
| 1:A:132:LEU:HD12 | 1:A:167:ASN:HD22 | 1.50 | 0.75 |
| 1:B:181:ILE:HG23 | 1:B:188:ASN:HD21 | 1.50 | 0.75 |
| 1:A:217:ASN:HB3 | 1:A:218:PRO:HD3 | 1.68 | 0.75 |
| 1:A:181:ILE:HG23 | 1:A:188:ASN:HD21 | 1.51 | 0.75 |
| 2:E:617:ILE:O | 2:E:620:ARG:HB2 | 1.87 | 0.75 |
| 1:B:81:GLU:HA | 1:B:188:ASN:HA | 1.68 | 0.75 |
| 1:B:37:ARG:HD3 | 1:B:101:ASN:HD21 | 1.52 | 0.74 |
| 1:A:217:ASN:CB | 2:D:536:VAL:HG11 | 2.18 | 0.74 |
| 2:F:668:VAL:HG23 | 5:F:213:HOH:O | 1.88 | 0.74 |
| 1:C:210:ALA:O | 1:C:214:LYS:HD2 | 1.86 | 0.74 |
| 2:E:532:TYR:C | 2:E:533:VAL:HG22 | 2.09 | 0.74 |
| 1:C:217:ASN:HB3 | 1:C:218:PRO:HD3 | 1.70 | 0.73 |
| 1:B:217:ASN:HB3 | 1:B:218:PRO:HD3 | 1.71 | 0.73 |
| 1:C:217:ASN:CB | 2:F:536:VAL:HG11 | 2.18 | 0.73 |
| 1:B:202:ASN:HA | 5:B:277:HOH:O | 1.88 | 0.72 |
| 1:A:51:HIS:HA | 1:A:54:GLU:HG2 | 1.71 | 0.72 |
| 2:D:617:ILE:O | 2:D:620:ARG:HB2 | 1.88 | 0.72 |
| 1:B:217:ASN:HB2 | 2:E:536:VAL:HG11 | 1.72 | 0.72 |
| 1:A:198:VAL:HG22 | 2:D:561:GLN:OE1 | 1.89 | 0.72 |
| 1:B:217:ASN:CB | 2:E:536:VAL:HG11 | 2.19 | 0.72 |
| 2:F:617:ILE:O | 2:F:620:ARG:HB2 | 1.90 | 0.72 |
| 4:D:678:GNP:O3G | 5:D:1:HOH:O | 2.08 | 0.72 |
| 1:C:197:VAL:HG21 | 2:F:534:PRO:HG2 | 1.71 | 0.72 |
| 1:C:191:THR:HB | 2:F:532:TYR:OH | 1.90 | 0.71 |
| 1:A:37:ARG:HD3 | 1:A:101:ASN:HD21 | 1.55 | 0.71 |
| 1:C:198:VAL:HG22 | 2:F:561:GLN:OE1 | 1.90 | 0.71 |
| 1:C:212:THR:HG22 | 1:C:213:LEU:H | 1.55 | 0.71 |
| 2:F:539:ASN:N | 2:F:539:ASN:HD22 | 1.88 | 0.71 |
| 1:A:217:ASN:HB2 | 2:D:536:VAL:HG11 | 1.71 | 0.71 |
| 1:B:213:LEU:HD22 | 5:E:24:HOH:O | 1.91 | 0.71 |
| 1:B:132:LEU:HD12 | 1:B:167:ASN:HD22 | 1.55 | 0.71 |
| 1:B:198:VAL:HG22 | 2:E:561:GLN:OE1 | 1.91 | 0.70 |
| 1:C:141:VAL:HG22 | 1:C:222:PHE:CD1 | 2.26 | 0.70 |
| 1:B:212:THR:HG22 | 1:B:213:LEU:H | 1.56 | 0.70 |
| 1:C:37:ARG:N | 1:C:38:PRO:HD3 | 2.03 | 0.70 |
| 1:C:217:ASN:HB2 | 2:F:536:VAL:HG11 | 1.72 | 0.70 |
| 2:F:569:PRO:HB3 | 2:F:604:HIS:NE2 | 2.05 | 0.70 |
| 1:B:40:LEU:HD23 | 1:B:101:ASN:HB3 | 1.73 | 0.70 |
| 1:A:191:THR:HB | 2:D:532:TYR:OH | 1.92 | 0.70 |
| 1:A:197:VAL:HG21 | 2:D:534:PRO:HG2 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:51:HIS:HA | 1:B:54:GLU:HG2 | 1.71 | 0.70 |
| 2:E:569:PRO:HB3 | 2:E:604:HIS:NE2 | 2.05 | 0.70 |
| 1:C:60:GLU:HB3 | 5:C:245:HOH:O | 1.91 | 0.70 |
| 2:E:539:ASN:N | 2:E:539:ASN:HD22 | 1.90 | 0.70 |
| 1:B:94:ARG:HG3 | 5:B:264:HOH:O | 1.92 | 0.70 |
| 1:B:211:ILE:HG13 | 1:B:212:THR:N | 2.06 | 0.70 |
| 2:D:501:PRO:HG3 | 2:D:550:PRO:HB2 | 1.74 | 0.69 |
| 2:D:569:PRO:HB3 | 2:D:604:HIS:NE2 | 2.07 | 0.69 |
| 1:C:181:ILE:HG23 | 1:C:188:ASN:HD21 | 1.56 | 0.69 |
| 1:C:51:HIS:HA | 1:C:54:GLU:HG2 | 1.73 | 0.69 |
| 1:A:44:GLN:HB2 | 1:A:100:TYR:HB3 | 1.74 | 0.69 |
| 1:B:141:VAL:HG22 | 1:B:222:PHE:CD1 | 2.27 | 0.69 |
| 1:C:37:ARG:HD3 | 1:C:101:ASN:HD21 | 1.58 | 0.69 |
| 1:C:44:GLN:HB2 | 1:C:100:TYR:HB3 | 1.74 | 0.69 |
| 1:C:132:LEU:HD12 | 1:C:167:ASN:HD22 | 1.58 | 0.69 |
| 2:F:501:PRO:HG3 | 2:F:550:PRO:HB2 | 1.74 | 0.69 |
| 1:A:108:PHE:HD1 | 1:A:116:LEU:HD23 | 1.58 | 0.68 |
| 1:A:141:VAL:HG22 | 1:A:222:PHE:CD2 | 2.28 | 0.68 |
| 2:D:539:ASN:N | 2:D:539:ASN:HD22 | 1.89 | 0.68 |
| 2:E:617:ILE:HD11 | 2:E:656:GLU:HB3 | 1.75 | 0.68 |
| 1:C:199:PHE:HB3 | 5:C:288:HOH:O | 1.93 | 0.68 |
| 2:F:617:ILE:HD11 | 2:F:656:GLU:HB3 | 1.76 | 0.68 |
| 1:B:37:ARG:NH1 | 1:B:97:GLN:HB3 | 2.09 | 0.68 |
| 1:C:40:LEU:HD23 | 1:C:101:ASN:HB3 | 1.76 | 0.68 |
| 2:F:667:ASN:ND2 | 5:F:213:HOH:O | 2.27 | 0.68 |
| 4:F:678:GNP:O3G | 5:F:3:HOH:O | 2.10 | 0.68 |
| 1:C:125:LEU:HD11 | 1:C:174:LEU:HD22 | 1.75 | 0.68 |
| 2:E:646:ALA:O | 2:E:649:LEU:N | 2.26 | 0.68 |
| 2:F:646:ALA:O | 2:F:649:LEU:N | 2.27 | 0.68 |
| 2:E:501:PRO:HG3 | 2:E:550:PRO:HB2 | 1.76 | 0.67 |
| 1:C:37:ARG:NH1 | 1:C:97:GLN:HB3 | 2.09 | 0.67 |
| 1:A:200:GLY:N | 1:A:201:PRO:HD2 | 2.10 | 0.67 |
| 1:C:200:GLY:N | 1:C:201:PRO:HD2 | 2.09 | 0.67 |
| 1:B:44:GLN:HB2 | 1:B:100:TYR:HB3 | 1.76 | 0.67 |
| 1:B:138:TYR:HA | 5:B:267:HOH:O | 1.94 | 0.67 |
| 1:B:108:PHE:HD1 | 1:B:116:LEU:HD23 | 1.58 | 0.67 |
| 1:A:40:LEU:HD23 | 1:A:101:ASN:HB3 | 1.75 | 0.66 |
| 1:B:48:SER:OG | 1:B:51:HIS:HB2 | 1.94 | 0.66 |
| 1:C:108:PHE:HD1 | 1:C:116:LEU:HD23 | 1.60 | 0.66 |
| 1:B:125:LEU:HD11 | 1:B:174:LEU:HD22 | 1.77 | 0.66 |
| 2:E:667:ASN:ND2 | 5:E:297:HOH:O | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:37:ARG:HD3 | 1:B:101:ASN:ND2 | 2.11 | 0.66 |
| 1:B:215:ALA:C | 1:B:216:ILE:HD12 | 2.16 | 0.66 |
| 2:D:633:LYS:HG2 | 2:D:634:GLN:HE21 | 1.61 | 0.66 |
| 1:B:188:ASN:O | 1:B:189:LYS:HB2 | 1.96 | 0.65 |
| 1:A:215:ALA:C | 1:A:216:ILE:HD12 | 2.17 | 0.65 |
| 2:D:617:ILE:HD11 | 2:D:656:GLU:HB3 | 1.78 | 0.65 |
| 1:C:215:ALA:C | 1:C:216:ILE:HD12 | 2.16 | 0.65 |
| 1:A:40:LEU:HD23 | 1:A:101:ASN:CB | 2.27 | 0.65 |
| 1:C:211:ILE:HG13 | 1:C:212:THR:N | 2.08 | 0.65 |
| 2:F:606:PRO:O | 2:F:607:LYS:HB2 | 1.96 | 0.65 |
| 1:A:37:ARG:HD3 | 1:A:101:ASN:ND2 | 2.11 | 0.65 |
| 1:B:212:THR:HG21 | 1:B:214:LYS:HE3 | 1.79 | 0.65 |
| 2:E:633:LYS:HG2 | 2:E:634:GLN:HE21 | 1.62 | 0.65 |
| 2:E:606:PRO:O | 2:E:607:LYS:HB2 | 1.95 | 0.65 |
| 1:C:48:SER:OG | 1:C:51:HIS:HB2 | 1.97 | 0.65 |
| 1:C:212:THR:HG21 | 1:C:214:LYS:HE3 | 1.79 | 0.65 |
| 2:D:633:LYS:HG2 | 2:D:634:GLN:NE2 | 2.12 | 0.64 |
| 1:B:169:GLN:HE21 | 1:B:169:GLN:HA | 1.61 | 0.64 |
| 1:B:191:THR:HB | 2:E:532:TYR:OH | 1.97 | 0.64 |
| 1:C:188:ASN:O | 1:C:189:LYS:HB2 | 1.96 | 0.64 |
| 2:F:633:LYS:HG2 | 2:F:634:GLN:HE21 | 1.63 | 0.64 |
| 1:A:188:ASN:O | 1:A:189:LYS:HB2 | 1.97 | 0.64 |
| 2:F:542:VAL:HA | 5:F:90:HOH:O | 1.98 | 0.64 |
| 2:D:646:ALA:O | 2:D:649:LEU:N | 2.30 | 0.64 |
| 1:A:37:ARG:NH1 | 1:A:97:GLN:HB3 | 2.13 | 0.64 |
| 1:A:217:ASN:CG | 2:D:536:VAL:HG11 | 2.18 | 0.64 |
| 1:C:37:ARG:HD3 | 1:C:101:ASN:ND2 | 2.11 | 0.64 |
| 1:C:40:LEU:HD23 | 1:C:101:ASN:CB | 2.28 | 0.63 |
| 2:D:612:LEU:HD23 | 2:D:654:TYR:HB2 | 1.80 | 0.63 |
| 1:B:40:LEU:HD23 | 1:B:101:ASN:CB | 2.28 | 0.63 |
| 1:B:78:LEU:HG | 5:B:263:HOH:O | 1.97 | 0.63 |
| 1:B:130:GLU:HG3 | 1:B:131:PRO:HD2 | 1.81 | 0.63 |
| 2:E:532:TYR:O | 2:E:533:VAL:HG13 | 1.99 | 0.63 |
| 1:C:217:ASN:CG | 2:F:536:VAL:HG11 | 2.17 | 0.63 |
| 1:A:169:GLN:HE21 | 1:A:169:GLN:HA | 1.63 | 0.63 |
| 2:D:674:LEU:HD12 | 2:D:674:LEU:O | 1.99 | 0.63 |
| 2:E:661:THR:HG21 | 2:E:663:ARG:HB3 | 1.80 | 0.63 |
| 1:B:47:VAL:HG13 | 1:B:52:LEU:HD21 | 1.81 | 0.63 |
| 2:E:674:LEU:HD12 | 2:E:674:LEU:O | 1.99 | 0.63 |
| 2:E:532:TYR:O | 2:E:533:VAL:HG22 | 1.98 | 0.62 |
| 1:A:211:ILE:HG13 | 1:A:212:THR:N | 2.09 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:661:THR:CG2 | 2:E:663:ARG:HB3 | 2.29 | 0.62 |
| 1:B:126:ARG:HG2 | 5:B:277:HOH:O | 1.98 | 0.62 |
| 2:E:633:LYS:HG2 | 2:E:634:GLN:NE2 | 2.14 | 0.62 |
| 1:B:200:GLY:N | 1:B:201:PRO:HD2 | 2.14 | 0.62 |
| 1:C:47:VAL:HG13 | 1:C:52:LEU:HD21 | 1.82 | 0.62 |
| 2:D:515:GLY:HA2 | 4:D:678:GNP:H8 | 1.82 | 0.62 |
| 1:B:216:ILE:HD13 | 2:E:537:PHE:CD1 | 2.35 | 0.62 |
| 2:E:668:VAL:HG23 | 5:E:297:HOH:O | 1.99 | 0.62 |
| 2:F:503:THR:O | 2:F:504:ILE:HG13 | 1.98 | 0.62 |
| 1:C:180:GLN:HG3 | 5:C:270:HOH:O | 2.00 | 0.62 |
| 1:A:47:VAL:HG13 | 1:A:52:LEU:HD21 | 1.81 | 0.62 |
| 2:D:503:THR:O | 2:D:504:ILE:HG13 | 1.98 | 0.62 |
| 2:E:668:VAL:HG12 | 2:E:669:PHE:CD2 | 2.35 | 0.62 |
| 1:C:179:VAL:HG21 | 1:C:230:GLN:HG3 | 1.81 | 0.62 |
| 1:A:125:LEU:HD11 | 1:A:174:LEU:HD22 | 1.82 | 0.62 |
| 2:E:518:CYS:HB3 | 2:E:528:PHE:CE2 | 2.35 | 0.62 |
| 1:C:169:GLN:HE21 | 1:C:169:GLN:HA | 1.63 | 0.62 |
| 2:F:653:LYS:HD2 | 2:F:655:VAL:HG12 | 1.82 | 0.62 |
