



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 10:19 AM EST

PDB ID : 1C3O
Title : CRYSTAL STRUCTURE OF THE CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT MUTANT C269S WITH BOUND GLUTAMINE
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Deposited on : 1999-07-28
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.36

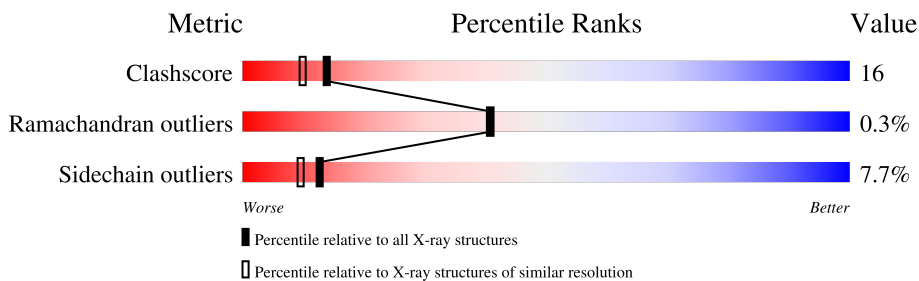
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 | 5710 (2.10-2.10) |
| Ramachandran outliers | 138981 | 5647 (2.10-2.10) |
| Sidechain outliers | 138945 | 5648 (2.10-2.10) |

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 $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1073 | |
| 1 | C | 1073 | |
| 1 | E | 1073 | |
| 1 | G | 1073 | |
| 2 | B | 382 | |
| 2 | D | 382 | |
| 2 | F | 382 | |
| 2 | H | 382 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 5 | CL | G | 4083 | - | - | X | - |

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48477 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 CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUB-UNIT.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|-----------|---------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 1058 | Total 8195 | C 5146 | N 1433 | O 1570 | S 46 | 0 | 6 | 0 |
| 1 | C | 1058 | Total 8192 | C 5144 | N 1428 | O 1575 | S 45 | 0 | 7 | 0 |
| 1 | E | 1058 | Total 8211 | C 5155 | N 1431 | O 1580 | S 45 | 0 | 10 | 0 |
| 1 | G | 1058 | Total 8180 | C 5135 | N 1425 | O 1574 | S 46 | 0 | 4 | 0 |

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUB-UNIT.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | B | 379 | Total 2895 | C 1825 | N 508 | O 553 | S 9 | 0 | 0 | 0 |
| 2 | D | 379 | Total 2895 | C 1825 | N 508 | O 553 | S 9 | 0 | 0 | 0 |
| 2 | F | 379 | Total 2895 | C 1825 | N 508 | O 553 | S 9 | 0 | 0 | 0 |
| 2 | H | 379 | Total 2895 | C 1825 | N 508 | O 553 | S 9 | 0 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 269 | SER | CYS | engineered mutation | UNP P00907 |
| D | 269 | SER | CYS | engineered mutation | UNP P00907 |
| F | 269 | SER | CYS | engineered mutation | UNP P00907 |
| H | 269 | SER | CYS | engineered mutation | UNP P00907 |

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | A | 3 | Total Mn 3 3 | 0 | 0 |
| 3 | C | 3 | Total Mn 3 3 | 0 | 0 |
| 3 | E | 3 | Total Mn 3 3 | 0 | 0 |
| 3 | G | 3 | Total Mn 3 3 | 0 | 0 |

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4 | A | 7 | Total K 7 7 | 0 | 0 |
| 4 | B | 1 | Total K 1 1 | 0 | 0 |
| 4 | C | 7 | Total K 7 7 | 0 | 0 |
| 4 | D | 1 | Total K 1 1 | 0 | 0 |
| 4 | E | 7 | Total K 7 7 | 0 | 0 |
| 4 | F | 1 | Total K 1 1 | 0 | 0 |
| 4 | G | 7 | Total K 7 7 | 0 | 0 |
| 4 | H | 1 | Total K 1 1 | 0 | 0 |

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

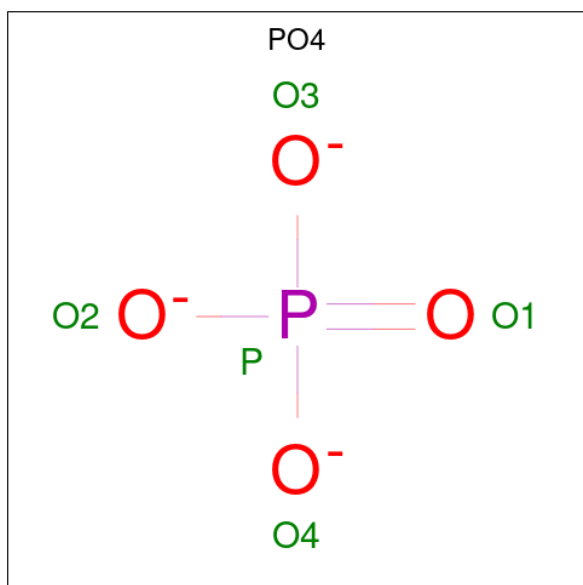
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | A | 3 | Total Cl 3 3 | 0 | 0 |
| 5 | B | 1 | Total Cl 1 1 | 0 | 0 |
| 5 | C | 3 | Total Cl 3 3 | 0 | 0 |
| 5 | D | 1 | Total Cl 1 1 | 0 | 0 |
| 5 | E | 3 | Total Cl 3 3 | 0 | 0 |
| 5 | F | 1 | Total Cl 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5 | G | 3 | Total | Cl | 0 | 0 |
| | | | 3 | 3 | | |
| 5 | H | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



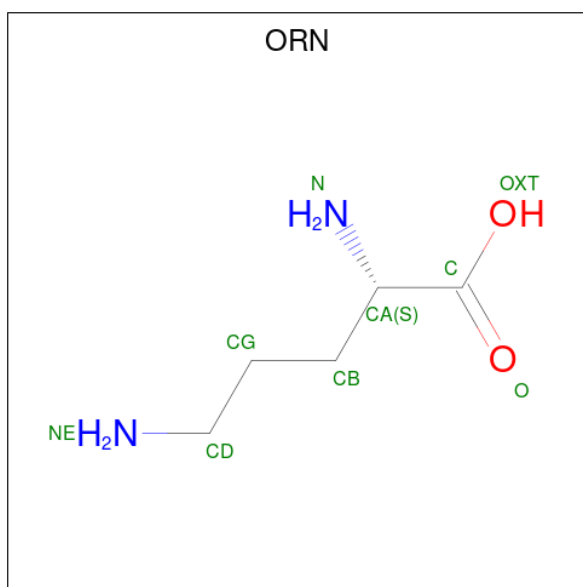
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6 | A | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 6 | C | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 6 | E | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 6 | E | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 6 | G | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



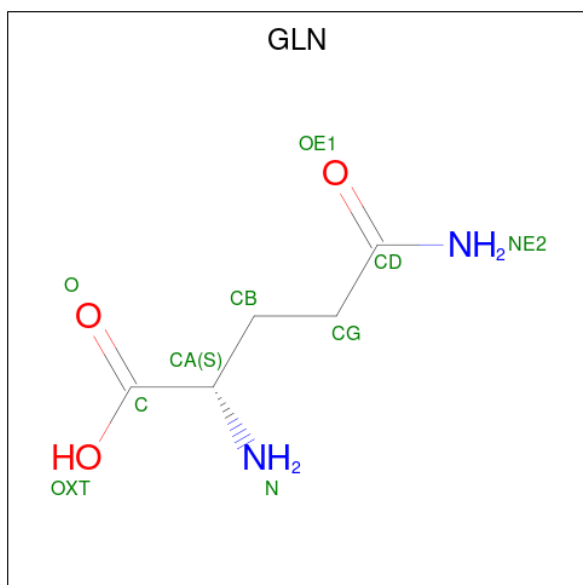
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| | | | Total | C | N | O | P | | |
| 7 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 7 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 7 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 7 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 7 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 7 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 7 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 7 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 8 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



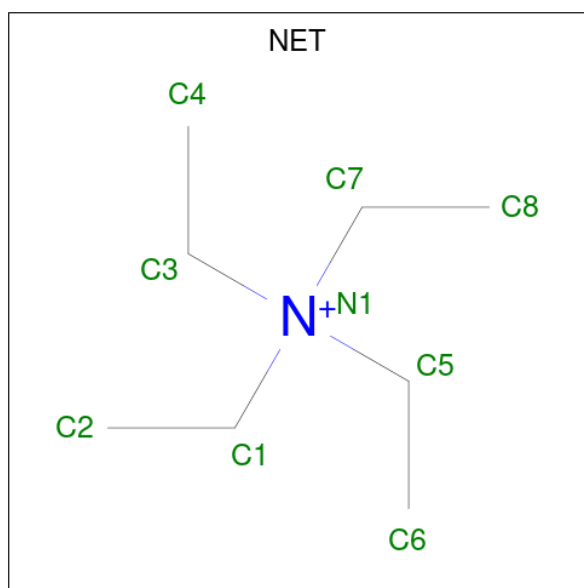
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|---|---|---|---------|---------|---|
| | | | Total | C | N | O | | | |
| 8 | A | 1 | Total | 9 | 5 | 2 | 2 | 0 | 0 |
| 8 | C | 1 | Total | 9 | 5 | 2 | 2 | 0 | 0 |
| 8 | E | 1 | Total | 9 | 5 | 2 | 2 | 0 | 0 |
| 8 | G | 1 | Total | 9 | 5 | 2 | 2 | 0 | 0 |

- Molecule 9 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 9 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |
| 9 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |
| 9 | C | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |
| 9 | D | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |
| 9 | E | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |
| 9 | F | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |
| 9 | G | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |
| 9 | H | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 2 | 3 | | |

- Molecule 10 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: C₈H₂₀N).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10 | A | 1 | Total | C | N | 0 | 0 |
| | | | 9 | 8 | 1 | | |
| 10 | C | 1 | Total | C | N | 0 | 0 |
| | | | 9 | 8 | 1 | | |
| 10 | E | 1 | Total | C | N | 0 | 0 |
| | | | 9 | 8 | 1 | | |
| 10 | G | 1 | Total | C | N | 0 | 0 |
| | | | 9 | 8 | 1 | | |

- Molecule 11 is water.

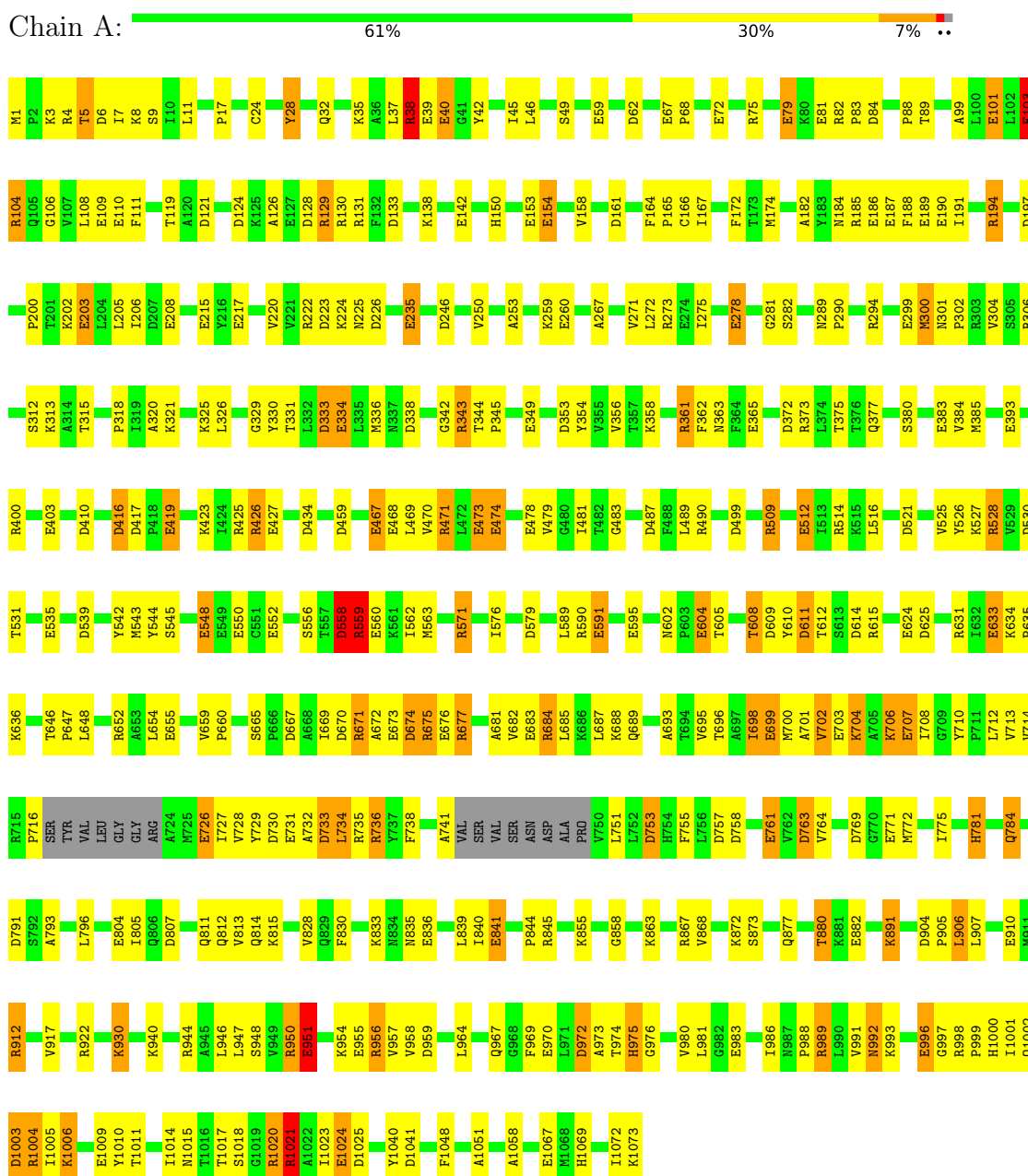
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 11 | A | 699 | Total O 699 699 | 0 | 0 |
| 11 | B | 231 | Total O 231 231 | 0 | 0 |
| 11 | C | 706 | Total O 706 706 | 0 | 0 |
| 11 | D | 250 | Total O 250 250 | 0 | 0 |
| 11 | E | 754 | Total O 754 754 | 0 | 0 |
| 11 | F | 231 | Total O 231 231 | 0 | 0 |
| 11 | G | 622 | Total O 622 622 | 0 | 0 |
| 11 | H | 173 | Total O 173 173 | 0 | 0 |

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.