| 2:F:668:VAL:HG12 | 2:F:669:PHE:CD2 | 2.35 | 0.62 |
| 2:D:668:VAL:HG12 | 2:D:669:PHE:CD2 | 2.34 | 0.61 |
| 1:C:130:GLU:HG3 | 1:C:131:PRO:HD2 | 1.82 | 0.61 |
| 1:C:153:VAL:N | 1:C:154:PRO:HD2 | 2.14 | 0.61 |
| 1:C:216:ILE:HD13 | 2:F:537:PHE:CD1 | 2.35 | 0.61 |
| 1:A:153:VAL:N | 1:A:154:PRO:HD2 | 2.15 | 0.61 |
| 2:D:661:THR:CG2 | 2:D:663:ARG:HB3 | 2.30 | 0.61 |
| 1:B:217:ASN:CG | 2:E:536:VAL:HG11 | 2.20 | 0.61 |
| 2:F:515:GLY:HA2 | 4:F:678:GNP:H8 | 1.81 | 0.61 |
| 2:F:649:LEU:O | 2:F:650:LYS:HB2 | 2.00 | 0.61 |
| 2:D:606:PRO:O | 2:D:607:LYS:HB2 | 1.99 | 0.61 |
| 2:D:653:LYS:HD3 | 2:D:654:TYR:O | 2.01 | 0.61 |
| 2:D:661:THR:HG21 | 2:D:663:ARG:HB3 | 1.83 | 0.61 |
| 2:F:653:LYS:HD3 | 2:F:654:TYR:O | 2.01 | 0.61 |
| 2:F:661:THR:HG21 | 2:F:663:ARG:HB3 | 1.83 | 0.61 |
| 2:D:535:THR:HG22 | 2:D:536:VAL:C | 2.21 | 0.61 |
| 1:B:104:LEU:HD12 | 1:B:105:PRO:HD2 | 1.82 | 0.61 |
| 1:B:99:LYS:NZ | 1:B:111:TYR:OH | 2.29 | 0.61 |
| 2:F:633:LYS:HG2 | 2:F:634:GLN:NE2 | 2.15 | 0.61 |
| 1:B:211:ILE:CG1 | 1:B:212:THR:H | 2.09 | 0.60 |
| 1:C:140:HIS:NE2 | 1:C:156:THR:OG1 | 2.34 | 0.60 |
| 2:E:622:ASP:O | 2:E:625:THR:OG1 | 2.19 | 0.60 |
| 1:B:153:VAL:N | 1:B:154:PRO:HD2 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:553:LEU:HD22 | 2:E:673:ILE:HD11 | 1.83 | 0.60 |
| 2:F:674:LEU:HD12 | 2:F:674:LEU:O | 2.02 | 0.60 |
| 2:E:515:GLY:HA2 | 4:E:678:GNP:H8 | 1.82 | 0.60 |
| 1:C:192:ASN:OD1 | 1:C:227:LEU:HB3 | 2.02 | 0.60 |
| 1:A:179:VAL:HG21 | 1:A:230:GLN:HG3 | 1.83 | 0.60 |
| 2:F:508:VAL:CG2 | 2:F:579:LEU:HD12 | 2.31 | 0.60 |
| 1:C:184:HIS:O | 1:C:187:GLN:HG2 | 2.02 | 0.60 |
| 2:D:518:CYS:HB3 | 2:D:528:PHE:CE2 | 2.37 | 0.60 |
| 2:E:653:LYS:HD2 | 2:E:655:VAL:HG12 | 1.83 | 0.60 |
| 1:A:216:ILE:HD13 | 2:D:537:PHE:CD1 | 2.36 | 0.60 |
| 1:B:211:ILE:O | 1:B:215:ALA:N | 2.34 | 0.60 |
| 2:F:661:THR:CG2 | 2:F:663:ARG:HB3 | 2.31 | 0.60 |
| 1:A:52:LEU:O | 1:A:56:ASN:HB2 | 2.02 | 0.59 |
| 1:A:130:GLU:HG3 | 1:A:131:PRO:HD2 | 1.84 | 0.59 |
| 1:A:217:ASN:CB | 1:A:218:PRO:HD3 | 2.33 | 0.59 |
| 2:D:542:VAL:HA | 5:D:52:HOH:O | 2.02 | 0.59 |
| 1:A:83:ILE:HD13 | 1:A:181:ILE:HD12 | 1.83 | 0.59 |
| 2:E:653:LYS:HD3 | 2:E:654:TYR:O | 2.02 | 0.59 |
| 1:C:78:LEU:HG | 5:C:270:HOH:O | 2.00 | 0.59 |
| 1:C:104:LEU:HD12 | 1:C:105:PRO:HD2 | 1.84 | 0.59 |
| 1:A:215:ALA:O | 1:A:216:ILE:HD12 | 2.02 | 0.59 |
| 1:C:215:ALA:O | 1:C:216:ILE:HD12 | 2.02 | 0.59 |
| 1:A:104:LEU:HD12 | 1:A:105:PRO:HD2 | 1.85 | 0.59 |
| 2:D:508:VAL:CG2 | 2:D:579:LEU:HD12 | 2.32 | 0.59 |
| 1:B:184:HIS:O | 1:B:187:GLN:HG2 | 2.03 | 0.59 |
| 1:A:43:GLN:HA | 1:A:101:ASN:HA | 1.85 | 0.59 |
| 1:C:99:LYS:NZ | 1:C:111:TYR:OH | 2.29 | 0.59 |
| 1:B:52:LEU:O | 1:B:56:ASN:HB2 | 2.03 | 0.59 |
| 1:A:119:VAL:HG23 | 1:A:120:ILE:HD13 | 1.85 | 0.58 |
| 1:C:211:ILE:O | 1:C:215:ALA:N | 2.36 | 0.58 |
| 1:A:100:TYR:CE2 | 1:A:106:VAL:HG21 | 2.38 | 0.58 |
| 1:B:37:ARG:NH1 | 1:B:45:PHE:HB2 | 2.18 | 0.58 |
| 2:E:503:THR:O | 2:E:504:ILE:HG13 | 2.03 | 0.58 |
| 2:E:535:THR:HG22 | 2:E:536:VAL:C | 2.22 | 0.58 |
| 2:E:649:LEU:O | 2:E:650:LYS:HB2 | 2.04 | 0.58 |
| 1:A:211:ILE:O | 1:A:215:ALA:N | 2.35 | 0.58 |
| 1:B:197:VAL:O | 2:E:564:TYR:HE2 | 1.86 | 0.58 |
| 2:F:547:GLY:N | 5:F:41:HOH:O | 2.33 | 0.58 |
| 1:A:181:ILE:HG23 | 1:A:188:ASN:ND2 | 2.18 | 0.58 |
| 1:A:216:ILE:HG22 | 2:D:536:VAL:HG13 | 1.84 | 0.58 |
| 2:F:518:CYS:HB3 | 2:F:528:PHE:CE2 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:48:SER:OG | 1:A:51:HIS:HB2 | 2.03 | 0.58 |
| 2:E:568:ARG:O | 2:E:571:SER:HB2 | 2.04 | 0.58 |
| 1:A:192:ASN:OD1 | 1:A:227:LEU:HB3 | 2.03 | 0.58 |
| 1:C:52:LEU:O | 1:C:56:ASN:HB2 | 2.03 | 0.58 |
| 1:C:132:LEU:HA | 1:C:167:ASN:ND2 | 2.19 | 0.58 |
| 1:B:179:VAL:HG21 | 1:B:230:GLN:HG3 | 1.84 | 0.58 |
| 1:C:197:VAL:O | 2:F:564:TYR:HE2 | 1.86 | 0.58 |
| 2:F:535:THR:HG22 | 2:F:536:VAL:C | 2.22 | 0.58 |
| 2:F:587:PRO:HG2 | 2:F:634:GLN:OE1 | 2.04 | 0.58 |
| 1:A:37:ARG:NH1 | 1:A:45:PHE:HB2 | 2.19 | 0.58 |
| 1:A:184:HIS:O | 1:A:187:GLN:HG2 | 2.03 | 0.58 |
| 1:B:215:ALA:O | 1:B:216:ILE:HD12 | 2.04 | 0.58 |
| 2:E:590:PHE:O | 2:E:593:VAL:HB | 2.04 | 0.58 |
| 1:B:43:GLN:HA | 1:B:101:ASN:HA | 1.85 | 0.57 |
| 1:B:192:ASN:OD1 | 1:B:227:LEU:HB3 | 2.04 | 0.57 |
| 2:F:612:LEU:HD23 | 2:F:654:TYR:HB2 | 1.85 | 0.57 |
| 2:F:655:VAL:CG2 | 2:F:668:VAL:HG22 | 2.32 | 0.57 |
| 1:C:213:LEU:HD22 | 5:F:47:HOH:O | 2.04 | 0.57 |
| 1:C:217:ASN:CB | 1:C:218:PRO:HD3 | 2.33 | 0.57 |
| 2:F:590:PHE:O | 2:F:593:VAL:HB | 2.04 | 0.57 |
| 1:A:197:VAL:O | 2:D:564:TYR:HE2 | 1.87 | 0.57 |
| 2:D:659:ALA:HB2 | 5:D:274:HOH:O | 2.04 | 0.57 |
| 1:A:60:GLU:HB3 | 5:A:245:HOH:O | 2.03 | 0.57 |
| 1:A:132:LEU:HA | 1:A:167:ASN:ND2 | 2.19 | 0.57 |
| 2:D:568:ARG:O | 2:D:571:SER:HB2 | 2.05 | 0.57 |
| 1:B:132:LEU:HA | 1:B:167:ASN:ND2 | 2.20 | 0.57 |
| 1:B:181:ILE:HG23 | 1:B:188:ASN:ND2 | 2.19 | 0.57 |
| 1:B:217:ASN:CB | 1:B:218:PRO:HD3 | 2.33 | 0.57 |
| 1:C:43:GLN:HA | 1:C:101:ASN:HA | 1.87 | 0.57 |
| 2:F:622:ASP:O | 2:F:625:THR:OG1 | 2.21 | 0.57 |
| 2:D:590:PHE:O | 2:D:593:VAL:HB | 2.05 | 0.57 |
| 1:B:81:GLU:CA | 1:B:188:ASN:HA | 2.35 | 0.57 |
| 1:B:96:VAL:HG13 | 1:B:106:VAL:HG11 | 1.87 | 0.57 |
| 2:D:653:LYS:HD2 | 2:D:655:VAL:HG12 | 1.86 | 0.56 |
| 1:A:40:LEU:HB3 | 1:A:41:PRO:CD | 2.30 | 0.56 |
| 1:B:96:VAL:HG13 | 1:B:106:VAL:CG1 | 2.35 | 0.56 |
| 1:A:102:MET:SD | 2:E:674:LEU:HD13 | 2.44 | 0.56 |
| 1:A:106:VAL:HB | 5:A:253:HOH:O | 2.04 | 0.56 |
| 2:D:509:VAL:HG12 | 2:D:558:THR:HG21 | 1.85 | 0.56 |
| 1:B:100:TYR:CE2 | 1:B:106:VAL:HG21 | 2.39 | 0.56 |
| 2:E:522:SER:HB3 | 2:E:665:LEU:HD21 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:590:PHE:CZ | 2:E:645:LEU:HG | 2.41 | 0.56 |
| 1:C:81:GLU:CA | 1:C:188:ASN:HA | 2.34 | 0.56 |
| 2:F:597:TRP:HA | 2:F:597:TRP:CE3 | 2.41 | 0.56 |
| 1:A:96:VAL:HG13 | 1:A:106:VAL:HG11 | 1.87 | 0.56 |
| 2:D:590:PHE:CZ | 2:D:645:LEU:HG | 2.40 | 0.56 |
| 1:A:157:LEU:HD21 | 1:A:232:GLU:O | 2.05 | 0.56 |
| 1:C:157:LEU:HD21 | 1:C:232:GLU:O | 2.06 | 0.56 |
| 1:C:215:ALA:HB1 | 2:F:567:LEU:HD22 | 1.87 | 0.56 |
| 2:F:522:SER:HB3 | 2:F:665:LEU:HD21 | 1.86 | 0.56 |
| 1:A:93:VAL:HG13 | 1:A:120:ILE:CD1 | 2.35 | 0.56 |
| 1:A:212:THR:HG21 | 1:A:214:LYS:HE3 | 1.86 | 0.56 |
| 2:F:610:PHE:O | 2:F:652:VAL:HG22 | 2.06 | 0.56 |
| 2:F:620:ARG:NH2 | 2:F:656:GLU:OE1 | 2.39 | 0.56 |
| 2:E:508:VAL:CG2 | 2:E:579:LEU:HD12 | 2.32 | 0.56 |
| 1:A:211:ILE:CG1 | 1:A:212:THR:H | 2.13 | 0.56 |
| 2:D:610:PHE:O | 2:D:652:VAL:HG22 | 2.06 | 0.56 |
| 2:D:649:LEU:O | 2:D:650:LYS:HB2 | 2.05 | 0.56 |
| 2:E:509:VAL:HG12 | 2:E:558:THR:HG21 | 1.88 | 0.56 |
| 2:E:512:GLY:O | 2:E:513:ALA:HB3 | 2.06 | 0.56 |
| 1:A:99:LYS:NZ | 1:A:111:TYR:OH | 2.30 | 0.55 |
| 2:D:655:VAL:CG2 | 2:D:668:VAL:HG22 | 2.29 | 0.55 |
| 1:C:37:ARG:NH1 | 1:C:45:PHE:HB2 | 2.21 | 0.55 |
| 2:F:590:PHE:CZ | 2:F:645:LEU:HG | 2.41 | 0.55 |
| 1:A:44:GLN:CB | 1:A:100:TYR:HB3 | 2.36 | 0.55 |
| 1:A:216:ILE:CG2 | 2:D:536:VAL:HG13 | 2.36 | 0.55 |
| 1:C:83:ILE:O | 1:C:85:ARG:N | 2.39 | 0.55 |
| 1:C:216:ILE:O | 1:C:218:PRO:HD2 | 2.06 | 0.55 |
| 1:C:217:ASN:ND2 | 2:F:536:VAL:HG11 | 2.21 | 0.55 |
| 2:D:522:SER:HB3 | 2:D:665:LEU:HD21 | 1.87 | 0.55 |
| 2:D:620:ARG:NH2 | 2:D:656:GLU:OE1 | 2.39 | 0.55 |
| 1:C:216:ILE:HG22 | 2:F:536:VAL:HG13 | 1.87 | 0.55 |
| 2:F:568:ARG:O | 2:F:571:SER:HB2 | 2.06 | 0.55 |
| 1:A:81:GLU:CA | 1:A:188:ASN:HA | 2.34 | 0.55 |
| 1:A:215:ALA:HB1 | 2:D:567:LEU:HD22 | 1.89 | 0.55 |
| 2:D:646:ALA:O | 2:D:647:ARG:C | 2.43 | 0.55 |
| 2:E:613:VAL:HA | 2:E:655:VAL:O | 2.07 | 0.55 |
| 2:F:646:ALA:O | 2:F:647:ARG:C | 2.44 | 0.55 |