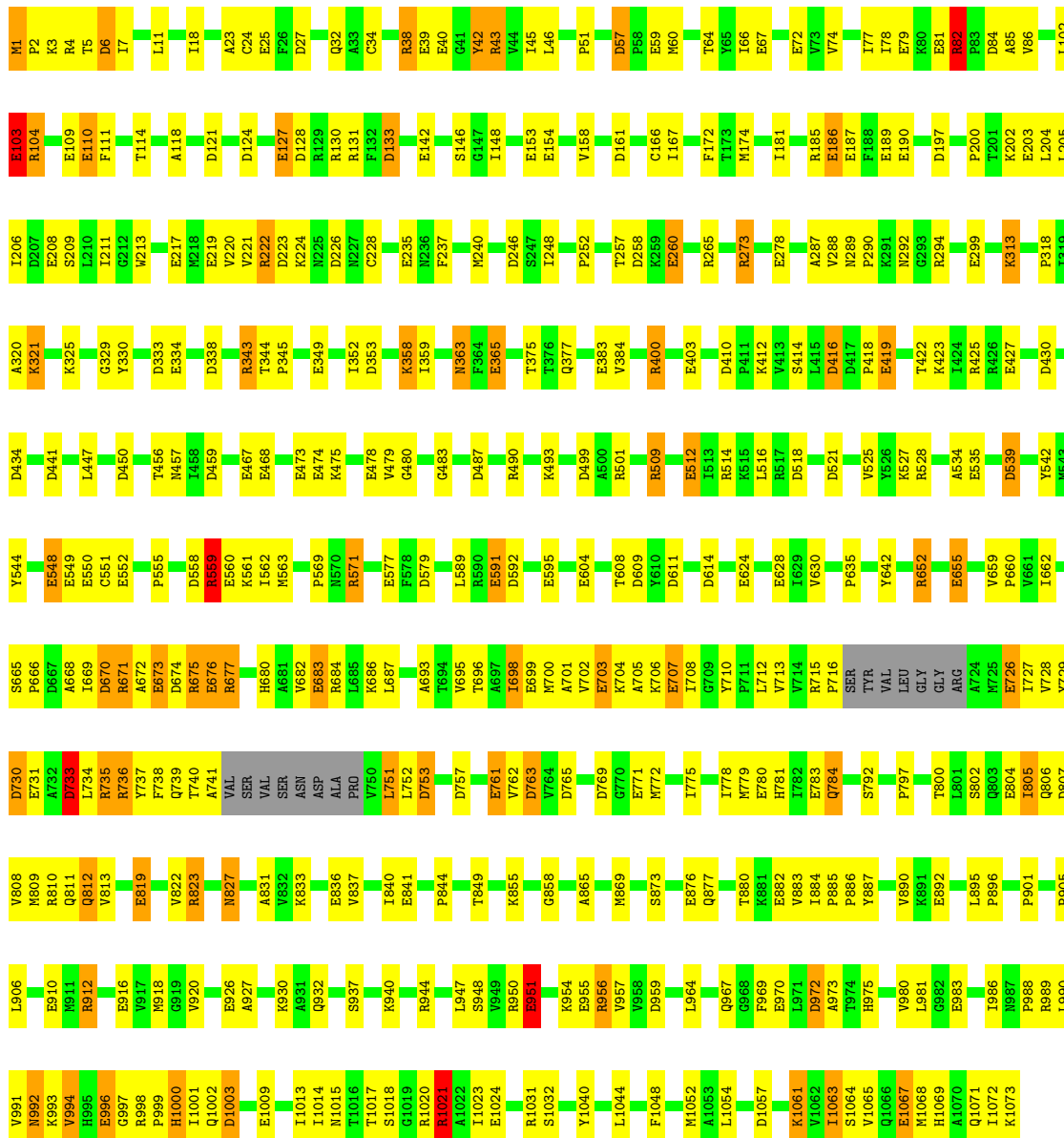
Note EDS was not executed.

- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



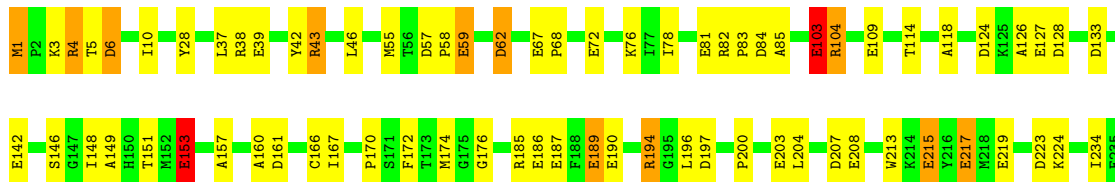
● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

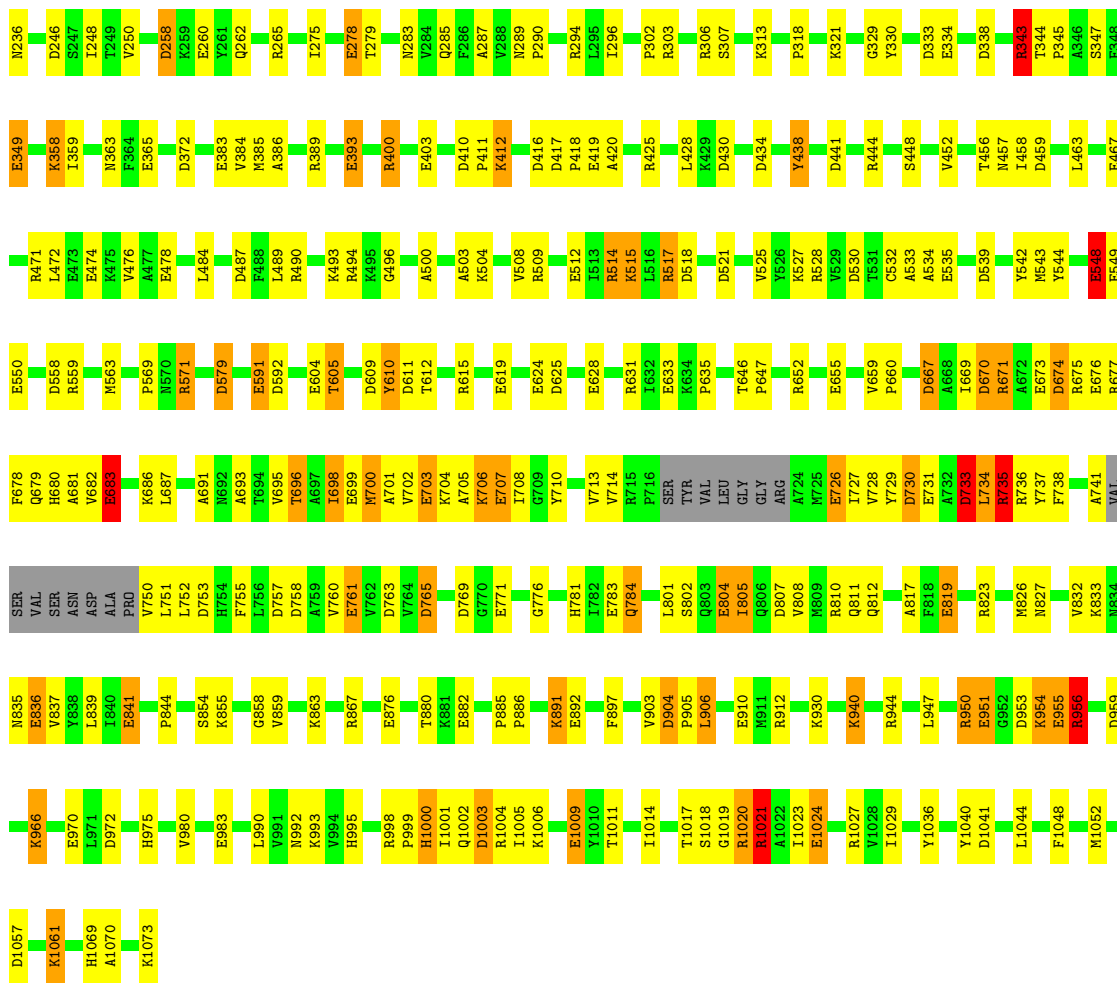
Chain C: 



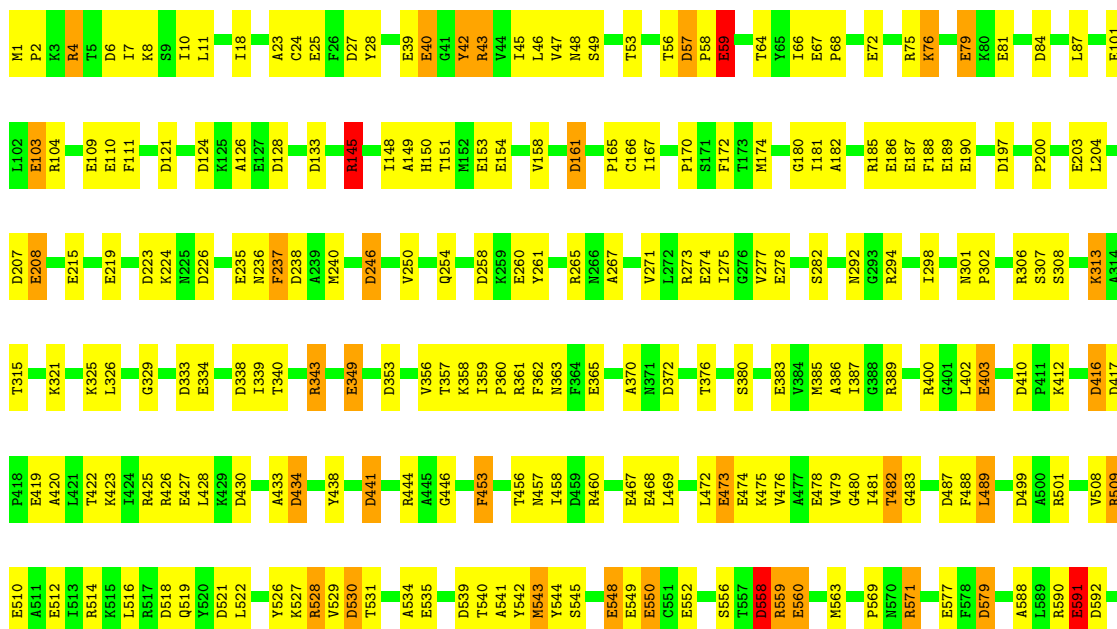
● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

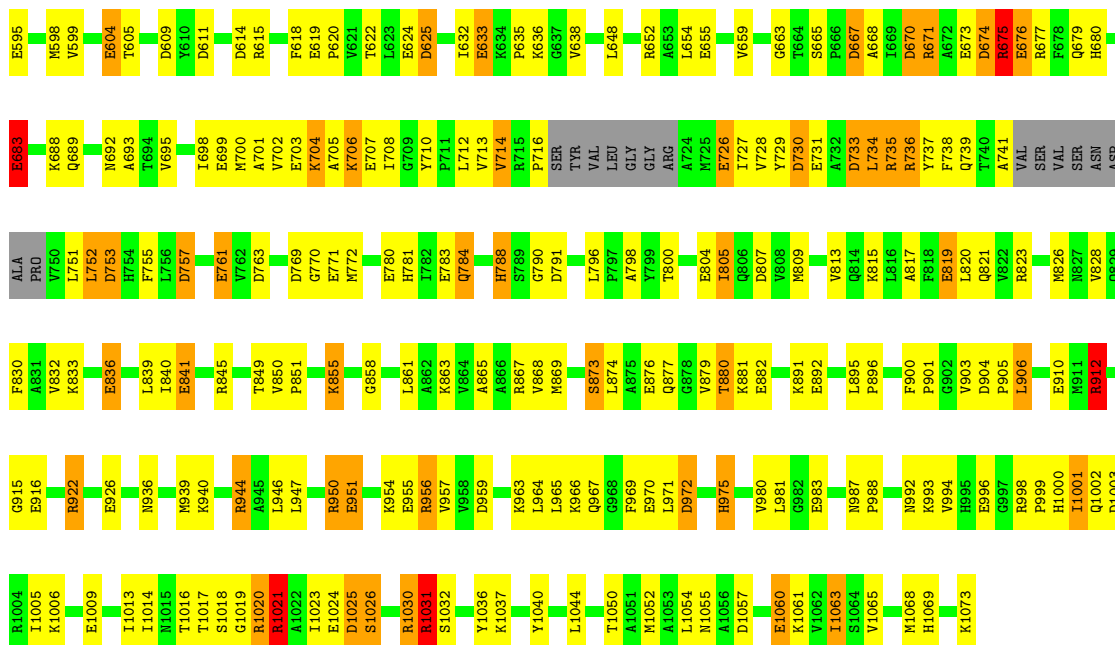
Chain E: 





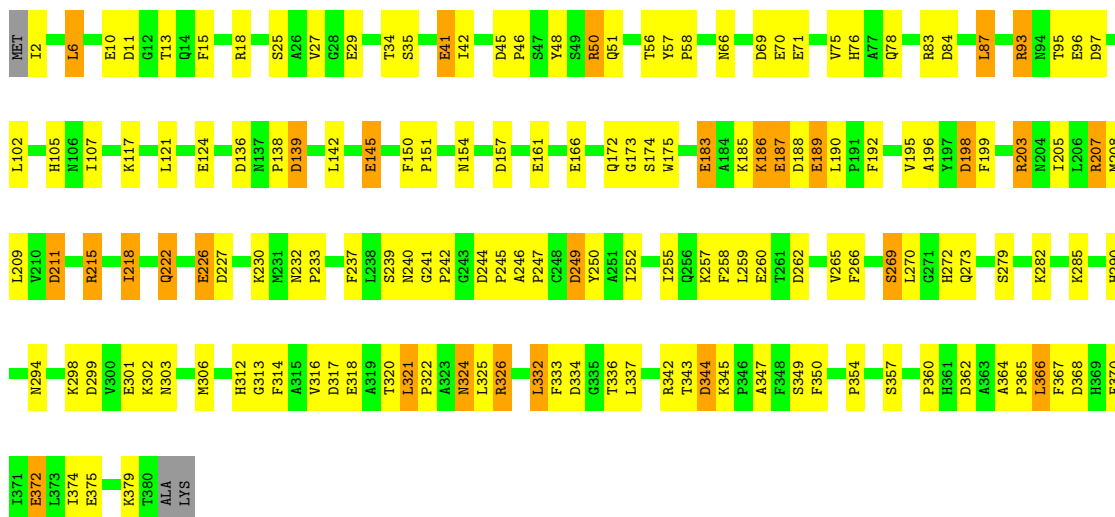
● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT





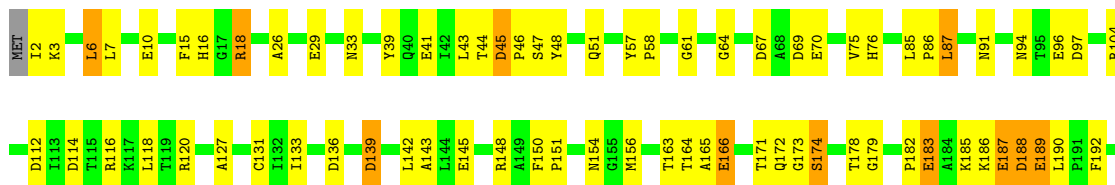
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain B: 58% 34% 7%



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

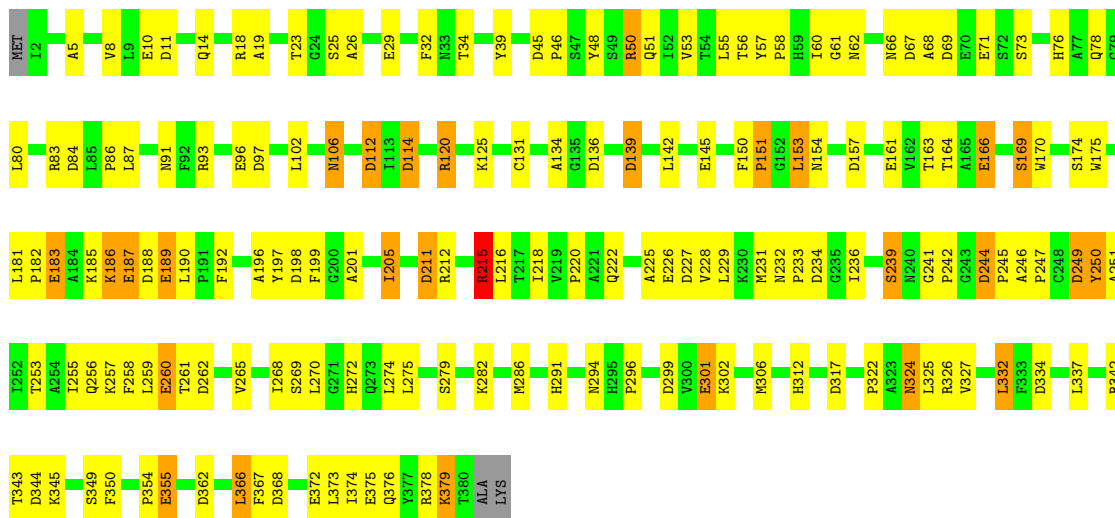
Chain D: 57% 36% 6%





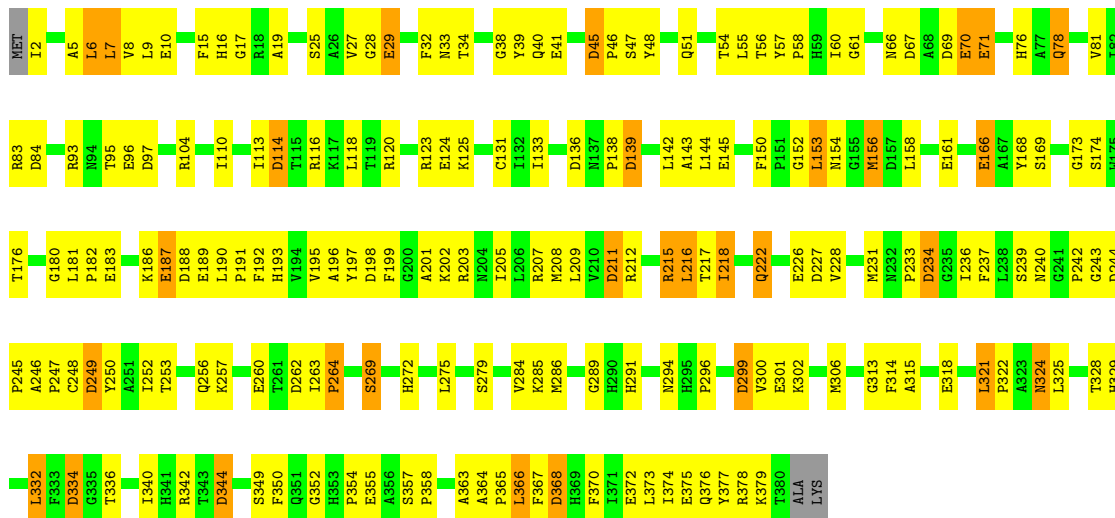
● Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain F: 55% 36% 7%



● Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 49% 42% 8%



4 Data and refinement statistics

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

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 152.50Å 164.40Å 332.60Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.10 | Depositor |
| % Data completeness (in resolution range) | 98.4 (30.00-2.10) | Depositor |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | TNT 5E | Depositor |
| R, R_{free} | 0.188 , 0.258 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| Total number of atoms | 48477 | wwPDB-VP |
| Average B, all atoms (Å ²) | 37.0 | 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: CL, NET, PO4, K, ORN, MN, ADP

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 1.04 | 72/8345 (0.9%) | 1.41 | 128/11276 (1.1%) |
| 1 | C | 1.04 | 77/8346 (0.9%) | 1.38 | 112/11281 (1.0%) |
| 1 | E | 1.05 | 68/8377 (0.8%) | 1.40 | 124/11320 (1.1%) |
| 1 | G | 1.01 | 79/8322 (0.9%) | 1.39 | 118/11249 (1.0%) |
| 2 | B | 0.90 | 18/2957 (0.6%) | 1.32 | 40/4016 (1.0%) |
| 2 | D | 0.94 | 15/2957 (0.5%) | 1.38 | 44/4016 (1.1%) |
| 2 | F | 0.92 | 15/2957 (0.5%) | 1.37 | 43/4016 (1.1%) |
| 2 | H | 0.91 | 18/2957 (0.6%) | 1.33 | 35/4016 (0.9%) |
| All | All | 1.01 | 362/45218 (0.8%) | 1.39 | 644/61190 (1.1%) |