| 1:A:178:LEU:HB3 | 1:A:195:LEU:HD13 | 1.88 | 0.55 |
| 2:D:587:PRO:HG2 | 2:D:634:GLN:OE1 | 2.06 | 0.55 |
| 1:B:216:ILE:HG22 | 2:E:536:VAL:HG13 | 1.87 | 0.55 |
| 1:B:216:ILE:CG2 | 2:E:536:VAL:HG13 | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:PRO:HG3 | 2:E:548:GLY:HA3 | 1.88 | 0.55 |
| 2:E:655:VAL:CG2 | 2:E:668:VAL:HG22 | 2.34 | 0.55 |
| 2:F:544:VAL:HG22 | 5:F:67:HOH:O | 2.06 | 0.55 |
| 1:B:93:VAL:HG13 | 1:B:120:ILE:CD1 | 2.36 | 0.55 |
| 1:B:178:LEU:HB3 | 1:B:195:LEU:HD13 | 1.87 | 0.55 |
| 2:E:597:TRP:HA | 2:E:597:TRP:CE3 | 2.42 | 0.55 |
| 1:C:119:VAL:HG23 | 1:C:120:ILE:HD13 | 1.89 | 0.55 |
| 1:C:144:PHE:CZ | 1:C:152:ARG:HD2 | 2.41 | 0.55 |
| 1:A:94:ARG:NH2 | 5:A:248:HOH:O | 2.40 | 0.54 |
| 1:A:83:ILE:O | 1:A:85:ARG:N | 2.40 | 0.54 |
| 2:E:573:PRO:HD3 | 5:E:257:HOH:O | 2.07 | 0.54 |
| 1:A:217:ASN:ND2 | 2:D:536:VAL:HG11 | 2.23 | 0.54 |
| 2:E:610:PHE:O | 2:E:652:VAL:HG22 | 2.06 | 0.54 |
| 2:E:645:LEU:HD13 | 2:E:649:LEU:HD12 | 1.90 | 0.54 |
| 2:D:595:GLU:O | 2:D:596:LYS:HB2 | 2.07 | 0.54 |
| 2:E:665:LEU:HD12 | 2:E:669:PHE:CE2 | 2.42 | 0.54 |
| 1:C:93:VAL:HG13 | 1:C:120:ILE:CD1 | 2.37 | 0.54 |
| 2:F:639:PRO:HA | 2:F:654:TYR:HE2 | 1.73 | 0.54 |
| 1:C:211:ILE:CG1 | 1:C:212:THR:H | 2.10 | 0.54 |
| 2:E:612:LEU:HD23 | 2:E:654:TYR:HB2 | 1.88 | 0.54 |
| 2:F:512:GLY:O | 2:F:513:ALA:HB3 | 2.07 | 0.54 |
| 2:F:509:VAL:HG12 | 2:F:558:THR:HG21 | 1.89 | 0.54 |
| 2:E:540:TYR:HB2 | 2:E:555:LEU:HB2 | 1.89 | 0.54 |
| 2:E:620:ARG:NH1 | 2:E:637:ILE:O | 2.41 | 0.54 |
| 2:E:653:LYS:HD2 | 2:E:655:VAL:CG1 | 2.37 | 0.54 |
| 2:F:613:VAL:HA | 2:F:655:VAL:O | 2.08 | 0.54 |
| 2:D:597:TRP:CE3 | 2:D:597:TRP:HA | 2.43 | 0.54 |
| 2:D:665:LEU:HD12 | 2:D:669:PHE:CE2 | 2.43 | 0.54 |
| 1:B:44:GLN:CB | 1:B:100:TYR:HB3 | 2.38 | 0.54 |
| 1:C:65:VAL:HG11 | 1:C:124:PHE:HB2 | 1.90 | 0.54 |
| 2:F:505:LYS:HB3 | 2:F:575:THR:HA | 1.89 | 0.54 |
| 1:A:189:LYS:HD3 | 2:D:532:TYR:CD1 | 2.43 | 0.53 |
| 2:D:582:PHE:HE1 | 2:D:584:VAL:HA | 1.73 | 0.53 |
| 1:B:216:ILE:O | 1:B:218:PRO:HD2 | 2.08 | 0.53 |
| 1:C:44:GLN:CB | 1:C:100:TYR:HB3 | 2.36 | 0.53 |
| 2:F:553:LEU:HD22 | 2:F:673:ILE:HD11 | 1.90 | 0.53 |
| 1:A:213:LEU:HD22 | 5:D:81:HOH:O | 2.08 | 0.53 |
| 2:D:620:ARG:NH1 | 2:D:637:ILE:O | 2.42 | 0.53 |
| 1:B:144:PHE:CZ | 1:B:152:ARG:HD2 | 2.44 | 0.53 |
| 2:E:649:LEU:C | 2:E:650:LYS:HD3 | 2.28 | 0.53 |
| 2:E:620:ARG:NH2 | 2:E:656:GLU:OE1 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:119:VAL:HG23 | 1:B:120:ILE:HD13 | 1.89 | 0.53 |
| 2:E:587:PRO:HG2 | 2:E:634:GLN:OE1 | 2.08 | 0.53 |
| 1:C:40:LEU:HB3 | 1:C:41:PRO:CD | 2.30 | 0.53 |
| 2:D:540:TYR:HB2 | 2:D:555:LEU:HB2 | 1.90 | 0.53 |
| 2:E:532:TYR:C | 2:E:533:VAL:CG2 | 2.77 | 0.53 |
| 1:A:70:VAL:O | 1:A:74:GLN:HG3 | 2.08 | 0.53 |
| 2:E:639:PRO:HA | 2:E:654:TYR:HE2 | 1.72 | 0.53 |
| 1:C:116:LEU:N | 1:C:117:PRO:CD | 2.72 | 0.53 |
| 2:D:582:PHE:CE1 | 2:D:584:VAL:HA | 2.44 | 0.53 |
| 2:D:645:LEU:HD13 | 2:D:649:LEU:HD12 | 1.91 | 0.53 |
| 1:B:215:ALA:HB1 | 2:E:567:LEU:HD22 | 1.91 | 0.53 |
| 1:B:83:ILE:O | 1:B:85:ARG:N | 2.42 | 0.53 |
| 2:F:568:ARG:NH2 | 5:F:279:HOH:O | 2.34 | 0.53 |
| 2:D:665:LEU:HD12 | 2:D:669:PHE:HE2 | 1.74 | 0.53 |
| 1:A:144:PHE:CZ | 1:A:152:ARG:HD2 | 2.43 | 0.53 |
| 1:C:96:VAL:HG13 | 1:C:106:VAL:CG1 | 2.39 | 0.53 |
| 1:C:125:LEU:CD1 | 1:C:174:LEU:HD22 | 2.39 | 0.53 |
| 1:C:178:LEU:HB3 | 1:C:195:LEU:HD13 | 1.91 | 0.53 |
| 2:F:572:TYR:N | 2:F:573:PRO:HD2 | 2.23 | 0.53 |
| 2:D:505:LYS:HB3 | 2:D:575:THR:HA | 1.91 | 0.52 |
| 1:A:96:VAL:HG13 | 1:A:106:VAL:CG1 | 2.38 | 0.52 |
| 2:D:572:TYR:N | 2:D:573:PRO:HD2 | 2.24 | 0.52 |
| 2:D:622:ASP:O | 2:D:625:THR:OG1 | 2.26 | 0.52 |
| 1:C:181:ILE:HG23 | 1:C:188:ASN:ND2 | 2.23 | 0.52 |
| 1:A:65:VAL:HG11 | 1:A:124:PHE:HB2 | 1.91 | 0.52 |
| 1:A:140:HIS:NE2 | 1:A:156:THR:OG1 | 2.39 | 0.52 |
| 2:D:613:VAL:HA | 2:D:655:VAL:O | 2.08 | 0.52 |
| 1:B:83:ILE:HD12 | 1:B:84:PHE:CD2 | 2.44 | 0.52 |
| 1:B:153:VAL:N | 1:B:154:PRO:CD | 2.73 | 0.52 |
| 1:C:153:VAL:N | 1:C:154:PRO:CD | 2.72 | 0.52 |
| 1:A:216:ILE:O | 1:A:218:PRO:HD2 | 2.10 | 0.52 |
| 2:D:516:LYS:HB2 | 4:D:678:GNP:O1B | 2.09 | 0.52 |
| 2:D:553:LEU:HD22 | 2:D:673:ILE:HD11 | 1.90 | 0.52 |
| 2:D:561:GLN:HG3 | 5:D:1:HOH:O | 2.09 | 0.52 |
| 1:B:157:LEU:HD21 | 1:B:232:GLU:O | 2.09 | 0.52 |
| 2:E:582:PHE:CE1 | 2:E:584:VAL:HA | 2.44 | 0.52 |
| 2:F:645:LEU:HD13 | 2:F:649:LEU:HD12 | 1.90 | 0.52 |
| 1:B:70:VAL:O | 1:B:74:GLN:HG3 | 2.09 | 0.52 |
| 2:F:620:ARG:NH1 | 2:F:637:ILE:O | 2.42 | 0.52 |
| 2:D:512:GLY:O | 2:D:513:ALA:HB3 | 2.09 | 0.52 |
| 1:B:116:LEU:N | 1:B:117:PRO:CD | 2.72 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:665:LEU:HD12 | 2:E:669:PHE:HE2 | 1.74 | 0.52 |
| 1:C:211:ILE:HB | 2:F:570:LEU:CD1 | 2.40 | 0.52 |
| 2:F:532:TYR:C | 2:F:533:VAL:HG22 | 2.29 | 0.52 |
| 2:F:582:PHE:CE1 | 2:F:584:VAL:HA | 2.45 | 0.52 |
| 1:B:40:LEU:HB3 | 1:B:41:PRO:CD | 2.31 | 0.52 |
| 1:A:116:LEU:N | 1:A:117:PRO:CD | 2.73 | 0.52 |
| 2:D:519:LEU:HD12 | 5:D:151:HOH:O | 2.08 | 0.52 |
| 1:B:217:ASN:ND2 | 2:E:536:VAL:HG11 | 2.24 | 0.52 |
| 2:E:582:PHE:HE1 | 2:E:584:VAL:HA | 1.74 | 0.52 |
| 2:D:503:THR:C | 2:D:504:ILE:HG13 | 2.30 | 0.52 |
| 1:B:65:VAL:HG11 | 1:B:124:PHE:HB2 | 1.92 | 0.52 |
| 1:B:177:PHE:O | 1:B:180:GLN:HG2 | 2.10 | 0.52 |
| 2:E:595:GLU:O | 2:E:596:LYS:HB2 | 2.10 | 0.52 |
| 1:C:107:ASP:C | 1:C:109:ASP:H | 2.14 | 0.52 |
| 1:C:216:ILE:CG2 | 1:C:217:ASN:H | 2.13 | 0.52 |
| 2:F:532:TYR:N | 2:F:533:VAL:HG22 | 2.25 | 0.52 |
| 1:A:153:VAL:N | 1:A:154:PRO:CD | 2.72 | 0.51 |
| 2:D:532:TYR:O | 2:D:533:VAL:CG1 | 2.56 | 0.51 |
| 2:D:532:TYR:C | 2:D:533:VAL:HG22 | 2.30 | 0.51 |
| 1:C:216:ILE:HG22 | 1:C:217:ASN:N | 2.17 | 0.51 |
| 2:F:582:PHE:HE1 | 2:F:584:VAL:HA | 1.75 | 0.51 |
| 2:E:572:TYR:N | 2:E:573:PRO:HD2 | 2.25 | 0.51 |
| 2:F:572:TYR:N | 2:F:573:PRO:CD | 2.73 | 0.51 |
| 1:C:216:ILE:CG2 | 2:F:536:VAL:HG13 | 2.39 | 0.51 |
| 2:F:503:THR:C | 2:F:504:ILE:HG13 | 2.30 | 0.51 |
| 2:F:653:LYS:HD2 | 2:F:655:VAL:CG1 | 2.40 | 0.51 |
| 2:F:665:LEU:HD12 | 2:F:669:PHE:CE2 | 2.45 | 0.51 |
| 1:C:70:VAL:HG22 | 1:C:177:PHE:CD2 | 2.45 | 0.51 |
| 1:C:100:TYR:CE2 | 1:C:106:VAL:HG21 | 2.46 | 0.51 |
| 1:A:70:VAL:HG22 | 1:A:177:PHE:CD2 | 2.46 | 0.51 |
| 2:D:595:GLU:O | 2:D:596:LYS:CB | 2.58 | 0.51 |
| 2:D:639:PRO:HA | 2:D:654:TYR:HE2 | 1.75 | 0.51 |
| 1:B:180:GLN:HG3 | 5:B:263:HOH:O | 2.11 | 0.51 |
| 2:D:559:ALA:HB3 | 2:D:564:TYR:CB | 2.41 | 0.51 |
| 2:D:568:ARG:N | 2:D:569:PRO:CD | 2.73 | 0.51 |
| 1:B:211:ILE:HB | 2:E:570:LEU:CD1 | 2.41 | 0.51 |
| 2:F:516:LYS:HB2 | 4:F:678:GNP:O1B | 2.10 | 0.51 |
| 2:D:508:VAL:HG12 | 2:D:516:LYS:HG2 | 1.93 | 0.51 |
| 2:F:508:VAL:HG12 | 2:F:516:LYS:HG2 | 1.93 | 0.51 |
| 2:F:595:GLU:O | 2:F:596:LYS:HB2 | 2.10 | 0.51 |
| 2:E:505:LYS:HB3 | 2:E:575:THR:HA | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:539:ASN:N | 2:E:539:ASN:ND2 | 2.59 | 0.51 |
| 2:E:632:ASN:O | 2:E:633:LYS:HD2 | 2.11 | 0.51 |
| 1:C:189:LYS:HZ3 | 2:F:532:TYR:HD1 | 1.58 | 0.51 |
| 1:B:70:VAL:HG22 | 1:B:177:PHE:CD2 | 2.46 | 0.51 |
| 1:B:125:LEU:CD1 | 1:B:174:LEU:HD22 | 2.41 | 0.51 |
| 1:C:189:LYS:HD3 | 2:F:532:TYR:CD1 | 2.46 | 0.51 |
| 2:F:665:LEU:HD12 | 2:F:669:PHE:HE2 | 1.76 | 0.51 |
| 2:D:539:ASN:N | 2:D:539:ASN:ND2 | 2.59 | 0.50 |
| 2:D:559:ALA:O | 2:D:568:ARG:NH2 | 2.43 | 0.50 |
| 2:F:532:TYR:O | 2:F:533:VAL:CG1 | 2.56 | 0.50 |
| 2:F:568:ARG:N | 2:F:569:PRO:CD | 2.74 | 0.50 |
| 1:A:151:GLN:HA | 1:A:154:PRO:HG2 | 1.93 | 0.50 |
| 1:C:70:VAL:O | 1:C:74:GLN:HG3 | 2.10 | 0.50 |
| 1:A:211:ILE:HB | 2:D:570:LEU:CD1 | 2.41 | 0.50 |