All (362) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|--------|-------------|----------|
| 1 | C | 419[A] | GLU | CD-OE2 | -10.50 | 1.14 | 1.25 |
| 1 | C | 419[B] | GLU | CD-OE2 | -10.50 | 1.14 | 1.25 |
| 1 | C | 110 | GLU | CD-OE1 | -10.46 | 1.14 | 1.25 |
| 1 | C | 1009 | GLU | CD-OE2 | 9.29 | 1.35 | 1.25 |
| 1 | A | 109 | GLU | CD-OE2 | 8.80 | 1.35 | 1.25 |
| 1 | A | 1009 | GLU | CD-OE2 | 8.74 | 1.35 | 1.25 |
| 1 | A | 186 | GLU | CD-OE2 | 8.57 | 1.35 | 1.25 |
| 1 | C | 1024 | GLU | CD-OE2 | 8.50 | 1.34 | 1.25 |
| 1 | E | 726 | GLU | CD-OE2 | 8.30 | 1.34 | 1.25 |
| 1 | G | 951 | GLU | CD-OE2 | 8.19 | 1.34 | 1.25 |
| 2 | H | 166 | GLU | CD-OE2 | 8.01 | 1.34 | 1.25 |
| 1 | E | 910 | GLU | CD-OE2 | 7.80 | 1.34 | 1.25 |
| 2 | B | 166 | GLU | CD-OE2 | 7.78 | 1.34 | 1.25 |
| 1 | E | 804 | GLU | CD-OE2 | 7.78 | 1.34 | 1.25 |
| 1 | A | 110 | GLU | CD-OE2 | 7.72 | 1.34 | 1.25 |
| 1 | E | 72 | GLU | CD-OE2 | 7.70 | 1.34 | 1.25 |
| 2 | F | 372 | GLU | CD-OE2 | 7.68 | 1.34 | 1.25 |
| 2 | B | 372 | GLU | CD-OE2 | 7.67 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2 | D | 226 | GLU | CD-OE2 | 7.60 | 1.34 | 1.25 |
| 1 | C | 655 | GLU | CD-OE2 | 7.51 | 1.33 | 1.25 |
| 1 | G | 1009 | GLU | CD-OE2 | 7.47 | 1.33 | 1.25 |
| 2 | D | 183 | GLU | CD-OE2 | 7.41 | 1.33 | 1.25 |
| 1 | G | 512 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | G | 1024 | GLU | CD-OE2 | 7.31 | 1.33 | 1.25 |
| 1 | E | 819 | GLU | CD-OE2 | 7.30 | 1.33 | 1.25 |
| 1 | G | 215 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 1 | C | 676 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 2 | F | 166 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 1 | C | 683 | GLU | CD-OE2 | 7.27 | 1.33 | 1.25 |
| 1 | A | 217 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | E | 59 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 1 | G | 110 | GLU | CD-OE2 | 7.24 | 1.33 | 1.25 |
| 1 | A | 604 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | C | 535 | GLU | CD-OE2 | 7.21 | 1.33 | 1.25 |
| 2 | H | 70 | GLU | CD-OE2 | 7.17 | 1.33 | 1.25 |
| 2 | H | 372 | GLU | CD-OE2 | 7.16 | 1.33 | 1.25 |
| 1 | C | 703 | GLU | CD-OE2 | 7.15 | 1.33 | 1.25 |
| 2 | D | 166 | GLU | CD-OE2 | 7.14 | 1.33 | 1.25 |
| 1 | G | 699 | GLU | CD-OE2 | 7.14 | 1.33 | 1.25 |
| 1 | G | 892 | GLU | CD-OE2 | 7.13 | 1.33 | 1.25 |
| 1 | G | 707 | GLU | CD-OE2 | 7.11 | 1.33 | 1.25 |
| 1 | C | 187 | GLU | CD-OE2 | 7.08 | 1.33 | 1.25 |
| 1 | G | 676 | GLU | CD-OE2 | 7.07 | 1.33 | 1.25 |
| 1 | G | 731 | GLU | CD-OE2 | 7.07 | 1.33 | 1.25 |
| 1 | C | 876 | GLU | CD-OE2 | 7.06 | 1.33 | 1.25 |
| 1 | C | 804 | GLU | CD-OE2 | 7.02 | 1.33 | 1.25 |
| 1 | A | 703 | GLU | CD-OE2 | 7.01 | 1.33 | 1.25 |
| 1 | E | 673 | GLU | CD-OE2 | 7.00 | 1.33 | 1.25 |
| 1 | A | 512 | GLU | CD-OE2 | 7.00 | 1.33 | 1.25 |
| 1 | G | 365 | GLU | CD-OE2 | 6.99 | 1.33 | 1.25 |
| 1 | E | 1024 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 |
| 1 | A | 591 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 |
| 1 | A | 699 | GLU | CD-OE2 | 6.97 | 1.33 | 1.25 |
| 1 | A | 683 | GLU | CD-OE2 | 6.97 | 1.33 | 1.25 |
| 1 | E | 771 | GLU | CD-OE2 | 6.96 | 1.33 | 1.25 |
| 1 | A | 955 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | E | 190 | GLU | CD-OE2 | 6.93 | 1.33 | 1.25 |
| 1 | E | 761 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | G | 876 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | C | 103 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 1 | C | 726 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | A | 655 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | G | 109 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | E | 403 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 1 | C | 983 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 2 | D | 301 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | C | 467 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | A | 836 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | C | 217 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | E | 349 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 2 | F | 301 | GLU | CD-OE2 | 6.80 | 1.33 | 1.25 |
| 1 | C | 699 | GLU | CD-OE2 | 6.80 | 1.33 | 1.25 |
| 1 | A | 1067 | GLU | CD-OE2 | 6.79 | 1.33 | 1.25 |
| 1 | G | 819 | GLU | CD-OE2 | 6.76 | 1.33 | 1.25 |
| 1 | A | 153 | GLU | CD-OE2 | 6.76 | 1.33 | 1.25 |
| 2 | H | 145 | GLU | CD-OE2 | 6.74 | 1.33 | 1.25 |
| 1 | G | 510 | GLU | CD-OE2 | 6.72 | 1.33 | 1.25 |
| 2 | D | 189 | GLU | CD-OE2 | 6.70 | 1.33 | 1.25 |
| 1 | E | 676 | GLU | CD-OE2 | 6.68 | 1.33 | 1.25 |
| 1 | G | 655 | GLU | CD-OE2 | 6.66 | 1.32 | 1.25 |
| 1 | G | 334 | GLU | CD-OE2 | 6.66 | 1.32 | 1.25 |
| 1 | E | 187 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | A | 535 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | E | 619 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | C | 951 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | E | 478[A] | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | E | 478[B] | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | E | 703 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | E | 707 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | E | 217 | GLU | CD-OE2 | 6.60 | 1.32 | 1.25 |
| 1 | C | 731 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | E | 208 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | E | 683 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 2 | B | 145 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 1 | C | 59 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 2 | F | 96 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 2 | B | 187 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | C | 955 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | A | 1024 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | G | 804 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |
| 1 | G | 726 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |
| 1 | G | 79 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|--------|-------|-------------|----------|
| 1 | A | 560 | GLU | CD-OE2 | 6.47 | 1.32 | 1.25 |
| 1 | A | 676 | GLU | CD-OE2 | 6.46 | 1.32 | 1.25 |
| 2 | D | 372 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 2 | H | 29 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | C | 25 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | A | 633 | GLU | CD-OE2 | 6.44 | 1.32 | 1.25 |
| 1 | A | 707 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 2 | H | 183 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | E | 278 | GLU | CD-OE2 | 6.40 | 1.32 | 1.25 |
| 1 | G | 591 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 2 | B | 183 | GLU | CD-OE2 | 6.38 | 1.32 | 1.25 |
| 2 | H | 187 | GLU | CD-OE2 | 6.38 | 1.32 | 1.25 |
| 1 | G | 619 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 1 | G | 190 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 1 | C | 836 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | G | 683 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | E | 731 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | G | 478 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | E | 1009[A] | GLU | CD-OE2 | 6.34 | 1.32 | 1.25 |
| 1 | E | 1009[B] | GLU | CD-OE2 | 6.34 | 1.32 | 1.25 |
| 2 | B | 260 | GLU | CD-OE2 | 6.33 | 1.32 | 1.25 |
| 1 | C | 153 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | C | 761 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | G | 186 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | C | 219 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | E | 951 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 2 | D | 41 | GLU | CD-OE2 | 6.31 | 1.32 | 1.25 |
| 1 | G | 419 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 2 | D | 145 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 1 | A | 81 | GLU | CD-OE2 | 6.29 | 1.32 | 1.25 |
| 1 | A | 365 | GLU | CD-OE2 | 6.27 | 1.32 | 1.25 |
| 2 | D | 355 | GLU | CD-OE2 | 6.27 | 1.32 | 1.25 |
| 1 | A | 478 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | E | 955 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 2 | F | 189 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | C | 771 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | A | 882 | GLU | CD-OE2 | 6.25 | 1.32 | 1.25 |
| 1 | G | 703 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 2 | B | 161 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 1 | G | 154 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 1 | A | 624 | GLU | CD-OE1 | -6.22 | 1.18 | 1.25 |
| 1 | E | 260 | GLU | CD-OE2 | 6.22 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 2 | H | 226 | GLU | CD-OE2 | 6.22 | 1.32 | 1.25 |
| 1 | A | 910 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |
| 1 | G | 474 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |
| 1 | A | 726 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | E | 699 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | C | 1067 | GLU | CD-OE2 | 6.17 | 1.32 | 1.25 |
| 1 | G | 549 | GLU | CD-OE2 | 6.17 | 1.32 | 1.25 |
| 2 | F | 226 | GLU | CD-OE2 | 6.17 | 1.32 | 1.25 |
| 1 | C | 474 | GLU | CD-OE2 | 6.17 | 1.32 | 1.25 |
| 1 | C | 970 | GLU | CD-OE2 | 6.17 | 1.32 | 1.25 |
| 1 | E | 983 | GLU | CD-OE2 | 6.16 | 1.32 | 1.25 |
| 2 | H | 301 | GLU | CD-OE2 | 6.16 | 1.32 | 1.25 |
| 1 | A | 624 | GLU | CD-OE2 | 6.15 | 1.32 | 1.25 |
| 1 | A | 39 | GLU | CD-OE2 | 6.15 | 1.32 | 1.25 |
| 1 | E | 365 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 1 | E | 836 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | G | 783 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | A | 208 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | E | 655[A] | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | E | 655[B] | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 2 | F | 145 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 2 | B | 70 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 2 | H | 71 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | C | 512 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | G | 624 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | C | 996 | GLU | CD-OE2 | 6.11 | 1.32 | 1.25 |
| 1 | E | 467 | GLU | CD-OE2 | 6.11 | 1.32 | 1.25 |
| 2 | B | 226 | GLU | CD-OE2 | 6.10 | 1.32 | 1.25 |
| 1 | C | 628 | GLU | CD-OE2 | 6.09 | 1.32 | 1.25 |
| 2 | H | 10 | GLU | CD-OE2 | 6.08 | 1.32 | 1.25 |
| 1 | A | 72 | GLU | CD-OE2 | 6.08 | 1.32 | 1.25 |
| 1 | C | 190 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 1 | G | 349 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 1 | C | 349 | GLU | CD-OE2 | 6.06 | 1.32 | 1.25 |
| 1 | A | 299 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 2 | B | 318 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | A | 190 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | C | 473 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 2 | B | 301 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | G | 633 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | G | 278 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | E | 189 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 467 | GLU | CD-OE2 | 6.01 | 1.32 | 1.25 |
| 1 | E | 334 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | C | 203 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | C | 819 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | C | 550 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | C | 882 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | C | 624 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | G | 103 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | E | 76 | LYS | CE-NZ | -5.98 | 1.34 | 1.49 |
| 1 | E | 876 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | C | 926 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 2 | F | 187 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | E | 970 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | E | 103 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | C | 109 | GLU | CD-OE2 | 5.95 | 1.32 | 1.25 |
| 1 | A | 299 | GLU | CD-OE1 | -5.94 | 1.19 | 1.25 |
| 1 | G | 153 | GLU | CD-OE2 | 5.94 | 1.32 | 1.25 |
| 1 | A | 59 | GLU | CD-OE2 | 5.93 | 1.32 | 1.25 |
| 1 | A | 673 | GLU | CD-OE2 | 5.92 | 1.32 | 1.25 |
| 1 | G | 983 | GLU | CD-OE2 | 5.92 | 1.32 | 1.25 |
| 1 | G | 595 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | A | 951 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 2 | D | 70 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | G | 761 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | A | 187 | GLU | CD-OE2 | 5.90 | 1.32 | 1.25 |
| 1 | E | 127 | GLU | CD-OE2 | 5.90 | 1.32 | 1.25 |
| 1 | A | 154 | GLU | CD-OE2 | 5.89 | 1.32 | 1.25 |
| 1 | C | 478 | GLU | CD-OE2 | 5.89 | 1.32 | 1.25 |
| 1 | E | 186 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | A | 334 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | E | 783 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | G | 836 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | G | 427 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | E | 512 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 2 | F | 71 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | C | 673 | GLU | CD-OE2 | 5.86 | 1.32 | 1.25 |
| 1 | C | 427 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | A | 731 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | C | 39 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | A | 970 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | E | 549 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | C | 72 | GLU | CD-OE2 | 5.81 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1 | C | 186 | GLU | CD-OE2 | 5.81 | 1.32 | 1.25 |
| 1 | G | 916 | GLU | CD-OE2 | 5.81 | 1.32 | 1.25 |
| 2 | H | 260 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | G | 473[A] | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | G | 473[B] | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | C | 560 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | G | 189 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | G | 560 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | A | 550 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | C | 910 | GLU | CD-OE2 | 5.77 | 1.31 | 1.25 |
| 1 | G | 604 | GLU | CD-OE2 | 5.77 | 1.31 | 1.25 |
| 2 | F | 375 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | E | 419 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | G | 970 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | G | 841 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | C | 79 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | C | 591 | GLU | CD-OE2 | 5.73 | 1.31 | 1.25 |
| 2 | H | 161 | GLU | CD-OE2 | 5.73 | 1.31 | 1.25 |
| 1 | A | 761 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | C | 916 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | E | 628 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | A | 474 | GLU | CD-OE2 | 5.70 | 1.31 | 1.25 |
| 1 | G | 208 | GLU | CD-OE2 | 5.70 | 1.31 | 1.25 |
| 1 | E | 393 | GLU | CD-OE2 | 5.69 | 1.31 | 1.25 |
| 1 | G | 910 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | C | 278 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | E | 215 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | G | 468 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 2 | B | 189 | GLU | CD-OE2 | 5.67 | 1.31 | 1.25 |
| 1 | A | 419 | GLU | CD-OE2 | 5.66 | 1.31 | 1.25 |
| 2 | F | 355 | GLU | CD-OE1 | -5.65 | 1.19 | 1.25 |
| 1 | E | 841 | GLU | CD-OE2 | 5.64 | 1.31 | 1.25 |
| 1 | A | 79 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | A | 771 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | A | 40 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | E | 624 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | A | 142 | GLU | CD-OE2 | 5.62 | 1.31 | 1.25 |
| 1 | G | 996 | GLU | CD-OE2 | 5.62 | 1.31 | 1.25 |
| 1 | A | 403 | GLU | CD-OE1 | -5.62 | 1.19 | 1.25 |
| 1 | G | 403 | GLU | CD-OE2 | 5.61 | 1.31 | 1.25 |
| 1 | E | 591 | GLU | CD-OE2 | 5.60 | 1.31 | 1.25 |
| 2 | D | 375 | GLU | CD-OE2 | 5.59 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 40 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 2 | H | 375 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 2 | B | 29 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | A | 393 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | C | 468 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 2 | D | 187 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 2 | B | 124 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | G | 219 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | C | 189 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | G | 926 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | E | 550 | GLU | CD-OE1 | -5.53 | 1.19 | 1.25 |
| 1 | C | 403 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | E | 548 | GLU | CD-OE1 | -5.51 | 1.19 | 1.25 |
| 2 | B | 96 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 2 | H | 96 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | A | 278 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | C | 67 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | C | 235 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | A | 804 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | E | 189 | GLU | CD-OE1 | -5.44 | 1.19 | 1.25 |
| 1 | C | 549 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | E | 203 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 2 | F | 10 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 1 | G | 59 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 1 | E | 474 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 2 | B | 375 | GLU | CD-OE2 | 5.41 | 1.31 | 1.25 |
| 1 | E | 219 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | G | 535 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | E | 39 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | A | 552 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | E | 109 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | G | 260 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | G | 955 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 2 | D | 29 | GLU | CD-OE2 | 5.36 | 1.31 | 1.25 |
| 2 | H | 318 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | E | 535 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | G | 673 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | C | 383 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | A | 996 | GLU | CD-OE2 | 5.31 | 1.31 | 1.25 |
| 1 | C | 142 | GLU | CD-OE2 | 5.30 | 1.31 | 1.25 |
| 2 | B | 10 | GLU | CD-OE2 | 5.30 | 1.31 | 1.25 |
| 1 | G | 550 | GLU | CD-OE2 | 5.29 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 2 | H | 41 | GLU | CD-OE2 | 5.29 | 1.31 | 1.25 |
| 1 | A | 427 | GLU | CD-OE2 | 5.29 | 1.31 | 1.25 |
| 1 | C | 577 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | C | 208 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | G | 577 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | E | 142 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | C | 783 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 2 | H | 124 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | G | 72 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 1 | G | 1060 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 1 | A | 189 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | A | 473 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | G | 187 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | C | 127 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | E | 403 | GLU | CD-OE1 | -5.24 | 1.19 | 1.25 |
| 1 | C | 595 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | G | 235 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | G | 771 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 2 | D | 96 | GLU | CD-OE2 | 5.23 | 1.31 | 1.25 |
| 1 | A | 841 | GLU | CD-OE2 | 5.23 | 1.31 | 1.25 |
| 1 | G | 39 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 2 | F | 260 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | A | 595 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | C | 260 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | A | 468 | GLU | CD-OE2 | 5.19 | 1.31 | 1.25 |
| 1 | A | 103 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 |
| 1 | A | 215 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | G | 552 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | E | 153[A] | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | E | 153[B] | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | A | 203 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | A | 101 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | C | 334 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 2 | F | 183 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | A | 235 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | G | 383 | GLU | CD-OE1 | -5.09 | 1.20 | 1.25 |
| 1 | G | 25 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | C | 707 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | C | 548 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 2 | D | 10 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | A | 260 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | C | 780 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 274 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 2 | B | 41 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | A | 983 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | A | 467 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | C | 235 | GLU | CD-OE1 | -5.01 | 1.20 | 1.25 |
| 1 | C | 552 | GLU | CD-OE1 | -5.01 | 1.20 | 1.25 |
| 1 | G | 101 | GLU | CD-OE2 | 5.00 | 1.31 | 1.25 |
| 2 | F | 161 | GLU | CD-OE2 | 5.00 | 1.31 | 1.25 |