| 1:A:133:LEU:O | 1:A:134:THR:CB | 2.60 | 0.50 |
| 2:D:666:LYS:HB2 | 5:D:17:HOH:O | 2.11 | 0.50 |
| 2:E:568:ARG:N | 2:E:569:PRO:CD | 2.74 | 0.50 |
| 1:C:157:LEU:HD23 | 1:C:233:LEU:HA | 1.93 | 0.50 |
| 2:F:595:GLU:O | 2:F:596:LYS:CB | 2.60 | 0.50 |
| 2:F:598:VAL:CB | 2:F:599:PRO:HD3 | 2.42 | 0.50 |
| 1:C:94:ARG:NH2 | 5:C:247:HOH:O | 2.43 | 0.50 |
| 2:F:653:LYS:HG2 | 2:F:654:TYR:H | 1.76 | 0.50 |
| 2:D:519:LEU:HB3 | 5:D:274:HOH:O | 2.11 | 0.50 |
| 1:B:63:PRO:O | 1:B:67:ARG:HG3 | 2.12 | 0.50 |
| 2:E:673:ILE:O | 2:E:677:LEU:HG | 2.11 | 0.50 |
| 2:D:547:GLY:N | 5:D:131:HOH:O | 2.38 | 0.50 |
| 2:F:646:ALA:O | 2:F:650:LYS:N | 2.44 | 0.50 |
| 1:A:216:ILE:HG22 | 1:A:217:ASN:N | 2.21 | 0.49 |
| 1:B:107:ASP:C | 1:B:109:ASP:H | 2.16 | 0.49 |
| 1:B:142:VAL:HG21 | 5:B:246:HOH:O | 2.12 | 0.49 |
| 1:C:63:PRO:O | 1:C:67:ARG:HG3 | 2.12 | 0.49 |
| 1:C:84:PHE:CD1 | 1:C:118:ALA:HB1 | 2.47 | 0.49 |
| 1:C:177:PHE:O | 1:C:180:GLN:HG2 | 2.12 | 0.49 |
| 1:A:45:PHE:HZ | 1:A:120:ILE:HG23 | 1.77 | 0.49 |
| 2:F:559:ALA:O | 2:F:568:ARG:NH2 | 2.43 | 0.49 |
| 1:B:217:ASN:HB3 | 1:B:218:PRO:CD | 2.41 | 0.49 |
| 2:E:523:TYR:HB2 | 2:E:665:LEU:HD11 | 1.94 | 0.49 |
| 1:A:107:ASP:C | 1:A:109:ASP:H | 2.15 | 0.49 |
| 1:B:81:GLU:HA | 1:B:188:ASN:CA | 2.39 | 0.49 |
| 1:C:83:ILE:HD12 | 1:C:84:PHE:CD2 | 2.48 | 0.49 |
| 1:C:189:LYS:HZ3 | 2:F:532:TYR:HB2 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:540:TYR:HB2 | 2:F:555:LEU:HB2 | 1.94 | 0.49 |
| 1:A:157:LEU:CD2 | 1:A:233:LEU:HA | 2.42 | 0.49 |
| 2:D:653:LYS:HD2 | 2:D:655:VAL:CG1 | 2.42 | 0.49 |
| 2:E:516:LYS:NZ | 4:E:678:GNP:O1G | 2.44 | 0.49 |
| 1:C:199:PHE:O | 1:C:202:ASN:HB2 | 2.13 | 0.49 |
| 1:A:200:GLY:N | 1:A:201:PRO:CD | 2.76 | 0.49 |
| 1:A:212:THR:CG2 | 1:A:213:LEU:H | 2.22 | 0.49 |
| 1:B:47:VAL:CG2 | 1:B:48:SER:N | 2.76 | 0.49 |
| 2:F:673:ILE:O | 2:F:677:LEU:HG | 2.12 | 0.49 |
| 1:A:84:PHE:CD1 | 1:A:118:ALA:HB1 | 2.46 | 0.49 |
| 1:A:177:PHE:O | 1:A:180:GLN:HG2 | 2.12 | 0.49 |
| 2:D:572:TYR:N | 2:D:573:PRO:CD | 2.74 | 0.49 |
| 2:E:646:ALA:O | 2:E:647:ARG:C | 2.50 | 0.49 |
| 1:C:133:LEU:O | 1:C:134:THR:CB | 2.61 | 0.49 |
| 2:D:649:LEU:C | 2:D:650:LYS:HD3 | 2.33 | 0.49 |
| 1:B:45:PHE:HZ | 1:B:120:ILE:HG23 | 1.77 | 0.49 |
| 1:B:92:VAL:O | 1:B:95:GLU:N | 2.44 | 0.49 |
| 2:E:598:VAL:HB | 2:E:599:PRO:HD3 | 1.95 | 0.49 |
| 2:E:564:TYR:HD1 | 2:E:567:LEU:HD12 | 1.78 | 0.48 |
| 2:F:501:PRO:HG3 | 2:F:550:PRO:CB | 2.43 | 0.48 |
| 2:D:653:LYS:HG2 | 2:D:654:TYR:H | 1.78 | 0.48 |
| 2:E:601:ILE:HG23 | 2:E:610:PHE:CE1 | 2.49 | 0.48 |
| 2:E:503:THR:C | 2:E:504:ILE:HG13 | 2.33 | 0.48 |
| 1:A:157:LEU:HD23 | 1:A:233:LEU:HA | 1.95 | 0.48 |
| 2:D:523:TYR:HB2 | 2:D:665:LEU:HD11 | 1.96 | 0.48 |
| 1:B:66:LEU:O | 1:B:70:VAL:HB | 2.14 | 0.48 |
| 1:A:83:ILE:CD1 | 1:A:181:ILE:HD12 | 2.43 | 0.48 |
| 2:D:501:PRO:HG3 | 2:D:550:PRO:CB | 2.43 | 0.48 |
| 2:D:509:VAL:HG12 | 2:D:558:THR:CG2 | 2.44 | 0.48 |
| 2:E:539:ASN:HD22 | 2:E:539:ASN:H | 1.61 | 0.48 |
| 2:D:673:ILE:O | 2:D:677:LEU:HG | 2.13 | 0.48 |
| 1:B:83:ILE:HD13 | 1:B:181:ILE:HD12 | 1.96 | 0.48 |
| 1:B:194:ASN:O | 1:B:197:VAL:HG23 | 2.13 | 0.48 |
| 2:E:646:ALA:HA | 2:E:651:ALA:HB3 | 1.95 | 0.48 |
| 2:D:598:VAL:CB | 2:D:599:PRO:HD3 | 2.44 | 0.48 |
| 2:E:572:TYR:N | 2:E:573:PRO:CD | 2.76 | 0.48 |
| 2:F:519:LEU:HD12 | 5:F:121:HOH:O | 2.13 | 0.48 |
| 1:A:165:GLU:OE2 | 1:A:169:GLN:OE1 | 2.31 | 0.48 |
| 1:A:217:ASN:HB3 | 1:A:218:PRO:CD | 2.41 | 0.48 |
| 2:D:646:ALA:O | 2:D:650:LYS:N | 2.43 | 0.48 |
| 1:A:38:PRO:HA | 1:A:39:PRO:HD2 | 1.62 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:104:LEU:CD1 | 1:B:105:PRO:HD2 | 2.42 | 0.48 |
| 2:E:583:SER:N | 2:E:589:SER:OG | 2.43 | 0.48 |
| 2:E:595:GLU:O | 2:E:596:LYS:CB | 2.61 | 0.48 |
| 2:E:597:TRP:O | 2:E:601:ILE:HB | 2.14 | 0.48 |
| 2:E:643:GLU:O | 2:E:644:LYS:C | 2.52 | 0.48 |
| 1:C:66:LEU:O | 1:C:70:VAL:HB | 2.14 | 0.48 |
| 1:C:217:ASN:HB3 | 1:C:218:PRO:CD | 2.42 | 0.48 |
| 2:F:598:VAL:HB | 2:F:599:PRO:HD3 | 1.94 | 0.48 |
| 1:C:45:PHE:HZ | 1:C:120:ILE:HG23 | 1.78 | 0.48 |
| 2:D:583:SER:N | 2:D:589:SER:OG | 2.43 | 0.47 |
| 1:B:211:ILE:HG13 | 2:E:570:LEU:HD13 | 1.96 | 0.47 |
| 1:C:194:ASN:HA | 1:C:197:VAL:HG23 | 1.95 | 0.47 |
| 1:C:211:ILE:HG13 | 2:F:570:LEU:HD13 | 1.95 | 0.47 |
| 2:F:622:ASP:HA | 2:F:623:PRO:HD2 | 1.83 | 0.47 |
| 1:B:133:LEU:O | 1:B:134:THR:CB | 2.62 | 0.47 |
| 1:A:81:GLU:HA | 1:A:188:ASN:CA | 2.39 | 0.47 |
| 2:E:611:LEU:HD23 | 2:E:653:LYS:O | 2.15 | 0.47 |
| 2:F:596:LYS:HE3 | 2:F:597:TRP:CZ2 | 2.49 | 0.47 |
| 2:F:632:ASN:O | 2:F:633:LYS:HD2 | 2.14 | 0.47 |
| 2:D:617:ILE:HD13 | 2:D:656:GLU:OE1 | 2.15 | 0.47 |
| 2:D:643:GLU:O | 2:D:644:LYS:C | 2.52 | 0.47 |
| 1:B:151:GLN:HA | 1:B:154:PRO:HG2 | 1.96 | 0.47 |
| 1:B:185:SER:O | 1:B:189:LYS:HA | 2.15 | 0.47 |
| 2:E:646:ALA:O | 2:E:650:LYS:N | 2.47 | 0.47 |
| 2:F:597:TRP:O | 2:F:601:ILE:HB | 2.14 | 0.47 |
| 1:A:66:LEU:O | 1:A:70:VAL:HB | 2.14 | 0.47 |
| 1:B:140:HIS:NE2 | 1:B:156:THR:OG1 | 2.40 | 0.47 |
| 1:C:104:LEU:CD1 | 1:C:105:PRO:HD2 | 2.44 | 0.47 |
| 2:F:516:LYS:NZ | 4:F:678:GNP:O1G | 2.46 | 0.47 |
| 2:F:539:ASN:N | 2:F:539:ASN:ND2 | 2.57 | 0.47 |
| 2:F:601:ILE:HG23 | 2:F:610:PHE:CE1 | 2.49 | 0.47 |
| 1:B:205:TRP:HZ3 | 5:B:277:HOH:O | 1.97 | 0.47 |
| 2:F:569:PRO:HG2 | 5:F:224:HOH:O | 2.13 | 0.47 |
| 1:A:199:PHE:O | 1:A:202:ASN:HB2 | 2.14 | 0.47 |
| 2:D:564:TYR:HD1 | 2:D:567:LEU:HD12 | 1.80 | 0.47 |
| 2:D:617:ILE:CD1 | 2:D:656:GLU:HB3 | 2.44 | 0.47 |
| 2:D:642:ALA:HB3 | 2:D:654:TYR:CE2 | 2.49 | 0.47 |
| 1:B:37:ARG:HH12 | 1:B:97:GLN:HB3 | 1.78 | 0.47 |
| 1:B:84:PHE:CD1 | 1:B:118:ALA:HB1 | 2.50 | 0.47 |
| 1:B:86:ARG:HG2 | 5:B:237:HOH:O | 2.15 | 0.47 |
| 2:E:653:LYS:HG2 | 2:E:654:TYR:H | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:151:GLN:HA | 1:C:154:PRO:HG2 | 1.95 | 0.47 |
| 2:F:590:PHE:CE1 | 2:F:645:LEU:HG | 2.50 | 0.47 |
| 1:A:83:ILE:HD12 | 1:A:84:PHE:CD2 | 2.49 | 0.47 |
| 2:D:596:LYS:HE3 | 2:D:597:TRP:CZ2 | 2.50 | 0.47 |
| 2:E:598:VAL:CB | 2:E:599:PRO:HD3 | 2.45 | 0.47 |
| 1:C:200:GLY:N | 1:C:201:PRO:CD | 2.77 | 0.47 |
| 2:F:564:TYR:HD1 | 2:F:567:LEU:HD12 | 1.80 | 0.47 |
| 2:F:583:SER:N | 2:F:589:SER:OG | 2.47 | 0.47 |
| 1:A:185:SER:O | 1:A:189:LYS:HA | 2.15 | 0.47 |
| 1:A:216:ILE:CG1 | 2:D:567:LEU:HD13 | 2.44 | 0.47 |
| 2:E:522:SER:HB3 | 2:E:665:LEU:CD2 | 2.45 | 0.47 |
| 1:C:113:GLU:O | 1:C:114:LEU:HB3 | 2.14 | 0.47 |
| 2:F:539:ASN:HD22 | 2:F:539:ASN:H | 1.59 | 0.47 |
| 1:A:193:THR:HG22 | 1:A:224:LYS:HD2 | 1.98 | 0.46 |
| 2:D:516:LYS:NZ | 4:D:678:GNP:O1G | 2.45 | 0.46 |
| 2:D:539:ASN:HD22 | 2:D:539:ASN:H | 1.60 | 0.46 |
| 2:F:523:TYR:HB2 | 2:F:665:LEU:HD11 | 1.97 | 0.46 |
| 1:A:63:PRO:O | 1:A:67:ARG:HG3 | 2.14 | 0.46 |
| 1:B:113:GLU:O | 1:B:114:LEU:HB3 | 2.14 | 0.46 |
| 1:C:96:VAL:HG13 | 1:C:106:VAL:HG11 | 1.96 | 0.46 |
| 2:F:649:LEU:C | 2:F:650:LYS:HD3 | 2.35 | 0.46 |
| 2:D:559:ALA:HB3 | 2:D:564:TYR:HB3 | 1.96 | 0.46 |
| 1:C:81:GLU:HA | 1:C:188:ASN:CA | 2.38 | 0.46 |
| 2:D:597:TRP:O | 2:D:601:ILE:HB | 2.16 | 0.46 |
| 1:B:38:PRO:HA | 1:B:39:PRO:HD2 | 1.63 | 0.46 |
| 1:B:60:GLU:HB3 | 5:B:257:HOH:O | 2.15 | 0.46 |
| 1:B:211:ILE:CG1 | 2:E:570:LEU:HD13 | 2.45 | 0.46 |
| 1:B:216:ILE:HG22 | 1:B:217:ASN:N | 2.19 | 0.46 |
| 2:E:559:ALA:HB3 | 2:E:564:TYR:CB | 2.45 | 0.46 |
| 2:E:617:ILE:HD13 | 2:E:656:GLU:OE1 | 2.15 | 0.46 |
| 1:B:189:LYS:HD3 | 2:E:532:TYR:CD1 | 2.51 | 0.46 |
| 1:B:216:ILE:CG1 | 2:E:567:LEU:HD13 | 2.46 | 0.46 |
| 1:C:157:LEU:CD2 | 1:C:233:LEU:HA | 2.45 | 0.46 |
| 1:A:125:LEU:CD1 | 1:A:174:LEU:HD22 | 2.45 | 0.46 |