All (644) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|--------|-------------|----------|
| 1 | A | 514 | ARG | NE-CZ-NH2 | -12.65 | 113.97 | 120.30 |
| 1 | G | 75 | ARG | NE-CZ-NH2 | -12.58 | 114.01 | 120.30 |
| 1 | G | 265 | ARG | NE-CZ-NH1 | 12.54 | 126.57 | 120.30 |
| 2 | D | 120 | ARG | NE-CZ-NH1 | 12.14 | 126.37 | 120.30 |
| 1 | E | 343 | ARG | NE-CZ-NH1 | 11.54 | 126.07 | 120.30 |
| 1 | G | 261 | TYR | CB-CG-CD2 | -10.78 | 114.53 | 121.00 |
| 1 | C | 223 | ASP | CB-CG-OD2 | -10.65 | 108.72 | 118.30 |
| 2 | B | 211 | ASP | CB-CG-OD2 | -10.18 | 109.14 | 118.30 |
| 1 | A | 223 | ASP | CB-CG-OD2 | -10.15 | 109.16 | 118.30 |
| 1 | A | 944 | ARG | NE-CZ-NH1 | 9.84 | 125.22 | 120.30 |
| 1 | E | 753 | ASP | CB-CG-OD2 | -9.78 | 109.50 | 118.30 |
| 1 | C | 736 | ARG | NE-CZ-NH1 | 9.53 | 125.06 | 120.30 |
| 1 | E | 514 | ARG | NE-CZ-NH2 | -9.48 | 115.56 | 120.30 |
| 1 | C | 490[A] | ARG | NE-CZ-NH1 | 9.47 | 125.04 | 120.30 |
| 1 | C | 490[B] | ARG | NE-CZ-NH1 | 9.47 | 125.04 | 120.30 |
| 1 | G | 75 | ARG | NE-CZ-NH1 | 9.36 | 124.98 | 120.30 |
| 1 | A | 194 | ARG | NE-CZ-NH2 | -9.15 | 115.72 | 120.30 |
| 2 | F | 97 | ASP | CB-CG-OD2 | -9.12 | 110.09 | 118.30 |
| 1 | G | 223 | ASP | CB-CG-OD2 | -9.11 | 110.10 | 118.30 |
| 2 | F | 67 | ASP | CB-CG-OD2 | -9.10 | 110.11 | 118.30 |
| 2 | H | 334 | ASP | CB-CG-OD2 | -9.00 | 110.20 | 118.30 |
| 1 | A | 1003 | ASP | CB-CG-OD2 | -8.96 | 110.23 | 118.30 |
| 1 | E | 494 | ARG | NE-CZ-NH1 | 8.95 | 124.78 | 120.30 |
| 2 | D | 334 | ASP | CB-CG-OD2 | -8.93 | 110.27 | 118.30 |
| 2 | D | 207 | ARG | NE-CZ-NH1 | 8.84 | 124.72 | 120.30 |
| 1 | A | 129 | ARG | NE-CZ-NH1 | 8.80 | 124.70 | 120.30 |
| 1 | E | 38 | ARG | NE-CZ-NH1 | 8.79 | 124.70 | 120.30 |
| 1 | C | 521 | ASP | CB-CG-OD1 | 8.75 | 126.18 | 118.30 |
| 1 | E | 904 | ASP | CB-CG-OD2 | -8.69 | 110.48 | 118.30 |
| 2 | H | 45 | ASP | CB-CG-OD1 | 8.65 | 126.08 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 368 | ASP | CB-CG-OD2 | -8.62 | 110.54 | 118.30 |
| 1 | A | 514 | ARG | NE-CZ-NH1 | 8.60 | 124.60 | 120.30 |
| 1 | C | 131 | ARG | NE-CZ-NH1 | 8.60 | 124.60 | 120.30 |
| 1 | C | 956 | ARG | NE-CZ-NH2 | -8.58 | 116.01 | 120.30 |
| 1 | G | 261 | TYR | CB-CG-CD1 | 8.57 | 126.14 | 121.00 |
| 1 | A | 867 | ARG | NE-CZ-NH1 | 8.56 | 124.58 | 120.30 |
| 1 | E | 197 | ASP | CB-CG-OD2 | -8.56 | 110.60 | 118.30 |
| 1 | C | 501 | ARG | NE-CZ-NH1 | 8.51 | 124.55 | 120.30 |
| 1 | E | 38 | ARG | NE-CZ-NH2 | -8.51 | 116.05 | 120.30 |
| 2 | H | 368 | ASP | CB-CG-OD2 | -8.50 | 110.65 | 118.30 |
| 1 | G | 333 | ASP | CB-CG-OD2 | -8.49 | 110.66 | 118.30 |
| 1 | E | 609 | ASP | CB-CG-OD2 | -8.47 | 110.68 | 118.30 |
| 1 | G | 161 | ASP | CB-CG-OD2 | -8.43 | 110.71 | 118.30 |
| 1 | E | 333 | ASP | CB-CG-OD1 | 8.41 | 125.87 | 118.30 |
| 1 | C | 972 | ASP | CB-CG-OD1 | 8.39 | 125.85 | 118.30 |
| 1 | C | 121 | ASP | CB-CG-OD1 | 8.35 | 125.82 | 118.30 |
| 1 | G | 614 | ASP | CB-CG-OD2 | -8.33 | 110.80 | 118.30 |
| 1 | E | 670 | ASP | CB-CG-OD2 | -8.31 | 110.82 | 118.30 |
| 1 | A | 124 | ASP | CB-CG-OD2 | -8.27 | 110.86 | 118.30 |
| 1 | C | 670 | ASP | CB-CG-OD2 | -8.27 | 110.86 | 118.30 |
| 1 | A | 904 | ASP | CB-CG-OD2 | -8.22 | 110.90 | 118.30 |
| 1 | C | 972 | ASP | CB-CG-OD2 | -8.20 | 110.92 | 118.30 |
| 1 | G | 667 | ASP | CB-CG-OD2 | -8.20 | 110.92 | 118.30 |
| 2 | F | 139 | ASP | CB-CG-OD2 | -8.20 | 110.92 | 118.30 |
| 1 | G | 609 | ASP | CB-CG-OD2 | -8.19 | 110.93 | 118.30 |
| 2 | D | 215 | ARG | NE-CZ-NH1 | 8.17 | 124.39 | 120.30 |
| 1 | C | 959 | ASP | CB-CG-OD2 | -8.17 | 110.95 | 118.30 |
| 2 | F | 139 | ASP | CB-CG-OD1 | 8.16 | 125.65 | 118.30 |
| 1 | C | 441 | ASP | CB-CG-OD2 | -8.14 | 110.97 | 118.30 |
| 1 | C | 501 | ARG | NE-CZ-NH2 | -8.13 | 116.24 | 120.30 |
| 1 | E | 43 | ARG | NE-CZ-NH2 | -8.11 | 116.25 | 120.30 |
| 1 | G | 460 | ARG | NE-CZ-NH1 | 8.09 | 124.35 | 120.30 |
| 2 | D | 18 | ARG | NE-CZ-NH2 | -8.07 | 116.26 | 120.30 |
| 1 | C | 6 | ASP | CB-CG-OD2 | -8.06 | 111.05 | 118.30 |
| 1 | E | 372 | ASP | CB-CG-OD2 | -8.01 | 111.09 | 118.30 |
| 1 | E | 104 | ARG | NE-CZ-NH1 | 7.95 | 124.28 | 120.30 |
| 1 | A | 867 | ARG | NE-CZ-NH2 | -7.94 | 116.33 | 120.30 |
| 1 | G | 57 | ASP | CB-CG-OD1 | 7.93 | 125.44 | 118.30 |
| 2 | F | 317 | ASP | CB-CG-OD2 | -7.90 | 111.19 | 118.30 |
| 1 | G | 434 | ASP | CB-CG-OD2 | -7.90 | 111.19 | 118.30 |
| 1 | G | 609 | ASP | CB-CG-OD1 | 7.88 | 125.39 | 118.30 |
| 1 | E | 625 | ASP | CB-CG-OD1 | 7.84 | 125.35 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 823 | ARG | NE-CZ-NH1 | 7.82 | 124.21 | 120.30 |
| 2 | F | 368 | ASP | CB-CG-OD2 | -7.81 | 111.27 | 118.30 |
| 1 | E | 410 | ASP | CB-CG-OD1 | 7.80 | 125.32 | 118.30 |
| 1 | E | 625 | ASP | CB-CG-OD2 | -7.75 | 111.32 | 118.30 |
| 1 | A | 128 | ASP | CB-CG-OD2 | -7.75 | 111.32 | 118.30 |
| 1 | G | 1030 | ARG | NE-CZ-NH2 | -7.71 | 116.44 | 120.30 |
| 2 | B | 249 | ASP | CB-CG-OD2 | -7.71 | 111.37 | 118.30 |
| 1 | E | 444 | ARG | NE-CZ-NH1 | 7.70 | 124.15 | 120.30 |
| 1 | A | 670 | ASP | CB-CG-OD2 | -7.69 | 111.38 | 118.30 |
| 1 | A | 197 | ASP | CB-CG-OD2 | -7.69 | 111.38 | 118.30 |
| 1 | C | 27 | ASP | CB-CG-OD1 | 7.67 | 125.21 | 118.30 |
| 1 | A | 246 | ASP | CB-CG-OD2 | -7.67 | 111.40 | 118.30 |
| 1 | G | 944 | ARG | NE-CZ-NH1 | 7.64 | 124.12 | 120.30 |
| 1 | G | 124 | ASP | CB-CG-OD1 | 7.64 | 125.18 | 118.30 |
| 1 | A | 539 | ASP | CB-CG-OD2 | -7.62 | 111.44 | 118.30 |
| 1 | G | 410 | ASP | CB-CG-OD2 | -7.61 | 111.45 | 118.30 |
| 1 | C | 528 | ARG | NE-CZ-NH1 | 7.58 | 124.09 | 120.30 |
| 2 | H | 97 | ASP | CB-CG-OD2 | -7.58 | 111.48 | 118.30 |
| 1 | G | 333 | ASP | CB-CG-OD1 | 7.56 | 125.11 | 118.30 |
| 1 | A | 1021 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |
| 1 | A | 959 | ASP | CB-CG-OD2 | -7.55 | 111.50 | 118.30 |
| 1 | A | 611 | ASP | CB-CG-OD1 | 7.55 | 125.10 | 118.30 |
| 2 | B | 362 | ASP | CB-CG-OD2 | -7.54 | 111.51 | 118.30 |
| 1 | E | 333 | ASP | CB-CG-OD2 | -7.54 | 111.52 | 118.30 |
| 1 | A | 129 | ARG | NE-CZ-NH2 | -7.53 | 116.54 | 120.30 |
| 1 | G | 1057 | ASP | CB-CG-OD2 | -7.52 | 111.53 | 118.30 |
| 1 | G | 670 | ASP | CB-CG-OD2 | -7.51 | 111.54 | 118.30 |
| 1 | G | 6 | ASP | CB-CG-OD2 | -7.49 | 111.56 | 118.30 |
| 1 | E | 6 | ASP | CB-CG-OD1 | 7.47 | 125.03 | 118.30 |
| 1 | A | 372 | ASP | CB-CG-OD2 | -7.46 | 111.59 | 118.30 |
| 1 | C | 614 | ASP | CB-CG-OD2 | -7.46 | 111.59 | 118.30 |
| 2 | D | 262 | ASP | CB-CG-OD2 | -7.46 | 111.59 | 118.30 |
| 2 | H | 264 | PRO | N-CA-CB | 7.44 | 112.22 | 103.30 |
| 1 | E | 509 | ARG | NE-CZ-NH1 | 7.42 | 124.01 | 120.30 |
| 1 | A | 677 | ARG | NE-CZ-NH2 | -7.40 | 116.60 | 120.30 |
| 2 | H | 299 | ASP | CB-CG-OD2 | -7.40 | 111.64 | 118.30 |
| 1 | E | 959 | ASP | CB-CG-OD1 | 7.39 | 124.95 | 118.30 |
| 2 | F | 334 | ASP | CB-CG-OD2 | -7.38 | 111.66 | 118.30 |
| 1 | C | 197 | ASP | CB-CG-OD2 | -7.37 | 111.67 | 118.30 |
| 1 | E | 944 | ARG | NE-CZ-NH1 | 7.35 | 123.97 | 120.30 |
| 1 | C | 133 | ASP | CB-CG-OD1 | 7.35 | 124.91 | 118.30 |
| 1 | A | 338 | ASP | CB-CG-OD2 | -7.33 | 111.70 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 1003 | ASP | CB-CG-OD2 | -7.31 | 111.72 | 118.30 |
| 2 | F | 120 | ARG | NE-CZ-NH2 | -7.31 | 116.64 | 120.30 |
| 2 | D | 67 | ASP | CB-CG-OD2 | -7.30 | 111.73 | 118.30 |
| 1 | G | 145 | ARG | NE-CZ-NH2 | -7.30 | 116.65 | 120.30 |
| 1 | A | 343 | ARG | NE-CZ-NH2 | -7.29 | 116.65 | 120.30 |
| 1 | E | 810 | ARG | NE-CZ-NH2 | -7.29 | 116.66 | 120.30 |
| 1 | A | 128 | ASP | CB-CG-OD1 | 7.28 | 124.85 | 118.30 |
| 1 | E | 487 | ASP | CB-CG-OD1 | 7.28 | 124.85 | 118.30 |
| 1 | E | 223 | ASP | CB-CG-OD1 | 7.28 | 124.85 | 118.30 |
| 1 | A | 716 | PRO | N-CA-CB | 7.27 | 112.02 | 103.30 |
| 1 | E | 416 | ASP | CB-CG-OD2 | -7.27 | 111.76 | 118.30 |
| 2 | F | 368 | ASP | CB-CG-OD1 | 7.26 | 124.83 | 118.30 |
| 2 | H | 211 | ASP | CB-CG-OD2 | -7.26 | 111.77 | 118.30 |
| 1 | A | 131 | ARG | NE-CZ-NH1 | 7.24 | 123.92 | 120.30 |
| 1 | A | 490 | ARG | NE-CZ-NH2 | -7.23 | 116.68 | 120.30 |
| 1 | G | 128 | ASP | CB-CG-OD1 | 7.23 | 124.81 | 118.30 |
| 2 | D | 368 | ASP | CB-CG-OD2 | -7.23 | 111.79 | 118.30 |
| 1 | G | 410 | ASP | CB-CG-OD1 | 7.23 | 124.81 | 118.30 |
| 2 | H | 139 | ASP | CB-CG-OD1 | 7.21 | 124.79 | 118.30 |
| 1 | E | 487 | ASP | CB-CG-OD2 | -7.20 | 111.82 | 118.30 |
| 1 | C | 558 | ASP | N-CA-CB | -7.19 | 97.66 | 110.60 |
| 1 | E | 124 | ASP | CB-CG-OD1 | 7.19 | 124.77 | 118.30 |
| 1 | C | 131 | ARG | NE-CZ-NH2 | -7.17 | 116.71 | 120.30 |
| 1 | E | 400 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 1 | A | 611 | ASP | CB-CG-OD2 | -7.16 | 111.86 | 118.30 |
| 1 | E | 410 | ASP | CB-CG-OD2 | -7.13 | 111.88 | 118.30 |
| 1 | A | 615 | ARG | NE-CZ-NH1 | 7.13 | 123.86 | 120.30 |
| 1 | E | 1003 | ASP | CB-CG-OD2 | -7.12 | 111.89 | 118.30 |
| 2 | D | 203 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 1 | C | 539 | ASP | CB-CG-OD2 | -7.12 | 111.89 | 118.30 |
| 1 | E | 265 | ARG | NE-CZ-NH1 | 7.09 | 123.85 | 120.30 |
| 1 | E | 1027 | ARG | NE-CZ-NH2 | -7.09 | 116.75 | 120.30 |
| 1 | A | 226 | ASP | CB-CG-OD2 | -7.09 | 111.92 | 118.30 |
| 1 | C | 128 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 2 | F | 45 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | E | 161 | ASP | CB-CG-OD2 | -7.05 | 111.95 | 118.30 |
| 1 | C | 223 | ASP | CB-CG-OD1 | 7.04 | 124.64 | 118.30 |
| 1 | C | 733 | ASP | CB-CG-OD2 | -7.04 | 111.96 | 118.30 |
| 1 | E | 128 | ASP | CB-CG-OD2 | -7.01 | 111.99 | 118.30 |
| 1 | C | 226 | ASP | CB-CG-OD2 | -7.00 | 112.00 | 118.30 |
| 1 | E | 82 | ARG | NE-CZ-NH2 | -7.00 | 116.80 | 120.30 |
| 2 | B | 326 | ARG | NE-CZ-NH2 | -7.00 | 116.80 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 763 | ASP | CB-CG-OD2 | -7.00 | 112.00 | 118.30 |
| 2 | D | 114 | ASP | CB-CG-OD1 | 6.99 | 124.59 | 118.30 |
| 1 | G | 223 | ASP | CB-CG-OD1 | 6.99 | 124.59 | 118.30 |
| 1 | E | 904 | ASP | CB-CG-OD1 | 6.98 | 124.58 | 118.30 |
| 1 | E | 769 | ASP | CB-CG-OD2 | -6.97 | 112.02 | 118.30 |
| 1 | E | 223 | ASP | CB-CG-OD2 | -6.95 | 112.04 | 118.30 |
| 2 | B | 368 | ASP | CB-CG-OD1 | 6.94 | 124.55 | 118.30 |
| 1 | E | 763 | ASP | CB-CG-OD2 | -6.94 | 112.05 | 118.30 |
| 1 | A | 736 | ARG | NE-CZ-NH1 | 6.91 | 123.75 | 120.30 |