| 1:A:175:THR:O | 1:A:179:VAL:HG23 | 2.15 | 0.46 |
| 1:A:191:THR:HB | 2:D:532:TYR:HH | 1.77 | 0.46 |
| 2:E:509:VAL:HG12 | 2:E:558:THR:CG2 | 2.46 | 0.46 |
| 1:A:189:LYS:NZ | 2:D:532:TYR:HD1 | 2.13 | 0.46 |
| 2:D:564:TYR:O | 2:D:568:ARG:HB2 | 2.15 | 0.46 |
| 1:B:94:ARG:NH2 | 5:B:247:HOH:O | 2.48 | 0.46 |
| 1:B:133:LEU:CB | 1:B:203:LEU:HD13 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:194:ASN:HA | 1:B:197:VAL:HG23 | 1.97 | 0.46 |
| 2:E:559:ALA:O | 2:E:568:ARG:NH2 | 2.46 | 0.46 |
| 1:C:175:THR:O | 1:C:179:VAL:HG23 | 2.16 | 0.46 |
| 1:C:194:ASN:O | 1:C:197:VAL:HG23 | 2.16 | 0.46 |
| 2:F:564:TYR:O | 2:F:568:ARG:HB2 | 2.15 | 0.46 |
| 2:D:601:ILE:HG23 | 2:D:610:PHE:CE1 | 2.50 | 0.46 |
| 1:C:83:ILE:HD13 | 1:C:181:ILE:HD12 | 1.96 | 0.46 |
| 2:F:522:SER:HB3 | 2:F:665:LEU:CD2 | 2.46 | 0.46 |
| 1:A:113:GLU:O | 1:A:114:LEU:HB3 | 2.15 | 0.46 |
| 1:A:189:LYS:HZ3 | 2:D:532:TYR:HB2 | 1.81 | 0.46 |
| 2:E:657:CYS:HA | 2:E:664:GLY:HA3 | 1.98 | 0.46 |
| 2:F:617:ILE:CD1 | 2:F:656:GLU:HB3 | 2.45 | 0.46 |
| 1:A:104:LEU:CD1 | 1:A:105:PRO:HD2 | 2.45 | 0.45 |
| 2:E:594:LYS:HG3 | 2:E:595:GLU:N | 2.31 | 0.45 |
| 1:C:37:ARG:HH12 | 1:C:97:GLN:CG | 2.29 | 0.45 |
| 1:C:211:ILE:CG1 | 2:F:570:LEU:HD13 | 2.46 | 0.45 |
| 2:F:615:THR:HG22 | 2:F:616:GLN:HG3 | 1.98 | 0.45 |
| 2:D:522:SER:HB3 | 2:D:665:LEU:CD2 | 2.45 | 0.45 |
| 2:D:598:VAL:HB | 2:D:599:PRO:HD3 | 1.98 | 0.45 |
| 1:B:141:VAL:HG22 | 1:B:222:PHE:CG | 2.51 | 0.45 |
| 2:F:509:VAL:HG12 | 2:F:558:THR:CG2 | 2.46 | 0.45 |
| 1:A:194:ASN:O | 1:A:197:VAL:HG23 | 2.17 | 0.45 |
| 2:D:509:VAL:HA | 2:D:558:THR:OG1 | 2.15 | 0.45 |
| 1:B:86:ARG:NH1 | 5:B:292:HOH:O | 2.50 | 0.45 |
| 1:C:165:GLU:OE2 | 1:C:169:GLN:OE1 | 2.34 | 0.45 |
| 2:D:590:PHE:CE1 | 2:D:645:LEU:HG | 2.50 | 0.45 |
| 2:E:515:GLY:HA2 | 4:E:678:GNP:C8 | 2.46 | 0.45 |
| 2:E:542:VAL:HA | 5:E:50:HOH:O | 2.16 | 0.45 |
| 2:E:642:ALA:HB3 | 2:E:654:TYR:CE2 | 2.52 | 0.45 |
| 2:E:666:LYS:HB2 | 5:E:53:HOH:O | 2.16 | 0.45 |
| 2:F:659:ALA:HB3 | 4:F:678:GNP:O6 | 2.16 | 0.45 |
| 1:A:72:TYR:O | 1:A:75:ALA:HB3 | 2.17 | 0.45 |
| 2:D:532:TYR:O | 2:D:532:TYR:CD2 | 2.70 | 0.45 |
| 1:C:216:ILE:CG1 | 2:F:567:LEU:HD13 | 2.47 | 0.45 |
| 2:D:611:LEU:HD23 | 2:D:653:LYS:O | 2.17 | 0.45 |
| 1:B:157:LEU:CD2 | 1:B:233:LEU:HA | 2.46 | 0.45 |
| 1:B:157:LEU:HD23 | 1:B:233:LEU:HA | 1.99 | 0.45 |
| 1:C:185:SER:O | 1:C:189:LYS:HA | 2.16 | 0.45 |
| 2:F:533:VAL:H | 2:F:534:PRO:HD3 | 1.82 | 0.45 |
| 1:B:116:LEU:N | 1:B:117:PRO:HD3 | 2.31 | 0.45 |
| 2:E:590:PHE:CE1 | 2:E:645:LEU:HG | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:650:LYS:HD3 | 2:E:650:LYS:N | 2.32 | 0.45 |
| 1:C:62:ILE:HA | 1:C:63:PRO:HD3 | 1.82 | 0.45 |
| 1:C:116:LEU:O | 1:C:120:ILE:HG12 | 2.17 | 0.45 |
| 2:F:559:ALA:HB3 | 2:F:564:TYR:CB | 2.47 | 0.45 |
| 2:E:532:TYR:O | 2:E:533:VAL:CG2 | 2.65 | 0.44 |
| 2:F:611:LEU:HD23 | 2:F:653:LYS:O | 2.17 | 0.44 |
| 1:C:106:VAL:HB | 5:C:240:HOH:O | 2.17 | 0.44 |
| 1:A:40:LEU:HD23 | 1:A:101:ASN:HB2 | 1.98 | 0.44 |
| 2:D:622:ASP:HA | 2:D:623:PRO:HD2 | 1.87 | 0.44 |
| 1:B:93:VAL:HG13 | 1:B:120:ILE:HD11 | 1.99 | 0.44 |
| 2:F:539:ASN:ND2 | 2:F:539:ASN:H | 2.15 | 0.44 |
| 2:F:642:ALA:HB3 | 2:F:654:TYR:CE2 | 2.53 | 0.44 |
| 2:E:532:TYR:O | 2:E:533:VAL:CG1 | 2.65 | 0.44 |
| 2:E:615:THR:HG22 | 2:E:616:GLN:HG3 | 2.00 | 0.44 |
| 2:E:617:ILE:CD1 | 2:E:656:GLU:HB3 | 2.46 | 0.44 |
| 1:C:150:SER:HA | 5:C:272:HOH:O | 2.17 | 0.44 |
| 1:A:189:LYS:NZ | 2:D:532:TYR:CD1 | 2.85 | 0.44 |
| 1:B:181:ILE:CG2 | 1:B:188:ASN:HD21 | 2.24 | 0.44 |
| 2:E:521:ILE:HG22 | 2:E:527:LYS:O | 2.17 | 0.44 |
| 2:E:596:LYS:HE3 | 2:E:597:TRP:CZ2 | 2.53 | 0.44 |
| 2:E:661:THR:O | 2:E:662:GLN:HB2 | 2.18 | 0.44 |
| 1:A:86:ARG:HG2 | 5:A:236:HOH:O | 2.17 | 0.44 |
| 2:D:515:GLY:HA2 | 4:D:678:GNP:C8 | 2.47 | 0.44 |
| 2:D:632:ASN:O | 2:D:633:LYS:HD2 | 2.17 | 0.44 |
| 1:B:165:GLU:OE2 | 1:B:169:GLN:OE1 | 2.35 | 0.44 |
| 2:E:622:ASP:HA | 2:E:623:PRO:HD2 | 1.82 | 0.44 |
| 1:C:191:THR:CB | 2:F:532:TYR:OH | 2.63 | 0.44 |
| 1:A:138:TYR:HB3 | 1:A:139:PRO:HD3 | 1.99 | 0.44 |
| 2:D:594:LYS:HB3 | 2:D:649:LEU:HD11 | 1.99 | 0.44 |
| 2:E:564:TYR:O | 2:E:568:ARG:HB2 | 2.17 | 0.44 |
| 1:A:47:VAL:CG2 | 1:A:48:SER:N | 2.81 | 0.44 |
| 2:F:509:VAL:HA | 2:F:558:THR:OG1 | 2.17 | 0.44 |
| 2:F:584:VAL:CG1 | 2:F:620:ARG:NH1 | 2.81 | 0.44 |
| 1:A:79:THR:O | 1:A:187:GLN:HG3 | 2.17 | 0.43 |
| 1:A:93:VAL:HG13 | 1:A:120:ILE:HD11 | 1.99 | 0.43 |
| 1:A:181:ILE:CG2 | 1:A:188:ASN:HD21 | 2.25 | 0.43 |
| 2:E:506:CYS:SG | 2:E:579:LEU:HG | 2.58 | 0.43 |
| 2:E:509:VAL:HA | 2:E:558:THR:OG1 | 2.17 | 0.43 |
| 2:E:561:GLN:HG3 | 5:E:2:HOH:O | 2.18 | 0.43 |
| 2:F:532:TYR:C | 2:F:532:TYR:CD2 | 2.91 | 0.43 |
| 1:A:40:LEU:CB | 1:A:41:PRO:HD2 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:212:THR:HG22 | 1:A:213:LEU:N | 2.28 | 0.43 |
| 2:E:568:ARG:N | 2:E:569:PRO:HD3 | 2.33 | 0.43 |
| 1:C:93:VAL:HG13 | 1:C:120:ILE:HD11 | 1.99 | 0.43 |
| 1:C:167:ASN:O | 1:C:171:LEU:HB2 | 2.18 | 0.43 |
| 1:A:141:VAL:HG22 | 1:A:222:PHE:CG | 2.52 | 0.43 |
| 1:A:194:ASN:HA | 1:A:197:VAL:HG23 | 1.99 | 0.43 |
| 2:D:568:ARG:N | 2:D:569:PRO:HD3 | 2.33 | 0.43 |
| 1:B:79:THR:O | 1:B:187:GLN:HG3 | 2.18 | 0.43 |
| 1:C:212:THR:CG2 | 1:C:213:LEU:H | 2.26 | 0.43 |
| 2:D:501:PRO:CG | 2:D:550:PRO:HB2 | 2.46 | 0.43 |
| 1:B:138:TYR:HB3 | 1:B:139:PRO:HD3 | 1.99 | 0.43 |
| 1:B:175:THR:O | 1:B:179:VAL:HG23 | 2.18 | 0.43 |
| 1:C:72:TYR:O | 1:C:75:ALA:HB3 | 2.18 | 0.43 |
| 1:C:169:GLN:NE2 | 1:C:172:ARG:HH21 | 2.17 | 0.43 |
| 1:C:218:PRO:HD2 | 5:C:276:HOH:O | 2.19 | 0.43 |
| 2:F:515:GLY:HA2 | 4:F:678:GNP:C8 | 2.47 | 0.43 |
| 2:F:568:ARG:N | 2:F:569:PRO:HD3 | 2.34 | 0.43 |
| 2:F:617:ILE:HD13 | 2:F:656:GLU:OE1 | 2.18 | 0.43 |
| 2:F:646:ALA:HA | 2:F:651:ALA:HB3 | 2.00 | 0.43 |
| 1:A:189:LYS:HD3 | 2:D:532:TYR:CE1 | 2.53 | 0.43 |
| 2:E:547:GLY:N | 5:E:60:HOH:O | 2.42 | 0.43 |
| 1:C:95:GLU:O | 1:C:96:VAL:C | 2.56 | 0.43 |
| 1:C:104:LEU:CG | 1:C:105:PRO:HD2 | 2.49 | 0.43 |
| 1:A:37:ARG:HH12 | 1:A:97:GLN:HB3 | 1.82 | 0.43 |
| 1:A:191:THR:CB | 2:D:532:TYR:OH | 2.66 | 0.43 |
| 2:D:532:TYR:O | 2:D:533:VAL:CB | 2.66 | 0.43 |
| 1:C:212:THR:HG22 | 1:C:213:LEU:N | 2.29 | 0.43 |
| 2:D:539:ASN:ND2 | 2:D:539:ASN:H | 2.16 | 0.43 |
| 2:D:615:THR:HG22 | 2:D:616:GLN:HG3 | 2.00 | 0.43 |
| 1:B:167:ASN:O | 1:B:171:LEU:HB2 | 2.19 | 0.43 |
| 1:C:49:LEU:HA | 1:C:52:LEU:HD12 | 2.01 | 0.43 |
| 1:A:169:GLN:NE2 | 1:A:172:ARG:HH21 | 2.17 | 0.43 |
| 1:A:218:PRO:HD2 | 5:A:274:HOH:O | 2.18 | 0.43 |
| 1:B:189:LYS:NZ | 2:E:532:TYR:HD1 | 2.17 | 0.43 |
| 2:E:576:ASP:O | 2:E:577:VAL:CB | 2.56 | 0.43 |
| 1:C:37:ARG:HH12 | 1:C:97:GLN:HB3 | 1.80 | 0.43 |
| 2:E:517:THR:HB | 4:E:678:GNP:O1A | 2.19 | 0.42 |
| 2:E:532:TYR:O | 2:E:533:VAL:CB | 2.66 | 0.42 |
| 2:E:584:VAL:CG1 | 2:E:620:ARG:NH1 | 2.82 | 0.42 |
| 1:B:199:PHE:O | 1:B:202:ASN:HB2 | 2.18 | 0.42 |
| 2:E:516:LYS:HB2 | 4:E:678:GNP:O1B | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:83:ILE:H | 1:C:83:ILE:HG13 | 1.74 | 0.42 |
| 2:F:532:TYR:O | 2:F:533:VAL:CB | 2.67 | 0.42 |
| 1:C:40:LEU:HD23 | 1:C:101:ASN:HB2 | 2.00 | 0.42 |
| 1:C:138:TYR:HB3 | 1:C:139:PRO:HD3 | 2.01 | 0.42 |
| 2:F:599:PRO:O | 2:F:603:HIS:HB3 | 2.19 | 0.42 |
| 2:F:643:GLU:O | 2:F:644:LYS:C | 2.57 | 0.42 |
| 2:D:584:VAL:CG1 | 2:D:620:ARG:NH1 | 2.82 | 0.42 |
| 2:E:507:VAL:HB | 2:E:556:PHE:HB2 | 2.00 | 0.42 |
| 1:C:189:LYS:HD3 | 2:F:532:TYR:HD1 | 1.84 | 0.42 |
| 2:F:521:ILE:HG22 | 2:F:527:LYS:O | 2.18 | 0.42 |
| 2:F:532:TYR:O | 2:F:532:TYR:CD2 | 2.72 | 0.42 |