| 2 | D | 112 | ASP | CB-CG-OD1 | 6.91 | 124.52 | 118.30 |
| 2 | D | 188 | ASP | CB-CG-OD2 | -6.91 | 112.08 | 118.30 |
| 2 | D | 188 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 |
| 1 | E | 6 | ASP | CB-CG-OD2 | -6.89 | 112.10 | 118.30 |
| 1 | A | 559 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | E | 539 | ASP | CB-CG-OD1 | 6.88 | 124.49 | 118.30 |
| 2 | H | 215 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 1 | C | 6 | ASP | CB-CG-OD1 | 6.84 | 124.46 | 118.30 |
| 1 | A | 558 | ASP | CB-CG-OD2 | -6.84 | 112.14 | 118.30 |
| 2 | B | 97 | ASP | CB-CG-OD1 | 6.83 | 124.45 | 118.30 |
| 1 | G | 226 | ASP | CB-CG-OD1 | 6.82 | 124.44 | 118.30 |
| 1 | C | 161 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 2 | F | 249 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 1 | G | 197 | ASP | CB-CG-OD2 | -6.80 | 112.17 | 118.30 |
| 1 | E | 736 | ARG | NE-CZ-NH1 | 6.80 | 123.70 | 120.30 |
| 1 | G | 674 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 2 | F | 67 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | G | 499 | ASP | CB-CG-OD2 | -6.76 | 112.21 | 118.30 |
| 2 | H | 84 | ASP | CB-CG-OD1 | 6.76 | 124.39 | 118.30 |
| 1 | E | 128 | ASP | CB-CG-OD1 | 6.75 | 124.38 | 118.30 |
| 2 | H | 136 | ASP | CB-CG-OD2 | -6.74 | 112.23 | 118.30 |
| 1 | G | 959 | ASP | CB-CG-OD1 | 6.74 | 124.36 | 118.30 |
| 1 | G | 425 | ARG | NE-CZ-NH1 | 6.73 | 123.67 | 120.30 |
| 1 | G | 959 | ASP | CB-CG-OD2 | -6.73 | 112.24 | 118.30 |
| 2 | F | 97 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | E | 610 | TYR | CB-CG-CD2 | 6.71 | 125.03 | 121.00 |
| 1 | E | 765 | ASP | CB-CG-OD1 | 6.70 | 124.33 | 118.30 |
| 1 | A | 223 | ASP | CB-CG-OD1 | 6.70 | 124.33 | 118.30 |
| 2 | D | 362 | ASP | CB-CG-OD2 | -6.70 | 112.27 | 118.30 |
| 2 | F | 120 | ARG | NE-CZ-NH1 | 6.70 | 123.65 | 120.30 |
| 1 | C | 674 | ASP | CB-CG-OD2 | -6.69 | 112.28 | 118.30 |
| 1 | E | 611 | ASP | CB-CG-OD1 | 6.68 | 124.31 | 118.30 |
| 1 | C | 222 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | E | 517 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 1 | A | 972 | ASP | CB-CG-OD2 | -6.66 | 112.30 | 118.30 |
| 1 | G | 258 | ASP | CB-CG-OD1 | 6.66 | 124.30 | 118.30 |
| 2 | F | 344 | ASP | CB-CG-OD1 | 6.66 | 124.29 | 118.30 |
| 1 | E | 611 | ASP | CB-CG-OD2 | -6.65 | 112.31 | 118.30 |
| 1 | C | 430 | ASP | CB-CG-OD2 | -6.65 | 112.32 | 118.30 |
| 1 | C | 518 | ASP | CB-CG-OD2 | -6.64 | 112.33 | 118.30 |
| 1 | A | 416 | ASP | CB-CG-OD2 | -6.63 | 112.33 | 118.30 |
| 2 | D | 299 | ASP | CB-CG-OD1 | 6.63 | 124.27 | 118.30 |
| 1 | E | 416 | ASP | CB-CG-OD1 | 6.63 | 124.27 | 118.30 |
| 1 | G | 972 | ASP | CB-CG-OD1 | 6.62 | 124.26 | 118.30 |
| 2 | D | 97 | ASP | CB-CG-OD1 | 6.61 | 124.25 | 118.30 |
| 1 | E | 197 | ASP | CB-CG-OD1 | 6.61 | 124.25 | 118.30 |
| 1 | A | 677 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | E | 592 | ASP | CB-CG-OD2 | -6.59 | 112.37 | 118.30 |
| 1 | C | 450 | ASP | CB-CG-OD2 | -6.57 | 112.39 | 118.30 |
| 1 | G | 614 | ASP | CB-CG-OD1 | 6.57 | 124.22 | 118.30 |
| 2 | D | 139 | ASP | CB-CG-OD1 | 6.57 | 124.21 | 118.30 |
| 2 | B | 262 | ASP | CB-CG-OD2 | -6.56 | 112.39 | 118.30 |
| 1 | G | 769 | ASP | CB-CG-OD2 | -6.55 | 112.41 | 118.30 |
| 1 | C | 197 | ASP | CB-CG-OD1 | 6.55 | 124.19 | 118.30 |
| 1 | G | 670 | ASP | CB-CG-OD1 | 6.54 | 124.18 | 118.30 |
| 1 | C | 558 | ASP | CB-CG-OD2 | -6.52 | 112.43 | 118.30 |
| 2 | F | 227 | ASP | CB-CG-OD2 | -6.52 | 112.43 | 118.30 |
| 1 | E | 133 | ASP | CB-CG-OD1 | 6.52 | 124.17 | 118.30 |
| 2 | D | 299 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 1 | G | 625 | ASP | CB-CG-OD1 | 6.51 | 124.16 | 118.30 |
| 1 | A | 499 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 2 | F | 211 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 1 | G | 226 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 2 | D | 227 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | G | 306 | ARG | NE-CZ-NH1 | 6.49 | 123.55 | 120.30 |
| 1 | G | 372 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |
| 1 | C | 104 | ARG | NE-CZ-NH1 | 6.49 | 123.55 | 120.30 |
| 1 | G | 972 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |
| 2 | H | 67 | ASP | CB-CG-OD2 | -6.48 | 112.47 | 118.30 |
| 1 | E | 558 | ASP | CB-CG-OD2 | -6.46 | 112.49 | 118.30 |
| 1 | A | 528 | ARG | NE-CZ-NH1 | 6.46 | 123.53 | 120.30 |
| 1 | A | 1041 | ASP | CB-CG-OD1 | 6.46 | 124.11 | 118.30 |
| 1 | C | 226 | ASP | CB-CG-OD1 | 6.45 | 124.11 | 118.30 |
| 1 | C | 124 | ASP | CB-CG-OD2 | -6.45 | 112.50 | 118.30 |
| 1 | C | 416 | ASP | CB-CG-OD2 | -6.45 | 112.50 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | C | 338 | ASP | CB-CG-OD2 | -6.44 | 112.50 | 118.30 |
| 1 | C | 944 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | E | 459 | ASP | CB-CG-OD1 | 6.44 | 124.09 | 118.30 |
| 2 | B | 211 | ASP | CB-CG-OD1 | 6.43 | 124.09 | 118.30 |
| 1 | A | 625 | ASP | CB-CG-OD2 | -6.43 | 112.52 | 118.30 |
| 2 | B | 139 | ASP | CB-CG-OD2 | -6.43 | 112.52 | 118.30 |
| 1 | G | 592 | ASP | CB-CG-OD2 | -6.42 | 112.52 | 118.30 |
| 1 | E | 84 | ASP | CB-CG-OD2 | -6.42 | 112.52 | 118.30 |
| 1 | E | 674 | ASP | CB-CG-OD2 | -6.42 | 112.53 | 118.30 |
| 2 | F | 188 | ASP | CB-CG-OD1 | 6.41 | 124.07 | 118.30 |
| 1 | C | 487 | ASP | CB-CG-OD2 | -6.41 | 112.53 | 118.30 |
| 1 | G | 128 | ASP | CB-CG-OD2 | -6.41 | 112.53 | 118.30 |
| 1 | G | 579 | ASP | CB-CG-OD2 | -6.40 | 112.54 | 118.30 |
| 2 | H | 116 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 2 | H | 188 | ASP | CB-CG-OD1 | 6.39 | 124.05 | 118.30 |
| 2 | B | 344 | ASP | CB-CG-OD2 | -6.39 | 112.55 | 118.30 |
| 1 | E | 758 | ASP | CB-CG-OD1 | 6.38 | 124.05 | 118.30 |
| 2 | D | 368 | ASP | CB-CG-OD1 | 6.38 | 124.05 | 118.30 |
| 1 | C | 539 | ASP | CB-CG-OD1 | 6.38 | 124.04 | 118.30 |
| 2 | F | 45 | ASP | CB-CG-OD1 | 6.37 | 124.04 | 118.30 |
| 1 | G | 133 | ASP | CB-CG-OD2 | -6.37 | 112.56 | 118.30 |
| 2 | H | 97 | ASP | CB-CG-OD1 | 6.37 | 124.04 | 118.30 |
| 2 | D | 114 | ASP | CB-CG-OD2 | -6.37 | 112.56 | 118.30 |
| 2 | D | 139 | ASP | CB-CG-OD2 | -6.37 | 112.57 | 118.30 |
| 2 | F | 227 | ASP | CB-CG-OD1 | 6.37 | 124.03 | 118.30 |
| 1 | E | 194 | ARG | NE-CZ-NH2 | -6.36 | 117.12 | 120.30 |
| 1 | A | 807 | ASP | CB-CG-OD2 | -6.36 | 112.58 | 118.30 |
| 1 | A | 459 | ASP | CB-CG-OD2 | -6.35 | 112.58 | 118.30 |
| 1 | A | 6 | ASP | CB-CG-OD1 | 6.35 | 124.02 | 118.30 |
| 1 | C | 614 | ASP | CB-CG-OD1 | 6.34 | 124.01 | 118.30 |
| 1 | G | 736 | ARG | NE-CZ-NH1 | 6.34 | 123.47 | 120.30 |
| 2 | D | 211 | ASP | CB-CG-OD2 | -6.32 | 112.61 | 118.30 |
| 1 | G | 956 | ARG | NE-CZ-NH1 | 6.32 | 123.46 | 120.30 |
| 2 | D | 192 | PHE | CB-CG-CD2 | 6.32 | 125.22 | 120.80 |
| 1 | E | 1041 | ASP | CB-CG-OD1 | 6.31 | 123.98 | 118.30 |
| 1 | G | 389 | ARG | NE-CZ-NH1 | 6.31 | 123.45 | 120.30 |
| 1 | C | 128 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | E | 769 | ASP | CB-CG-OD1 | 6.29 | 123.96 | 118.30 |
| 1 | A | 185 | ARG | NE-CZ-NH1 | 6.28 | 123.44 | 120.30 |
| 1 | A | 333 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 2 | F | 244 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 1 | G | 757[A] | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | G | 757[B] | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 2 | D | 262 | ASP | CB-CG-OD1 | 6.27 | 123.95 | 118.30 |
| 1 | C | 441 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 2 | F | 211 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | G | 57 | ASP | CB-CG-OD2 | -6.27 | 112.66 | 118.30 |
| 2 | H | 299 | ASP | CB-CG-OD1 | 6.26 | 123.93 | 118.30 |
| 2 | F | 198 | ASP | CB-CG-OD1 | 6.25 | 123.93 | 118.30 |
| 1 | E | 438 | TYR | CB-CG-CD1 | 6.25 | 124.75 | 121.00 |
| 1 | E | 343 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 1 | E | 959 | ASP | CB-CG-OD2 | -6.24 | 112.69 | 118.30 |
| 1 | C | 1003 | ASP | CB-CG-OD1 | 6.23 | 123.91 | 118.30 |
| 1 | A | 333 | ASP | CB-CG-OD1 | 6.23 | 123.91 | 118.30 |
| 1 | C | 84 | ASP | CB-CG-OD2 | -6.23 | 112.69 | 118.30 |
| 2 | H | 212 | ARG | NE-CZ-NH1 | 6.23 | 123.42 | 120.30 |
| 1 | C | 609 | ASP | CB-CG-OD2 | -6.23 | 112.69 | 118.30 |
| 1 | A | 410 | ASP | CB-CG-OD2 | -6.22 | 112.70 | 118.30 |
| 1 | G | 667 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | A | 194 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 1 | E | 539 | ASP | CB-CG-OD2 | -6.21 | 112.71 | 118.30 |
| 1 | A | 956[A] | ARG | NE-CZ-NH2 | -6.21 | 117.20 | 120.30 |
| 1 | A | 956[B] | ARG | NE-CZ-NH2 | -6.21 | 117.20 | 120.30 |
| 1 | A | 539 | ASP | CB-CG-OD1 | 6.20 | 123.88 | 118.30 |
| 2 | D | 112 | ASP | CB-CG-OD2 | -6.19 | 112.73 | 118.30 |
| 2 | F | 262 | ASP | CB-CG-OD2 | -6.17 | 112.74 | 118.30 |
| 1 | C | 82 | ARG | CA-CB-CG | -6.17 | 99.82 | 113.40 |
| 1 | C | 684 | ARG | NE-CZ-NH2 | -6.17 | 117.21 | 120.30 |
| 1 | A | 124 | ASP | CB-CG-OD1 | 6.17 | 123.85 | 118.30 |
| 1 | E | 670 | ASP | CB-CG-OD1 | 6.17 | 123.85 | 118.30 |
| 1 | A | 763 | ASP | CB-CG-OD2 | -6.15 | 112.76 | 118.30 |
| 1 | C | 133 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | C | 769 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | G | 43 | ARG | NE-CZ-NH2 | -6.14 | 117.23 | 120.30 |
| 1 | E | 521 | ASP | CB-CG-OD1 | 6.14 | 123.82 | 118.30 |
| 2 | B | 136 | ASP | CB-CG-OD1 | 6.13 | 123.82 | 118.30 |
| 1 | E | 438 | TYR | CB-CG-CD2 | -6.12 | 117.33 | 121.00 |
| 1 | C | 487 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 1 | G | 730 | ASP | CB-CG-OD2 | -6.11 | 112.80 | 118.30 |
| 1 | C | 670 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 2 | B | 227 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | E | 441 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | A | 509 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 2 | D | 192 | PHE | CB-CG-CD1 | -6.10 | 116.53 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | C | 27 | ASP | CB-CG-OD2 | -6.09 | 112.81 | 118.30 |
| 1 | C | 763 | ASP | CB-CG-OD1 | 6.09 | 123.78 | 118.30 |
| 1 | A | 1041 | ASP | CB-CG-OD2 | -6.09 | 112.82 | 118.30 |
| 1 | G | 625 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 2 | H | 378 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 2 | H | 227 | ASP | CB-CG-OD2 | -6.07 | 112.83 | 118.30 |