| 1:A:211:ILE:CG1 | 2:D:570:LEU:HD13 | 2.50 | 0.42 |
| 1:C:92:VAL:O | 1:C:95:GLU:N | 2.44 | 0.42 |
| 1:A:70:VAL:HG22 | 1:A:177:PHE:CE2 | 2.55 | 0.42 |
| 1:B:169:GLN:NE2 | 1:B:172:ARG:HH21 | 2.17 | 0.42 |
| 2:E:638:THR:HA | 2:E:639:PRO:HD3 | 1.90 | 0.42 |
| 2:F:608:THR:HA | 2:F:609:PRO:HD2 | 1.64 | 0.42 |
| 1:A:189:LYS:HD3 | 2:D:532:TYR:HD1 | 1.83 | 0.42 |
| 2:D:521:ILE:HG22 | 2:D:527:LYS:O | 2.19 | 0.42 |
| 2:D:522:SER:O | 2:D:526:ASN:HA | 2.20 | 0.42 |
| 2:D:532:TYR:O | 2:D:533:VAL:HG22 | 2.19 | 0.42 |
| 1:B:189:LYS:HZ3 | 2:E:532:TYR:HB2 | 1.85 | 0.42 |
| 2:E:659:ALA:HB3 | 4:E:678:GNP:O6 | 2.20 | 0.42 |
| 1:C:126:ARG:CG | 1:C:202:ASN:OD1 | 2.67 | 0.42 |
| 1:C:140:HIS:CE1 | 1:C:222:PHE:HE1 | 2.38 | 0.42 |
| 1:C:211:ILE:CG1 | 1:C:212:THR:N | 2.76 | 0.42 |
| 2:D:599:PRO:O | 2:D:603:HIS:HB3 | 2.20 | 0.42 |
| 2:D:659:ALA:HB3 | 4:D:678:GNP:O6 | 2.20 | 0.42 |
| 1:B:193:THR:HG22 | 1:B:224:LYS:HD2 | 2.01 | 0.42 |
| 2:E:599:PRO:O | 2:E:603:HIS:HB3 | 2.20 | 0.42 |
| 2:D:598:VAL:HG21 | 2:D:649:LEU:HD13 | 2.01 | 0.42 |
| 1:B:169:GLN:CD | 1:B:172:ARG:HH21 | 2.23 | 0.42 |
| 1:C:116:LEU:N | 1:C:117:PRO:HD3 | 2.35 | 0.42 |
| 1:C:133:LEU:CB | 1:C:203:LEU:HD13 | 2.50 | 0.42 |
| 1:A:216:ILE:HG13 | 2:D:567:LEU:HD13 | 2.02 | 0.41 |
| 1:B:104:LEU:CG | 1:B:105:PRO:HD2 | 2.50 | 0.41 |
| 1:C:141:VAL:HG22 | 1:C:222:PHE:CG | 2.54 | 0.41 |
| 2:F:661:THR:O | 2:F:662:GLN:HB2 | 2.20 | 0.41 |
| 1:A:133:LEU:CB | 1:A:203:LEU:HD13 | 2.51 | 0.41 |
| 2:E:611:LEU:HD23 | 2:E:611:LEU:HA | 1.81 | 0.41 |
| 1:C:79:THR:O | 1:C:187:GLN:HG3 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:167:ASN:O | 1:A:171:LEU:HB2 | 2.20 | 0.41 |
| 1:A:211:ILE:HG13 | 2:D:570:LEU:HD13 | 2.02 | 0.41 |
| 2:D:585:VAL:O | 2:D:629:LEU:HD22 | 2.21 | 0.41 |
| 1:B:70:VAL:HG22 | 1:B:177:PHE:CE2 | 2.54 | 0.41 |
| 1:B:72:TYR:O | 1:B:75:ALA:HB3 | 2.19 | 0.41 |
| 1:B:217:ASN:ND2 | 2:E:536:VAL:HG21 | 2.35 | 0.41 |
| 2:E:594:LYS:HB3 | 2:E:649:LEU:HD11 | 2.01 | 0.41 |
| 2:E:564:TYR:CD1 | 2:E:567:LEU:HD12 | 2.54 | 0.41 |
| 1:C:38:PRO:HA | 1:C:39:PRO:HD2 | 1.62 | 0.41 |
| 2:F:501:PRO:CG | 2:F:550:PRO:HB2 | 2.47 | 0.41 |
| 2:F:584:VAL:HG13 | 2:F:620:ARG:NH1 | 2.35 | 0.41 |
| 1:A:140:HIS:CE1 | 1:A:222:PHE:HE2 | 2.39 | 0.41 |
| 2:D:507:VAL:HB | 2:D:556:PHE:HB2 | 2.02 | 0.41 |
| 2:D:584:VAL:HG13 | 2:D:620:ARG:NH1 | 2.36 | 0.41 |
| 2:E:559:ALA:HB3 | 2:E:564:TYR:HB3 | 2.01 | 0.41 |
| 1:C:207:LYS:HG3 | 5:C:239:HOH:O | 2.20 | 0.41 |
| 1:C:217:ASN:ND2 | 2:F:536:VAL:HG21 | 2.35 | 0.41 |
| 2:F:654:TYR:OH | 2:F:656:GLU:OE2 | 2.36 | 0.41 |
| 2:D:516:LYS:HB2 | 4:D:678:GNP:O2B | 2.20 | 0.41 |
| 2:D:650:LYS:HD3 | 2:D:650:LYS:N | 2.36 | 0.41 |
| 1:B:140:HIS:CE1 | 1:B:156:THR:HG1 | 2.35 | 0.41 |
| 1:B:191:THR:HB | 2:E:532:TYR:HH | 1.84 | 0.41 |
| 1:B:197:VAL:CG2 | 2:E:534:PRO:HG2 | 2.45 | 0.41 |
| 2:E:508:VAL:HG12 | 2:E:516:LYS:HG2 | 2.03 | 0.41 |
| 2:F:594:LYS:HB3 | 2:F:649:LEU:HD11 | 2.01 | 0.41 |
| 2:F:643:GLU:OE2 | 2:F:654:TYR:HB3 | 2.21 | 0.41 |
| 1:B:83:ILE:H | 1:B:83:ILE:HG13 | 1.74 | 0.41 |
| 1:B:189:LYS:HZ3 | 2:E:532:TYR:HD1 | 1.62 | 0.41 |
| 2:E:532:TYR:O | 2:E:532:TYR:CD2 | 2.73 | 0.41 |
| 1:C:132:LEU:HB3 | 5:C:278:HOH:O | 2.21 | 0.41 |
| 2:D:657:CYS:HA | 2:D:664:GLY:HA3 | 2.02 | 0.41 |
| 1:B:95:GLU:O | 1:B:96:VAL:C | 2.59 | 0.41 |
| 2:E:572:TYR:H | 2:E:573:PRO:HD2 | 1.85 | 0.41 |
| 1:C:169:GLN:CD | 1:C:172:ARG:HH21 | 2.24 | 0.41 |
| 2:F:501:PRO:O | 2:F:502:GLN:C | 2.59 | 0.41 |
| 2:F:638:THR:HA | 2:F:639:PRO:HD3 | 1.89 | 0.41 |
| 1:A:104:LEU:CG | 1:A:105:PRO:HD2 | 2.50 | 0.41 |
| 2:D:564:TYR:CD1 | 2:D:567:LEU:HD12 | 2.55 | 0.41 |
| 2:D:646:ALA:HA | 2:D:651:ALA:HB3 | 2.03 | 0.41 |
| 1:B:62:ILE:HA | 1:B:63:PRO:HD3 | 1.83 | 0.41 |
| 1:B:81:GLU:HA | 1:B:188:ASN:CB | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:218:PRO:HD2 | 5:B:275:HOH:O | 2.21 | 0.41 |
| 1:B:222:PHE:CE2 | 1:B:226:LEU:HD11 | 2.56 | 0.41 |
| 1:C:189:LYS:NZ | 2:F:532:TYR:HD1 | 2.17 | 0.41 |
| 2:F:507:VAL:HB | 2:F:556:PHE:HB2 | 2.02 | 0.41 |
| 2:F:511:ASP:O | 2:F:514:VAL:HG13 | 2.20 | 0.41 |
| 1:A:189:LYS:NZ | 2:D:532:TYR:HB2 | 2.35 | 0.41 |
| 1:B:140:HIS:CE1 | 1:B:222:PHE:HE1 | 2.39 | 0.41 |
| 2:E:501:PRO:HG3 | 2:E:550:PRO:CB | 2.45 | 0.41 |
| 2:E:606:PRO:O | 2:E:607:LYS:CB | 2.68 | 0.41 |
| 2:F:585:VAL:O | 2:F:629:LEU:HD22 | 2.21 | 0.41 |
| 1:A:95:GLU:O | 1:A:96:VAL:C | 2.58 | 0.40 |
| 2:D:517:THR:HB | 4:D:678:GNP:O1A | 2.22 | 0.40 |
| 2:D:661:THR:O | 2:D:662:GLN:HB2 | 2.21 | 0.40 |
| 1:B:44:GLN:CG | 1:B:100:TYR:HB3 | 2.51 | 0.40 |
| 2:E:608:THR:HA | 2:E:609:PRO:HD2 | 1.61 | 0.40 |
| 2:F:572:TYR:H | 2:F:573:PRO:HD2 | 1.85 | 0.40 |
| 1:A:49:LEU:HA | 1:A:52:LEU:HD12 | 2.03 | 0.40 |
| 1:B:96:VAL:CG1 | 1:B:106:VAL:HG11 | 2.52 | 0.40 |
| 1:C:189:LYS:CE | 2:F:532:TYR:HD1 | 2.35 | 0.40 |
| 1:A:44:GLN:CG | 1:A:100:TYR:HB3 | 2.50 | 0.40 |
| 2:D:532:TYR:C | 2:D:532:TYR:CD2 | 2.94 | 0.40 |
| 2:D:611:LEU:HD23 | 2:D:611:LEU:HA | 1.77 | 0.40 |
| 1:B:37:ARG:HH12 | 1:B:97:GLN:CG | 2.35 | 0.40 |
| 1:B:45:PHE:CD1 | 1:B:97:GLN:HG2 | 2.57 | 0.40 |
| 1:B:56:ASN:HA | 1:B:57:PRO:HD2 | 1.89 | 0.40 |
| 2:E:585:VAL:O | 2:E:629:LEU:HD22 | 2.22 | 0.40 |
| 1:A:86:ARG:NH1 | 5:A:267:HOH:O | 2.54 | 0.40 |
| 1:B:200:GLY:N | 1:B:201:PRO:CD | 2.80 | 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 | 197/199 (99%) | 157 (80%) | 29 (15%) | 11 (6%) | 2 3 |
| 1 | B | 197/199 (99%) | 157 (80%) | 29 (15%) | 11 (6%) | 2 3 |
| 1 | C | 197/199 (99%) | 159 (81%) | 26 (13%) | 12 (6%) | 1 2 |
| 2 | D | 170/177 (96%) | 137 (81%) | 21 (12%) | 12 (7%) | 1 1 |
| 2 | E | 170/177 (96%) | 136 (80%) | 22 (13%) | 12 (7%) | 1 1 |
| 2 | F | 170/177 (96%) | 136 (80%) | 22 (13%) | 12 (7%) | 1 1 |
| All | All | 1101/1128 (98%) | 882 (80%) | 149 (14%) | 70 (6%) | 1 2 |

All (70) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 209 | ALA |
| 1 | A | 210 | ALA |
| 1 | A | 211 | ILE |
| 1 | A | 216 | ILE |
| 1 | A | 217 | ASN |
| 2 | D | 533 | VAL |
| 2 | D | 577 | VAL |
| 2 | D | 596 | LYS |
| 1 | B | 209 | ALA |
| 1 | B | 210 | ALA |
| 1 | B | 211 | ILE |
| 1 | B | 216 | ILE |
| 1 | B | 217 | ASN |
| 2 | E | 533 | VAL |
| 2 | E | 577 | VAL |
| 2 | E | 596 | LYS |
| 1 | C | 209 | ALA |
| 1 | C | 210 | ALA |
| 1 | C | 211 | ILE |
| 1 | C | 216 | ILE |
| 1 | C | 217 | ASN |
| 2 | F | 533 | VAL |
| 2 | F | 577 | VAL |
| 2 | F | 596 | LYS |
| 1 | A | 84 | PHE |
| 2 | D | 502 | GLN |
| 2 | D | 546 | ILE |
| 2 | D | 633 | LYS |
| 1 | B | 84 | PHE |
| 2 | E | 502 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 546 | ILE |
| 2 | E | 633 | LYS |
| 1 | C | 84 | PHE |
| 2 | F | 502 | GLN |
| 2 | F | 546 | ILE |
| 2 | F | 548 | GLY |
| 2 | F | 633 | LYS |
| 1 | A | 75 | ALA |
| 2 | D | 607 | LYS |
| 2 | D | 646 | ALA |
| 1 | B | 75 | ALA |
| 2 | E | 548 | GLY |
| 2 | E | 607 | LYS |
| 2 | E | 609 | PRO |
| 2 | E | 623 | PRO |
| 2 | E | 646 | ALA |
| 1 | C | 75 | ALA |
| 2 | F | 607 | LYS |
| 2 | F | 646 | ALA |
| 1 | A | 114 | LEU |
| 1 | A | 212 | THR |
| 2 | D | 609 | PRO |
| 2 | D | 623 | PRO |
| 1 | B | 114 | LEU |
| 1 | C | 114 | LEU |
| 2 | F | 609 | PRO |
| 2 | F | 623 | PRO |
| 2 | D | 548 | GLY |
| 1 | B | 129 | PRO |
| 1 | B | 212 | THR |
| 1 | C | 129 | PRO |
| 1 | C | 212 | THR |
| 1 | A | 129 | PRO |
| 2 | E | 536 | VAL |
| 2 | F | 536 | VAL |
| 1 | A | 39 | PRO |
| 2 | D | 536 | VAL |
| 1 | B | 39 | PRO |
| 1 | C | 39 | PRO |
| 1 | C | 164 | PRO |

5.3.2 Protein sidechains [\(i\)](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|-----------|-------------|