| 1 | G | 42 | TYR | CB-CG-CD1 | -6.07 | 117.36 | 121.00 |
| 2 | B | 203 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 2 | H | 234 | ASP | CB-CG-OD2 | -6.05 | 112.85 | 118.30 |
| 2 | B | 69 | ASP | CB-CG-OD2 | -6.05 | 112.85 | 118.30 |
| 1 | C | 343 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 1 | G | 757[A] | ASP | CB-CG-OD1 | 6.05 | 123.75 | 118.30 |
| 1 | G | 757[B] | ASP | CB-CG-OD1 | 6.05 | 123.75 | 118.30 |
| 1 | A | 300 | MET | CG-SD-CE | 6.05 | 109.88 | 100.20 |
| 1 | A | 416 | ASP | CB-CG-OD1 | 6.05 | 123.75 | 118.30 |
| 1 | C | 410 | ASP | CB-CG-OD1 | 6.05 | 123.74 | 118.30 |
| 1 | E | 1021 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | A | 763 | ASP | CB-CG-OD1 | 6.04 | 123.73 | 118.30 |
| 2 | H | 114 | ASP | CB-CG-OD2 | -6.03 | 112.87 | 118.30 |
| 1 | E | 430 | ASP | CB-CG-OD2 | -6.02 | 112.88 | 118.30 |
| 1 | E | 579 | ASP | CB-CG-OD2 | -6.01 | 112.89 | 118.30 |
| 1 | G | 1021 | ARG | NE-CZ-NH1 | 6.01 | 123.31 | 120.30 |
| 1 | C | 912 | ARG | NE-CZ-NH1 | 6.01 | 123.30 | 120.30 |
| 1 | E | 807 | ASP | CB-CG-OD2 | -6.00 | 112.90 | 118.30 |
| 2 | B | 317 | ASP | CB-CG-OD1 | 6.00 | 123.70 | 118.30 |
| 2 | H | 344 | ASP | CB-CG-OD1 | 6.00 | 123.70 | 118.30 |
| 1 | A | 38[A] | ARG | NE-CZ-NH2 | -5.99 | 117.30 | 120.30 |
| 1 | A | 38[B] | ARG | NE-CZ-NH2 | -5.99 | 117.30 | 120.30 |
| 1 | A | 487 | ASP | CB-CG-OD2 | -5.99 | 112.91 | 118.30 |
| 2 | D | 136 | ASP | CB-CG-OD1 | 5.99 | 123.69 | 118.30 |
| 1 | A | 684 | ARG | NE-CZ-NH2 | -5.98 | 117.31 | 120.30 |
| 2 | B | 227 | ASP | CB-CG-OD2 | -5.98 | 112.92 | 118.30 |
| 1 | C | 514 | ARG | NE-CZ-NH2 | -5.98 | 117.31 | 120.30 |
| 1 | G | 514 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | E | 609 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | C | 1021 | ARG | NE-CZ-NH1 | 5.95 | 123.27 | 120.30 |
| 2 | H | 211 | ASP | CB-CG-OD1 | 5.94 | 123.64 | 118.30 |
| 1 | E | 592 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | E | 674 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | G | 716 | PRO | N-CA-CB | 5.93 | 110.41 | 103.30 |
| 1 | E | 133 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 1 | A | 614 | ASP | CB-CG-OD1 | 5.92 | 123.62 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | C | 989 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 2 | F | 157 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | C | 514 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 2 | H | 249 | ASP | CB-CG-OD2 | -5.88 | 113.00 | 118.30 |
| 1 | A | 372 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | E | 124 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | A | 425 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | A | 758 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 2 | H | 136 | ASP | CB-CG-OD1 | 5.87 | 123.59 | 118.30 |
| 1 | G | 674 | ASP | CB-CG-OD1 | 5.86 | 123.57 | 118.30 |
| 2 | F | 362 | ASP | CB-CG-OD2 | -5.86 | 113.03 | 118.30 |
| 1 | G | 124 | ASP | CB-CG-OD2 | -5.84 | 113.05 | 118.30 |
| 1 | G | 416 | ASP | CB-CG-OD2 | -5.83 | 113.05 | 118.30 |
| 2 | D | 104 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 1 | E | 1027 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 1 | G | 161 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 2 | B | 262 | ASP | CB-CG-OD1 | 5.83 | 123.54 | 118.30 |
| 1 | C | 459 | ASP | CB-CG-OD1 | 5.83 | 123.54 | 118.30 |
| 1 | E | 459 | ASP | CB-CG-OD2 | -5.82 | 113.06 | 118.30 |
| 1 | E | 956[A] | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | E | 956[B] | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | G | 753 | ASP | CB-CG-OD2 | -5.82 | 113.06 | 118.30 |
| 1 | E | 294 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 2 | F | 188 | ASP | CB-CG-OD2 | -5.82 | 113.07 | 118.30 |
| 2 | B | 299 | ASP | CB-CG-OD2 | -5.81 | 113.07 | 118.30 |
| 2 | F | 262 | ASP | CB-CG-OD1 | 5.81 | 123.53 | 118.30 |
| 1 | A | 579 | ASP | CB-CG-OD2 | -5.80 | 113.08 | 118.30 |
| 2 | F | 234 | ASP | CB-CG-OD1 | 5.80 | 123.52 | 118.30 |
| 2 | B | 69 | ASP | CB-CG-OD1 | 5.79 | 123.51 | 118.30 |
| 1 | E | 425 | ARG | NE-CZ-NH1 | 5.79 | 123.19 | 120.30 |
| 1 | G | 521 | ASP | CB-CG-OD2 | -5.79 | 113.09 | 118.30 |
| 2 | H | 198 | ASP | CB-CG-OD2 | -5.78 | 113.09 | 118.30 |
| 1 | E | 765 | ASP | CB-CG-OD2 | -5.78 | 113.10 | 118.30 |
| 1 | G | 246 | ASP | CB-CG-OD1 | 5.76 | 123.49 | 118.30 |
| 2 | H | 139 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | A | 670 | ASP | CB-CG-OD1 | 5.76 | 123.49 | 118.30 |
| 2 | D | 136 | ASP | CB-CG-OD2 | -5.76 | 113.12 | 118.30 |
| 1 | G | 922 | ARG | NE-CZ-NH1 | 5.75 | 123.18 | 120.30 |
| 1 | A | 667 | ASP | CB-CG-OD1 | 5.75 | 123.48 | 118.30 |
| 2 | F | 114 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | G | 426[A] | ARG | NE-CZ-NH2 | -5.75 | 117.43 | 120.30 |
| 1 | G | 426[B] | ARG | NE-CZ-NH2 | -5.75 | 117.43 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | B | 188 | ASP | CB-CG-OD2 | -5.74 | 113.13 | 118.30 |
| 1 | C | 333 | ASP | CB-CG-OD2 | -5.74 | 113.13 | 118.30 |
| 2 | D | 67 | ASP | CB-CG-OD1 | 5.74 | 123.47 | 118.30 |
| 1 | E | 1036 | TYR | CB-CG-CD2 | -5.74 | 117.56 | 121.00 |
| 1 | A | 434 | ASP | CB-CG-OD2 | -5.74 | 113.14 | 118.30 |
| 1 | A | 490 | ARG | NE-CZ-NH1 | 5.74 | 123.17 | 120.30 |
| 1 | E | 265 | ARG | NE-CZ-NH2 | -5.73 | 117.43 | 120.30 |
| 1 | G | 904 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | G | 1031 | ARG | NE-CZ-NH2 | -5.73 | 117.43 | 120.30 |
| 1 | A | 791 | ASP | CB-CG-OD1 | 5.73 | 123.45 | 118.30 |
| 1 | A | 922 | ARG | NE-CZ-NH2 | -5.72 | 117.44 | 120.30 |
| 1 | G | 487 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 2 | B | 50 | ARG | NE-CZ-NH2 | -5.72 | 117.44 | 120.30 |
| 1 | G | 246 | ASP | CB-CG-OD2 | -5.72 | 113.16 | 118.30 |
| 2 | D | 45 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |
| 1 | A | 609 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |
| 1 | G | 121 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |
| 1 | A | 609 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 2 | F | 84 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 2 | H | 262 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | E | 735 | ARG | NE-CZ-NH2 | -5.70 | 117.45 | 120.30 |
| 2 | D | 234 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | A | 471 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 2 | F | 84 | ASP | CB-CG-OD1 | 5.68 | 123.42 | 118.30 |
| 1 | E | 631 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 1 | C | 716 | PRO | N-CA-CB | 5.68 | 110.11 | 103.30 |
| 2 | F | 11 | ASP | CB-CG-OD1 | 5.68 | 123.41 | 118.30 |
| 1 | G | 237 | PHE | CB-CG-CD2 | 5.67 | 124.77 | 120.80 |
| 1 | C | 246 | ASP | CB-CG-OD1 | 5.67 | 123.40 | 118.30 |
| 2 | H | 198 | ASP | CB-CG-OD1 | 5.67 | 123.40 | 118.30 |
| 1 | E | 972 | ASP | CB-CG-OD2 | -5.66 | 113.20 | 118.30 |
| 1 | C | 333 | ASP | CB-CG-OD1 | 5.65 | 123.39 | 118.30 |
| 1 | E | 1041 | ASP | CB-CG-OD2 | -5.65 | 113.21 | 118.30 |
| 1 | A | 631 | ARG | NE-CZ-NH1 | 5.65 | 123.13 | 120.30 |
| 2 | B | 84 | ASP | CB-CG-OD1 | 5.65 | 123.39 | 118.30 |
| 2 | D | 69 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | A | 426 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | G | 539 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 2 | D | 227 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 2 | H | 249 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | A | 400 | ARG | NE-CZ-NH1 | 5.63 | 123.12 | 120.30 |
| 1 | G | 27 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | G | 675 | ARG | NE-CZ-NH1 | 5.63 | 123.11 | 120.30 |
| 1 | G | 791 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | G | 453 | PHE | CB-CG-CD2 | -5.62 | 116.86 | 120.80 |
| 1 | G | 1025 | ASP | CB-CG-OD2 | -5.61 | 113.25 | 118.30 |
| 1 | E | 303 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | C | 265 | ARG | NE-CZ-NH2 | -5.60 | 117.50 | 120.30 |
| 1 | C | 753 | ASP | CB-CG-OD2 | -5.60 | 113.26 | 118.30 |
| 1 | A | 104 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | A | 530 | ASP | CB-CG-OD1 | 5.60 | 123.34 | 118.30 |
| 1 | G | 956 | ARG | NE-CZ-NH2 | -5.59 | 117.50 | 120.30 |
| 1 | A | 590 | ARG | NE-CZ-NH2 | -5.59 | 117.50 | 120.30 |
| 1 | A | 75 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 1 | A | 119 | THR | CA-CB-CG2 | -5.59 | 104.58 | 112.40 |
| 2 | B | 45 | ASP | CB-CG-OD1 | 5.59 | 123.33 | 118.30 |
| 1 | G | 730 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | G | 416 | ASP | CB-CG-OD1 | 5.57 | 123.31 | 118.30 |
| 1 | A | 197 | ASP | CB-CG-OD1 | 5.57 | 123.31 | 118.30 |
| 1 | G | 528 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |
| 1 | A | 1003 | ASP | CB-CG-OD1 | 5.56 | 123.30 | 118.30 |
| 1 | A | 769 | ASP | CB-CG-OD2 | -5.56 | 113.30 | 118.30 |
| 1 | A | 959 | ASP | CB-CG-OD1 | 5.56 | 123.30 | 118.30 |
| 1 | E | 471 | ARG | NE-CZ-NH2 | -5.55 | 117.52 | 120.30 |
| 1 | G | 611 | ASP | CB-CG-OD2 | -5.55 | 113.30 | 118.30 |
| 1 | A | 84 | ASP | CB-CG-OD1 | 5.55 | 123.29 | 118.30 |
| 1 | E | 258 | ASP | CB-CG-OD2 | -5.54 | 113.31 | 118.30 |
| 1 | C | 246 | ASP | CB-CG-OD2 | -5.54 | 113.32 | 118.30 |
| 1 | G | 499 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 1 | A | 28 | TYR | CB-CG-CD1 | -5.53 | 117.69 | 121.00 |
| 1 | C | 450 | ASP | CB-CG-OD1 | 5.52 | 123.27 | 118.30 |
| 1 | C | 42 | TYR | CB-CG-CD1 | -5.52 | 117.69 | 121.00 |
| 1 | A | 361 | ARG | NE-CZ-NH1 | 5.52 | 123.06 | 120.30 |
| 1 | A | 354 | TYR | CB-CG-CD2 | 5.52 | 124.31 | 121.00 |
| 1 | E | 605 | THR | CA-CB-CG2 | -5.52 | 104.67 | 112.40 |
| 2 | D | 148 | ARG | NE-CZ-NH1 | 5.52 | 123.06 | 120.30 |
| 1 | E | 730 | ASP | CB-CG-OD2 | -5.52 | 113.34 | 118.30 |
| 1 | C | 609 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | C | 642 | TYR | CB-CG-CD2 | -5.51 | 117.69 | 121.00 |
| 1 | A | 807 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | E | 733 | ASP | CB-CG-OD2 | -5.50 | 113.35 | 118.30 |
| 1 | G | 590 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | C | 559 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 2 | D | 317 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | F | 317 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | A | 361 | ARG | NE-CZ-NH2 | -5.49 | 117.55 | 120.30 |