| 1 | A | 175/180 (97%) | 143 (82%) | 32 (18%) | 1 4 |
| 1 | B | 175/180 (97%) | 141 (81%) | 34 (19%) | 1 3 |
| 1 | C | 175/180 (97%) | 139 (79%) | 36 (21%) | 1 3 |
| 2 | D | 147/157 (94%) | 102 (69%) | 45 (31%) | 0 0 |
| 2 | E | 147/157 (94%) | 102 (69%) | 45 (31%) | 0 0 |
| 2 | F | 147/157 (94%) | 100 (68%) | 47 (32%) | 0 0 |
| All | All | 966/1011 (96%) | 727 (75%) | 239 (25%) | 0 2 |

All (239) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 37 | ARG |
| 1 | A | 40 | LEU |
| 1 | A | 43 | GLN |
| 1 | A | 47 | VAL |
| 1 | A | 53 | GLN |
| 1 | A | 64 | ILE |
| 1 | A | 68 | GLU |
| 1 | A | 78 | LEU |
| 1 | A | 80 | THR |
| 1 | A | 81 | GLU |
| 1 | A | 83 | ILE |
| 1 | A | 86 | ARG |
| 1 | A | 90 | THR |
| 1 | A | 94 | ARG |
| 1 | A | 102 | MET |
| 1 | A | 112 | ASN |
| 1 | A | 121 | LEU |
| 1 | A | 137 | LEU |
| 1 | A | 142 | VAL |
| 1 | A | 146 | ASN |
| 1 | A | 147 | ILE |
| 1 | A | 151 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 159 | VAL |
| 1 | A | 161 | GLN |
| 1 | A | 169 | GLN |
| 1 | A | 171 | LEU |
| 1 | A | 180 | GLN |
| 1 | A | 181 | ILE |
| 1 | A | 187 | GLN |
| 1 | A | 190 | MET |
| 1 | A | 197 | VAL |
| 1 | A | 213 | LEU |
| 2 | D | 505 | LYS |
| 2 | D | 507 | VAL |
| 2 | D | 509 | VAL |
| 2 | D | 511 | ASP |
| 2 | D | 516 | LYS |
| 2 | D | 519 | LEU |
| 2 | D | 522 | SER |
| 2 | D | 527 | LYS |
| 2 | D | 533 | VAL |
| 2 | D | 539 | ASN |
| 2 | D | 557 | ASP |
| 2 | D | 563 | ASP |
| 2 | D | 567 | LEU |
| 2 | D | 568 | ARG |
| 2 | D | 574 | GLN |
| 2 | D | 576 | ASP |
| 2 | D | 579 | LEU |
| 2 | D | 584 | VAL |
| 2 | D | 589 | SER |
| 2 | D | 591 | GLU |
| 2 | D | 594 | LYS |
| 2 | D | 595 | GLU |
| 2 | D | 596 | LYS |
| 2 | D | 601 | ILE |
| 2 | D | 603 | HIS |
| 2 | D | 607 | LYS |
| 2 | D | 611 | LEU |
| 2 | D | 612 | LEU |
| 2 | D | 617 | ILE |
| 2 | D | 620 | ARG |
| 2 | D | 623 | PRO |
| 2 | D | 633 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 635 | LYS |
| 2 | D | 640 | GLU |
| 2 | D | 641 | THR |
| 2 | D | 643 | GLU |
| 2 | D | 645 | LEU |
| 2 | D | 647 | ARG |
| 2 | D | 648 | ASP |
| 2 | D | 650 | LYS |
| 2 | D | 663 | ARG |
| 2 | D | 666 | LYS |
| 2 | D | 667 | ASN |
| 2 | D | 668 | VAL |
| 2 | D | 677 | LEU |
| 1 | B | 37 | ARG |
| 1 | B | 40 | LEU |
| 1 | B | 43 | GLN |
| 1 | B | 47 | VAL |
| 1 | B | 53 | GLN |
| 1 | B | 64 | ILE |
| 1 | B | 68 | GLU |
| 1 | B | 78 | LEU |
| 1 | B | 80 | THR |
| 1 | B | 81 | GLU |
| 1 | B | 83 | ILE |
| 1 | B | 86 | ARG |
| 1 | B | 90 | THR |
| 1 | B | 94 | ARG |
| 1 | B | 102 | MET |
| 1 | B | 112 | ASN |
| 1 | B | 121 | LEU |
| 1 | B | 137 | LEU |
| 1 | B | 142 | VAL |
| 1 | B | 146 | ASN |
| 1 | B | 147 | ILE |
| 1 | B | 151 | GLN |
| 1 | B | 159 | VAL |
| 1 | B | 161 | GLN |
| 1 | B | 169 | GLN |
| 1 | B | 171 | LEU |
| 1 | B | 180 | GLN |
| 1 | B | 181 | ILE |
| 1 | B | 187 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 189 | LYS |
| 1 | B | 190 | MET |
| 1 | B | 197 | VAL |
| 1 | B | 213 | LEU |
| 1 | B | 229 | HIS |
| 2 | E | 505 | LYS |
| 2 | E | 507 | VAL |
| 2 | E | 509 | VAL |
| 2 | E | 511 | ASP |
| 2 | E | 516 | LYS |
| 2 | E | 519 | LEU |
| 2 | E | 522 | SER |
| 2 | E | 527 | LYS |
| 2 | E | 533 | VAL |
| 2 | E | 539 | ASN |
| 2 | E | 557 | ASP |
| 2 | E | 563 | ASP |
| 2 | E | 566 | ARG |
| 2 | E | 567 | LEU |
| 2 | E | 574 | GLN |
| 2 | E | 576 | ASP |
| 2 | E | 579 | LEU |
| 2 | E | 584 | VAL |
| 2 | E | 589 | SER |
| 2 | E | 591 | GLU |
| 2 | E | 594 | LYS |
| 2 | E | 595 | GLU |
| 2 | E | 596 | LYS |
| 2 | E | 601 | ILE |
| 2 | E | 603 | HIS |
| 2 | E | 607 | LYS |
| 2 | E | 611 | LEU |
| 2 | E | 612 | LEU |
| 2 | E | 617 | ILE |
| 2 | E | 620 | ARG |
| 2 | E | 623 | PRO |
| 2 | E | 633 | LYS |
| 2 | E | 635 | LYS |
| 2 | E | 640 | GLU |
| 2 | E | 641 | THR |
| 2 | E | 643 | GLU |
| 2 | E | 645 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 647 | ARG |
| 2 | E | 648 | ASP |
| 2 | E | 650 | LYS |
| 2 | E | 663 | ARG |
| 2 | E | 666 | LYS |
| 2 | E | 667 | ASN |
| 2 | E | 668 | VAL |
| 2 | E | 677 | LEU |
| 1 | C | 37 | ARG |
| 1 | C | 40 | LEU |
| 1 | C | 43 | GLN |
| 1 | C | 47 | VAL |
| 1 | C | 53 | GLN |
| 1 | C | 64 | ILE |
| 1 | C | 68 | GLU |
| 1 | C | 78 | LEU |
| 1 | C | 80 | THR |
| 1 | C | 81 | GLU |
| 1 | C | 83 | ILE |
| 1 | C | 86 | ARG |
| 1 | C | 90 | THR |
| 1 | C | 94 | ARG |
| 1 | C | 102 | MET |
| 1 | C | 112 | ASN |
| 1 | C | 121 | LEU |
| 1 | C | 137 | LEU |
| 1 | C | 142 | VAL |
| 1 | C | 146 | ASN |
| 1 | C | 147 | ILE |
| 1 | C | 151 | GLN |
| 1 | C | 159 | VAL |
| 1 | C | 161 | GLN |
| 1 | C | 162 | THR |
| 1 | C | 169 | GLN |
| 1 | C | 171 | LEU |
| 1 | C | 180 | GLN |
| 1 | C | 181 | ILE |
| 1 | C | 187 | GLN |
| 1 | C | 189 | LYS |
| 1 | C | 190 | MET |
| 1 | C | 197 | VAL |
| 1 | C | 212 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 213 | LEU |
| 1 | C | 229 | HIS |
| 2 | F | 505 | LYS |
| 2 | F | 507 | VAL |
| 2 | F | 509 | VAL |
| 2 | F | 511 | ASP |
| 2 | F | 516 | LYS |
| 2 | F | 519 | LEU |
| 2 | F | 522 | SER |
| 2 | F | 527 | LYS |
| 2 | F | 533 | VAL |
| 2 | F | 539 | ASN |
| 2 | F | 557 | ASP |
| 2 | F | 563 | ASP |
| 2 | F | 566 | ARG |
| 2 | F | 567 | LEU |
| 2 | F | 568 | ARG |
| 2 | F | 574 | GLN |
| 2 | F | 576 | ASP |
| 2 | F | 579 | LEU |
| 2 | F | 584 | VAL |
| 2 | F | 589 | SER |
| 2 | F | 591 | GLU |
| 2 | F | 594 | LYS |
| 2 | F | 595 | GLU |
| 2 | F | 596 | LYS |
| 2 | F | 601 | ILE |
| 2 | F | 603 | HIS |
| 2 | F | 607 | LYS |
| 2 | F | 611 | LEU |
| 2 | F | 612 | LEU |
| 2 | F | 617 | ILE |
| 2 | F | 620 | ARG |
| 2 | F | 623 | PRO |
| 2 | F | 633 | LYS |
| 2 | F | 635 | LYS |
| 2 | F | 640 | GLU |
| 2 | F | 641 | THR |
| 2 | F | 643 | GLU |
| 2 | F | 645 | LEU |
| 2 | F | 647 | ARG |
| 2 | F | 648 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 650 | LYS |
| 2 | F | 653 | LYS |
| 2 | F | 663 | ARG |
| 2 | F | 666 | LYS |
| 2 | F | 667 | ASN |
| 2 | F | 668 | VAL |
| 2 | F | 677 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 110 | GLN |
| 1 | A | 146 | ASN |
| 1 | A | 167 | ASN |
| 1 | A | 169 | GLN |
| 1 | A | 230 | GLN |
| 2 | D | 539 | ASN |
| 2 | D | 592 | ASN |
| 2 | D | 634 | GLN |
| 1 | B | 110 | GLN |
| 1 | B | 146 | ASN |
| 1 | B | 167 | ASN |
| 1 | B | 169 | GLN |
| 1 | B | 230 | GLN |
| 2 | E | 539 | ASN |
| 2 | E | 592 | ASN |
| 2 | E | 634 | GLN |
| 2 | E | 667 | ASN |
| 1 | C | 110 | GLN |
| 1 | C | 146 | ASN |
| 1 | C | 167 | ASN |
| 1 | C | 169 | GLN |
| 1 | C | 230 | GLN |
| 2 | F | 539 | ASN |
| 2 | F | 592 | ASN |
| 2 | F | 667 | ASN |

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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 |
| 4 | GNP | F | 678 | 3 | 29,34,34 | 3.77 | 18 (62%) | 33,54,54 | 3.96 | 16 (48%) |
| 4 | GNP | E | 678 | 3 | 29,34,34 | 3.50 | 16 (55%) | 33,54,54 | 4.06 | 18 (54%) |
| 4 | GNP | D | 678 | 3 | 29,34,34 | 3.58 | 15 (51%) | 33,54,54 | 4.11 | 19 (57%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | GNP | F | 678 | 3 | - | 8/14/38/38 | 0/3/3/3 |
| 4 | GNP | E | 678 | 3 | - | 8/14/38/38 | 0/3/3/3 |
| 4 | GNP | D | 678 | 3 | - | 8/14/38/38 | 0/3/3/3 |

All (49) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | F | 678 | GNP | PB-O2B | -9.02 | 1.32 | 1.56 |
| 4 | D | 678 | GNP | PB-O2B | -8.54 | 1.33 | 1.56 |
| 4 | F | 678 | GNP | PG-O1G | 8.49 | 1.59 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | E | 678 | GNP | PB-O2B | -8.28 | 1.34 | 1.56 |
| 4 | D | 678 | GNP | C2-N1 | 8.08 | 1.49 | 1.35 |
| 4 | F | 678 | GNP | C2-N1 | 7.90 | 1.49 | 1.35 |
| 4 | E | 678 | GNP | C2-N1 | 7.35 | 1.48 | 1.35 |
| 4 | E | 678 | GNP | PG-O1G | 6.73 | 1.56 | 1.46 |
| 4 | D | 678 | GNP | PG-O1G | 6.36 | 1.56 | 1.46 |
| 4 | D | 678 | GNP | PB-N3B | 5.59 | 1.78 | 1.63 |
| 4 | F | 678 | GNP | PB-N3B | 5.51 | 1.77 | 1.63 |
| 4 | E | 678 | GNP | PB-N3B | 5.47 | 1.77 | 1.63 |
| 4 | F | 678 | GNP | PG-O2G | -4.95 | 1.43 | 1.56 |
| 4 | D | 678 | GNP | O6-C6 | 4.68 | 1.36 | 1.24 |
| 4 | D | 678 | GNP | PG-O2G | -4.67 | 1.44 | 1.56 |
| 4 | E | 678 | GNP | O6-C6 | 4.56 | 1.36 | 1.24 |
| 4 | F | 678 | GNP | O6-C6 | 4.45 | 1.35 | 1.24 |
| 4 | E | 678 | GNP | O4'-C1' | 4.36 | 1.47 | 1.41 |
| 4 | D | 678 | GNP | C2'-C1' | 4.34 | 1.60 | 1.53 |
| 4 | F | 678 | GNP | O4'-C1' | 4.30 | 1.47 | 1.41 |
| 4 | F | 678 | GNP | C2'-C1' | 4.22 | 1.60 | 1.53 |
| 4 | F | 678 | GNP | O3'-C3' | 4.22 | 1.52 | 1.43 |
| 4 | E | 678 | GNP | C2'-C1' | 4.18 | 1.60 | 1.53 |
| 4 | E | 678 | GNP | PG-O2G | -4.17 | 1.45 | 1.56 |
| 4 | D | 678 | GNP | PB-O3A | -4.04 | 1.54 | 1.59 |
| 4 | D | 678 | GNP | O4'-C1' | 3.99 | 1.46 | 1.41 |
| 4 | E | 678 | GNP | O3'-C3' | 3.91 | 1.52 | 1.43 |
| 4 | D | 678 | GNP | O3'-C3' | 3.63 | 1.51 | 1.43 |
| 4 | E | 678 | GNP | C2-N2 | -3.09 | 1.27 | 1.33 |
| 4 | D | 678 | GNP | C4-N3 | -3.08 | 1.30 | 1.35 |
| 4 | D | 678 | GNP | C2-N2 | -3.01 | 1.27 | 1.33 |
| 4 | F | 678 | GNP | C2-N2 | -3.00 | 1.27 | 1.33 |
| 4 | E | 678 | GNP | PB-O3A | -2.96 | 1.55 | 1.59 |
| 4 | D | 678 | GNP | C8-N7 | 2.94 | 1.39 | 1.34 |
| 4 | F | 678 | GNP | C4-N3 | -2.87 | 1.31 | 1.35 |
| 4 | E | 678 | GNP | C4-N3 | -2.86 | 1.31 | 1.35 |
| 4 | F | 678 | GNP | PB-O3A | -2.67 | 1.55 | 1.59 |
| 4 | F | 678 | GNP | C8-N7 | 2.63 | 1.39 | 1.34 |
| 4 | E | 678 | GNP | C8-N7 | 2.61 | 1.39 | 1.34 |
| 4 | E | 678 | GNP | C2'-C3' | 2.46 | 1.60 | 1.53 |
| 4 | E | 678 | GNP | C2-N3 | -2.42 | 1.23 | 1.34 |
| 4 | F | 678 | GNP | C2'-C3' | 2.39 | 1.59 | 1.53 |
| 4 | F | 678 | GNP | PB-O1B | 2.30 | 1.49 | 1.46 |
| 4 | D | 678 | GNP | C2'-C3' | 2.25 | 1.59 | 1.53 |
| 4 | E | 678 | GNP | O2'-C2' | 2.21 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | F | 678 | GNP | C2-N3 | -2.18 | 1.24 | 1.34 |
| 4 | F | 678 | GNP | O2'-C2' | 2.18 | 1.48 | 1.43 |
| 4 | D | 678 | GNP | C2-N3 | -2.16 | 1.25 | 1.34 |
| 4 | F | 678 | GNP | C5'-C4' | -2.03 | 1.45 | 1.51 |

All (53) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 4 | E | 678 | GNP | C4-C5-C6 | -13.20 | 108.20 | 120.80 |
| 4 | D | 678 | GNP | C4-C5-C6 | -12.43 | 108.93 | 120.80 |
| 4 | F | 678 | GNP | C4-C5-C6 | -12.36 | 109.00 | 120.80 |
| 4 | D | 678 | GNP | C2-N3-C4 | 7.98 | 124.47 | 115.36 |
| 4 | E | 678 | GNP | C2-N3-C4 | 7.84 | 124.31 | 115.36 |
| 4 | F | 678 | GNP | C2-N3-C4 | 7.72 | 124.17 | 115.36 |
| 4 | E | 678 | GNP | C4-C5-N7 | -7.66 | 101.42 | 109.40 |
| 4 | F | 678 | GNP | C4-C5-N7 | -7.41 | 101.68 | 109.40 |
| 4 | D | 678 | GNP | C4-C5-N7 | -7.35 | 101.74 | 109.40 |
| 4 | D | 678 | GNP | N2-C2-N3 | 7.26 | 129.63 | 117.79 |
| 4 | F | 678 | GNP | N2-C2-N3 | 6.96 | 129.14 | 117.79 |
| 4 | D | 678 | GNP | N3-C2-N1 | -6.87 | 118.06 | 127.22 |
| 4 | F | 678 | GNP | N3-C2-N1 | -6.75 | 118.22 | 127.22 |
| 4 | E | 678 | GNP | N2-C2-N3 | 6.67 | 128.67 | 117.79 |
| 4 | E | 678 | GNP | N3-C2-N1 | -6.30 | 118.82 | 127.22 |
| 4 | D | 678 | GNP | O3'-C3'-C4' | -5.13 | 96.21 | 111.05 |
| 4 | D | 678 | GNP | O1G-PG-N3B | -4.93 | 104.50 | 111.77 |
| 4 | E | 678 | GNP | O3'-C3'-C4' | -4.84 | 97.06 | 111.05 |
| 4 | F | 678 | GNP | O3'-C3'-C4' | -4.76 | 97.29 | 111.05 |
| 4 | E | 678 | GNP | O1G-PG-N3B | -4.66 | 104.91 | 111.77 |
| 4 | F | 678 | GNP | O3'-C3'-C2' | -4.36 | 97.73 | 111.82 |
| 4 | F | 678 | GNP | O1G-PG-N3B | -4.32 | 105.41 | 111.77 |
| 4 | D | 678 | GNP | O3G-PG-O1G | -4.16 | 102.99 | 113.45 |
| 4 | D | 678 | GNP | O3'-C3'-C2' | -4.10 | 98.57 | 111.82 |
| 4 | E | 678 | GNP | O3'-C3'-C2' | -4.04 | 98.75 | 111.82 |
| 4 | D | 678 | GNP | C2'-C3'-C4' | 3.94 | 110.29 | 102.64 |
| 4 | E | 678 | GNP | C2'-C3'-C4' | 3.94 | 110.29 | 102.64 |
| 4 | F | 678 | GNP | O3G-PG-O1G | -3.61 | 104.38 | 113.45 |
| 4 | F | 678 | GNP | C2'-C3'-C4' | 3.56 | 109.55 | 102.64 |
| 4 | E | 678 | GNP | O3G-PG-O1G | -3.43 | 104.84 | 113.45 |
| 4 | E | 678 | GNP | C5-C6-N1 | 3.21 | 127.83 | 123.43 |
| 4 | D | 678 | GNP | N2-C2-N1 | -3.18 | 112.31 | 117.25 |
| 4 | D | 678 | GNP | C5-C6-N1 | 3.10 | 127.68 | 123.43 |
| 4 | E | 678 | GNP | O2'-C2'-C1' | -3.10 | 99.42 | 110.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | E | 678 | GNP | N2-C2-N1 | -3.05 | 112.50 | 117.25 |
| 4 | D | 678 | GNP | O2'-C2'-C1' | -2.97 | 99.89 | 110.85 |
| 4 | F | 678 | GNP | N2-C2-N1 | -2.96 | 112.64 | 117.25 |
| 4 | F | 678 | GNP | O2'-C2'-C1' | -2.95 | 99.95 | 110.85 |
| 4 | F | 678 | GNP | C5-C6-N1 | 2.81 | 127.27 | 123.43 |
| 4 | D | 678 | GNP | O2G-PG-O3G | 2.79 | 115.06 | 107.64 |
| 4 | D | 678 | GNP | O2B-PB-O3A | 2.71 | 113.67 | 104.64 |
| 4 | F | 678 | GNP | O2G-PG-O1G | -2.66 | 106.77 | 113.45 |
| 4 | E | 678 | GNP | O4'-C4'-C3' | -2.65 | 99.87 | 105.11 |
| 4 | E | 678 | GNP | O2G-PG-O1G | -2.55 | 107.04 | 113.45 |
| 4 | D | 678 | GNP | O4'-C4'-C3' | -2.53 | 100.10 | 105.11 |
| 4 | F | 678 | GNP | O2A-PA-O1A | 2.45 | 124.38 | 112.24 |
| 4 | E | 678 | GNP | O2A-PA-O1A | 2.34 | 123.83 | 112.24 |
| 4 | E | 678 | GNP | O2G-PG-O3G | 2.31 | 113.80 | 107.64 |
| 4 | D | 678 | GNP | O2G-PG-O1G | -2.29 | 107.69 | 113.45 |
| 4 | D | 678 | GNP | O2A-PA-O1A | 2.25 | 123.38 | 112.24 |
| 4 | E | 678 | GNP | O3A-PB-N3B | 2.24 | 112.80 | 106.59 |
| 4 | F | 678 | GNP | O4'-C4'-C3' | -2.24 | 100.69 | 105.11 |
| 4 | D | 678 | GNP | O3A-PB-N3B | 2.08 | 112.37 | 106.59 |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 4 | D | 678 | GNP | PB-N3B-PG-O1G |
| 4 | D | 678 | GNP | PG-N3B-PB-O1B |
| 4 | D | 678 | GNP | PG-N3B-PB-O3A |
| 4 | D | 678 | GNP | C5'-O5'-PA-O2A |
| 4 | D | 678 | GNP | O4'-C4'-C5'-O5' |
| 4 | E | 678 | GNP | PB-N3B-PG-O1G |
| 4 | E | 678 | GNP | PG-N3B-PB-O1B |
| 4 | E | 678 | GNP | PG-N3B-PB-O3A |
| 4 | E | 678 | GNP | C5'-O5'-PA-O2A |
| 4 | E | 678 | GNP | O4'-C4'-C5'-O5' |
| 4 | F | 678 | GNP | PB-N3B-PG-O1G |
| 4 | F | 678 | GNP | PG-N3B-PB-O1B |
| 4 | F | 678 | GNP | PG-N3B-PB-O3A |
| 4 | F | 678 | GNP | C5'-O5'-PA-O2A |
| 4 | F | 678 | GNP | O4'-C4'-C5'-O5' |
| 4 | D | 678 | GNP | C3'-C4'-C5'-O5' |
| 4 | E | 678 | GNP | C3'-C4'-C5'-O5' |
| 4 | F | 678 | GNP | C3'-C4'-C5'-O5' |

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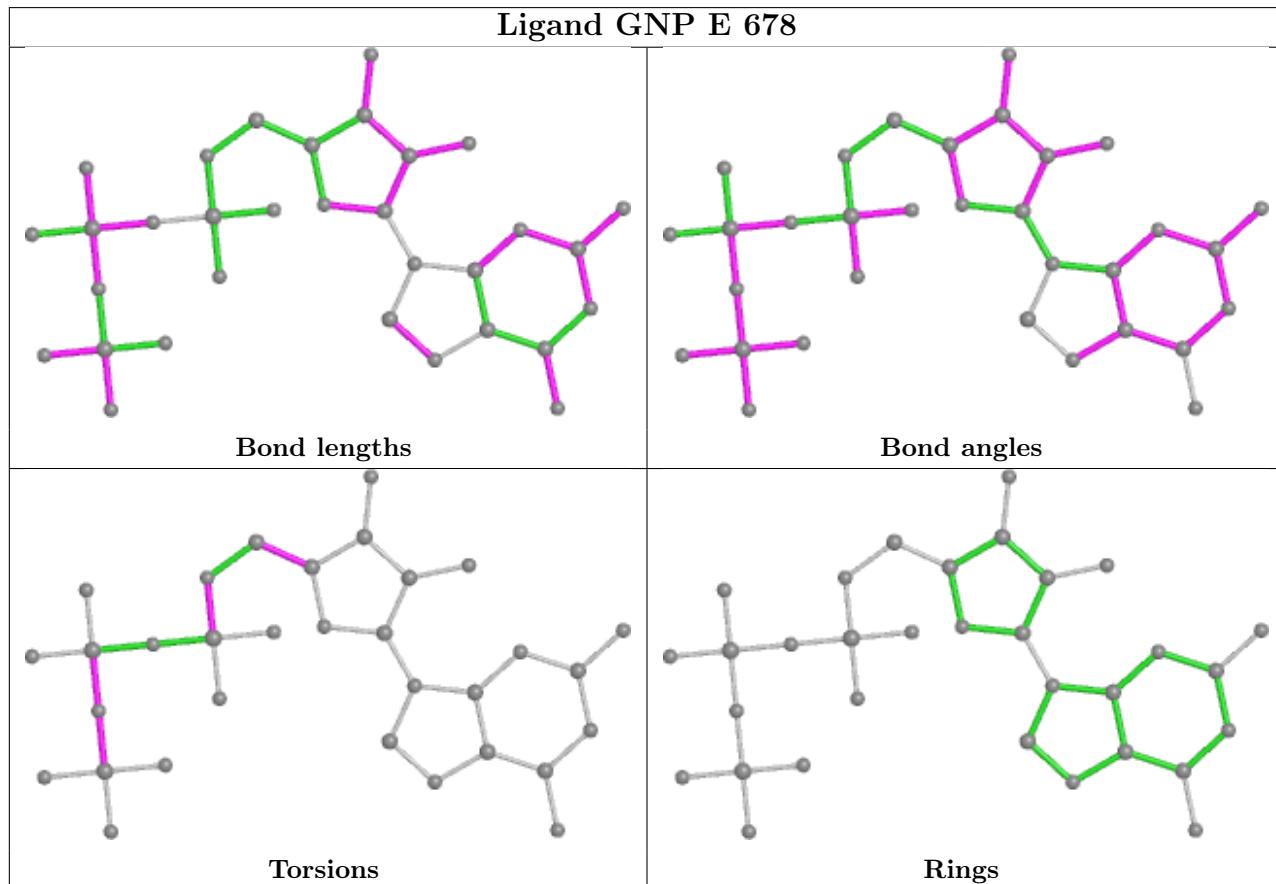
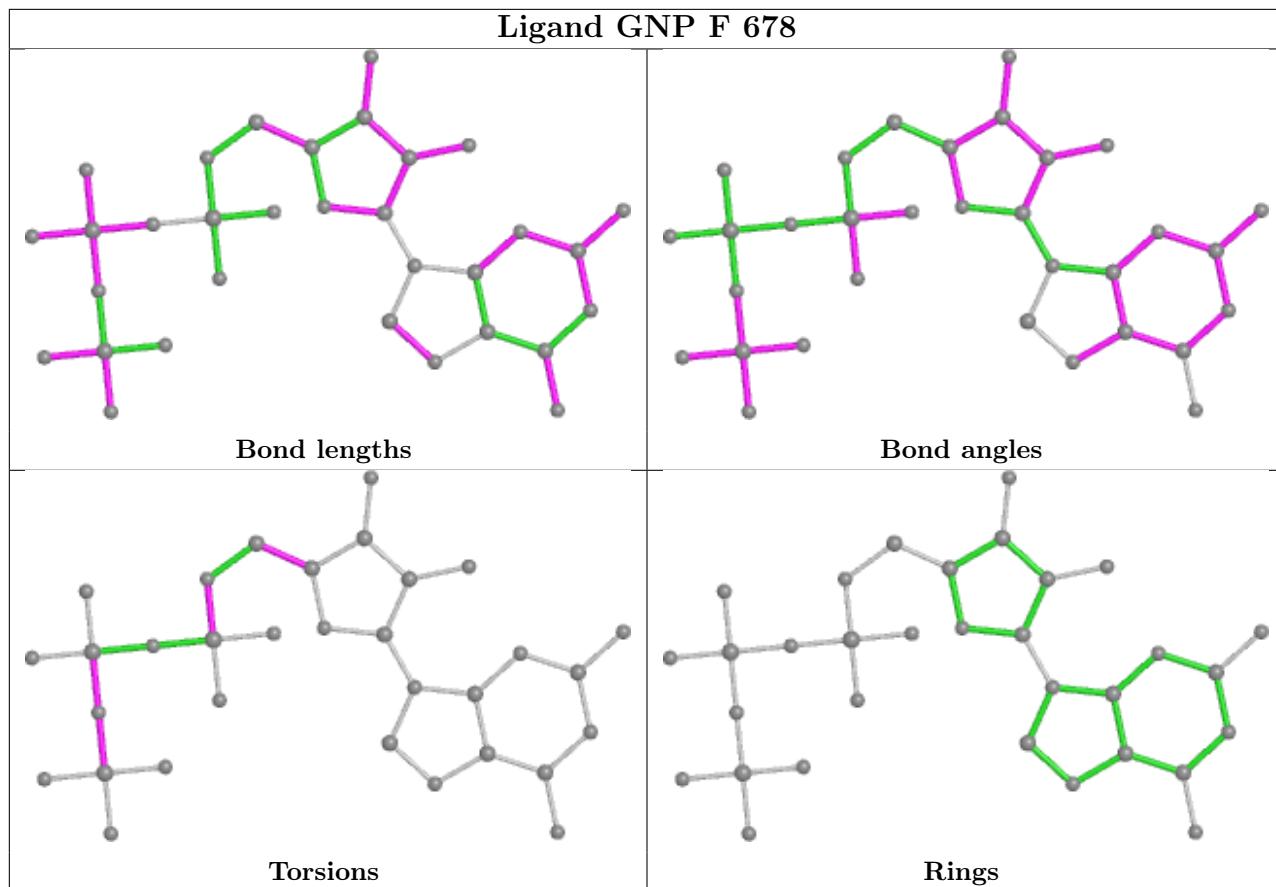
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 4 | D | 678 | GNP | C5'-O5'-PA-O3A |
| 4 | E | 678 | GNP | C5'-O5'-PA-O3A |
| 4 | F | 678 | GNP | C5'-O5'-PA-O3A |
| 4 | D | 678 | GNP | C5'-O5'-PA-O1A |
| 4 | E | 678 | GNP | C5'-O5'-PA-O1A |
| 4 | F | 678 | GNP | C5'-O5'-PA-O1A |

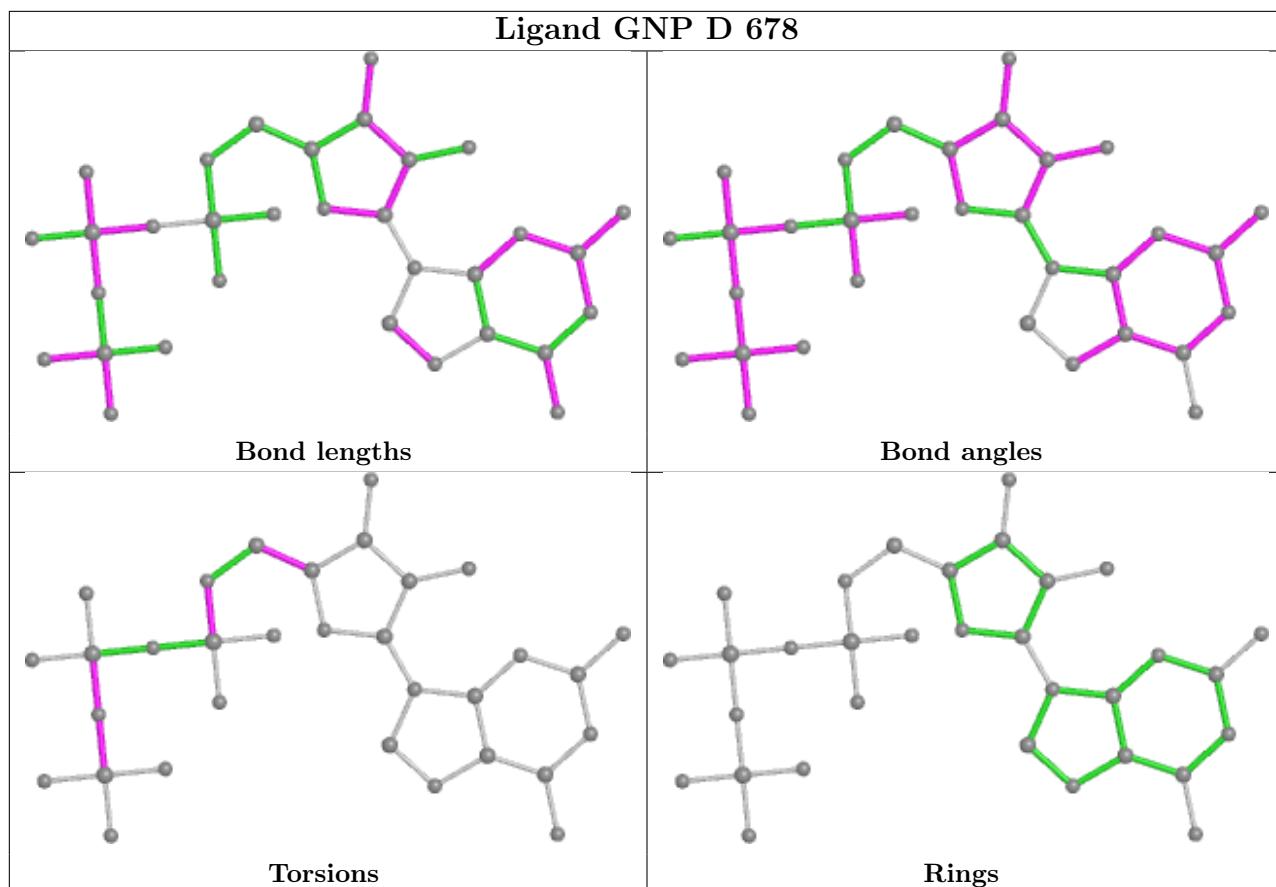
There are no ring outliers.

3 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | F | 678 | GNP | 7 | 0 |
| 4 | E | 678 | GNP | 7 | 0 |
| 4 | D | 678 | GNP | 9 | 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.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [\(i\)](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

EDS was not executed - this section is therefore empty.