| 1 | A | 1025 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | E | 730 | ASP | CB-CG-OD1 | 5.48 | 123.24 | 118.30 |
| 1 | C | 769 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | G | 530 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | C | 434 | ASP | CB-CG-OD2 | -5.47 | 113.38 | 118.30 |
| 1 | G | 237 | PHE | CB-CG-CD1 | -5.47 | 116.97 | 120.80 |
| 2 | B | 157 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 1 | E | 62 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 1 | G | 430 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 1 | G | 1057 | ASP | CB-CG-OD1 | 5.46 | 123.21 | 118.30 |
| 2 | H | 215 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 2 | B | 93 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 1 | G | 675 | ARG | NE-CZ-NH2 | -5.45 | 117.57 | 120.30 |
| 1 | G | 27 | ASP | CB-CG-OD1 | 5.44 | 123.20 | 118.30 |
| 1 | E | 807 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 1 | G | 912 | ARG | NE-CZ-NH1 | 5.43 | 123.02 | 120.30 |
| 1 | E | 530 | ASP | CB-CG-OD2 | -5.43 | 113.41 | 118.30 |
| 1 | C | 807 | ASP | CB-CG-OD1 | 5.42 | 123.18 | 118.30 |
| 1 | C | 499 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 2 | B | 136 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 1 | C | 161 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 2 | H | 69 | ASP | CB-CG-OD2 | -5.41 | 113.44 | 118.30 |
| 1 | C | 82 | ARG | CG-CD-NE | -5.40 | 100.45 | 111.80 |
| 1 | C | 959 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | C | 807 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | E | 434 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 2 | B | 244 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | E | 279 | THR | CA-CB-CG2 | -5.40 | 104.84 | 112.40 |
| 1 | C | 82 | ARG | NE-CZ-NH2 | -5.40 | 117.60 | 120.30 |
| 1 | E | 84 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 1 | G | 441 | ASP | CB-CG-OD2 | -5.39 | 113.44 | 118.30 |
| 1 | A | 769 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 2 | D | 344 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 2 | B | 11 | ASP | CB-CG-OD2 | -5.39 | 113.45 | 118.30 |
| 2 | B | 188 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 1 | E | 444 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 2 | F | 378 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 1 | E | 1021 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 1 | G | 121 | ASP | CB-CG-OD1 | 5.37 | 123.14 | 118.30 |
| 1 | E | 189 | GLU | CA-CB-CG | -5.37 | 101.59 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 1057 | ASP | CB-CG-OD1 | 5.37 | 123.13 | 118.30 |
| 1 | A | 758 | ASP | CB-CG-OD1 | 5.36 | 123.13 | 118.30 |
| 1 | C | 57 | ASP | CB-CG-OD2 | -5.36 | 113.47 | 118.30 |
| 1 | C | 434 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | A | 226 | ASP | CB-CG-OD1 | 5.35 | 123.12 | 118.30 |
| 1 | G | 84 | ASP | CB-CG-OD2 | -5.35 | 113.48 | 118.30 |
| 1 | E | 558 | ASP | N-CA-CB | -5.35 | 100.97 | 110.60 |
| 1 | E | 579 | ASP | CB-CG-OD1 | 5.35 | 123.11 | 118.30 |
| 1 | C | 204 | LEU | CB-CA-C | -5.34 | 100.05 | 110.20 |
| 2 | F | 250 | TYR | CB-CG-CD2 | -5.34 | 117.80 | 121.00 |
| 2 | B | 344 | ASP | CB-CG-OD1 | 5.34 | 123.10 | 118.30 |
| 1 | A | 904 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | A | 509 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 1 | E | 763 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | E | 434 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | G | 133 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 2 | B | 249 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | C | 677 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 1 | C | 425 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 2 | F | 198 | ASP | CB-CG-OD2 | -5.29 | 113.53 | 118.30 |
| 1 | G | 81 | GLU | CG-CD-OE2 | -5.29 | 107.72 | 118.30 |
| 1 | A | 625 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | C | 459 | ASP | CB-CG-OD2 | -5.28 | 113.55 | 118.30 |
| 1 | C | 674 | ASP | CB-CG-OD1 | 5.28 | 123.05 | 118.30 |
| 2 | F | 69 | ASP | CB-CG-OD1 | 5.28 | 123.05 | 118.30 |
| 1 | A | 161 | ASP | CB-CG-OD2 | -5.26 | 113.56 | 118.30 |
| 1 | A | 521 | ASP | CB-CG-OD2 | -5.26 | 113.56 | 118.30 |
| 1 | A | 753 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | C | 258 | ASP | CB-CG-OD2 | -5.26 | 113.57 | 118.30 |
| 1 | A | 373 | ARG | NE-CZ-NH2 | -5.25 | 117.67 | 120.30 |
| 1 | G | 558 | ASP | CB-CG-OD2 | -5.25 | 113.57 | 118.30 |
| 1 | A | 133 | ASP | CB-CG-OD2 | -5.25 | 113.58 | 118.30 |
| 1 | C | 273 | ARG | NE-CZ-NH2 | -5.25 | 117.68 | 120.30 |
| 1 | E | 246 | ASP | CB-CG-OD2 | -5.25 | 113.58 | 118.30 |
| 1 | E | 1057 | ASP | CB-CG-OD2 | -5.24 | 113.58 | 118.30 |
| 1 | G | 769 | ASP | CB-CG-OD1 | 5.24 | 123.02 | 118.30 |
| 1 | A | 306 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | A | 989 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | A | 667 | ASP | CB-CG-OD2 | -5.23 | 113.59 | 118.30 |
| 1 | A | 830 | PHE | CB-CG-CD1 | -5.23 | 117.14 | 120.80 |
| 2 | B | 198 | ASP | CB-CG-OD2 | -5.23 | 113.59 | 118.30 |
| 1 | E | 287 | ALA | N-CA-CB | 5.22 | 117.41 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 548 | GLU | CG-CD-OE2 | -5.22 | 107.87 | 118.30 |
| 1 | A | 121 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 2 | F | 50 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 2 | F | 234 | ASP | CB-CG-OD2 | -5.20 | 113.62 | 118.30 |
| 2 | D | 211 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 2 | B | 95 | THR | CA-CB-CG2 | -5.20 | 105.13 | 112.40 |
| 1 | E | 338 | ASP | CB-CG-OD2 | -5.19 | 113.63 | 118.30 |
| 1 | G | 238 | ASP | CB-CG-OD1 | 5.19 | 122.97 | 118.30 |
| 1 | G | 400 | ARG | NE-CZ-NH1 | 5.19 | 122.90 | 120.30 |
| 1 | A | 6 | ASP | CB-CG-OD2 | -5.19 | 113.63 | 118.30 |
| 2 | D | 249 | ASP | CB-CG-OD1 | 5.19 | 122.97 | 118.30 |
| 1 | A | 5 | THR | CA-CB-CG2 | -5.18 | 105.15 | 112.40 |
| 1 | C | 677 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 1 | C | 124 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | C | 338 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | G | 487 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | G | 807 | ASP | CB-CG-OD1 | 5.17 | 122.95 | 118.30 |
| 2 | F | 215 | ARG | NE-CZ-NH1 | 5.17 | 122.88 | 120.30 |
| 1 | G | 518 | ASP | CB-CG-OD2 | -5.17 | 113.65 | 118.30 |
| 2 | D | 120 | ARG | CD-NE-CZ | 5.17 | 130.83 | 123.60 |
| 1 | G | 530 | ASP | CB-CG-OD2 | -5.16 | 113.65 | 118.30 |
| 1 | A | 674 | ASP | CB-CG-OD2 | -5.16 | 113.66 | 118.30 |
| 1 | A | 133 | ASP | CB-CG-OD1 | 5.16 | 122.94 | 118.30 |
| 2 | D | 334 | ASP | CB-CG-OD1 | 5.15 | 122.93 | 118.30 |
| 1 | A | 62 | ASP | CB-CG-OD1 | 5.15 | 122.93 | 118.30 |
| 1 | A | 684 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 1 | E | 667 | ASP | CB-CG-OD2 | -5.14 | 113.67 | 118.30 |
| 2 | B | 316 | VAL | CA-CB-CG1 | -5.14 | 103.19 | 110.90 |
| 1 | A | 39 | GLU | CB-CA-C | -5.14 | 100.12 | 110.40 |
| 2 | B | 203 | ARG | NE-CZ-NH2 | -5.14 | 117.73 | 120.30 |
| 1 | G | 1016 | THR | CA-CB-CG2 | -5.13 | 105.21 | 112.40 |
| 1 | C | 84 | ASP | CB-CG-OD1 | 5.13 | 122.92 | 118.30 |
| 1 | A | 608 | THR | CA-CB-CG2 | -5.13 | 105.22 | 112.40 |
| 2 | F | 136 | ASP | CB-CG-OD2 | -5.13 | 113.68 | 118.30 |
| 1 | C | 592 | ASP | CB-CG-OD2 | -5.13 | 113.69 | 118.30 |
| 1 | C | 730 | ASP | CB-CG-OD2 | -5.13 | 113.69 | 118.30 |
| 1 | E | 118 | ALA | N-CA-CB | 5.12 | 117.26 | 110.10 |
| 1 | C | 579 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | G | 1025 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | A | 338 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 2 | B | 97 | ASP | CB-CG-OD2 | -5.10 | 113.71 | 118.30 |
| 2 | B | 45 | ASP | CB-CG-OD2 | -5.09 | 113.72 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 781 | HIS | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | A | 1004 | ARG | NE-CZ-NH2 | -5.09 | 117.76 | 120.30 |
| 1 | E | 880 | THR | CA-CB-CG2 | -5.09 | 105.28 | 112.40 |
| 2 | H | 114 | ASP | CB-CG-OD1 | 5.09 | 122.88 | 118.30 |
| 1 | A | 130 | ARG | NE-CZ-NH2 | -5.08 | 117.76 | 120.30 |
| 1 | E | 306 | ARG | NE-CZ-NH1 | 5.08 | 122.84 | 120.30 |
| 2 | H | 262 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | A | 791 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | G | 338 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | E | 389 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 2 | D | 326 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 1 | C | 994 | VAL | CG1-CB-CG2 | -5.06 | 102.80 | 110.90 |
| 2 | B | 207 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | G | 438 | TYR | CB-CG-CD2 | -5.05 | 117.97 | 121.00 |
| 2 | B | 320 | THR | CA-CB-CG2 | -5.03 | 105.35 | 112.40 |
| 1 | C | 912 | ARG | NE-CZ-NH2 | -5.03 | 117.78 | 120.30 |
| 2 | F | 112 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | E | 518 | ASP | CB-CG-OD1 | 5.03 | 122.82 | 118.30 |
| 1 | C | 400 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | E | 823 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | G | 353 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |
| 2 | H | 344 | ASP | CB-CG-OD2 | -5.01 | 113.79 | 118.30 |
| 1 | E | 372 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |
| 1 | A | 471 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |
| 2 | D | 344 | ASP | CB-CG-OD2 | -5.00 | 113.80 | 118.30 |
| 1 | A | 521 | ASP | CB-CG-OD1 | 5.00 | 122.80 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 8195 | 0 | 8247 | 239 | 0 |
| 1 | C | 8192 | 0 | 8230 | 247 | 0 |
| 1 | E | 8211 | 0 | 8245 | 225 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | G | 8180 | 0 | 8214 | 291 | 0 |
| 2 | B | 2895 | 0 | 2861 | 91 | 0 |
| 2 | D | 2895 | 0 | 2861 | 98 | 0 |
| 2 | F | 2895 | 0 | 2861 | 107 | 0 |
| 2 | H | 2895 | 0 | 2861 | 134 | 0 |
| 3 | A | 3 | 0 | 0 | 0 | 0 |
| 3 | C | 3 | 0 | 0 | 0 | 0 |
| 3 | E | 3 | 0 | 0 | 0 | 0 |
| 3 | G | 3 | 0 | 0 | 0 | 0 |
| 4 | A | 7 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 7 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | E | 7 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | G | 7 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 3 | 0 | 0 | 1 | 0 |
| 5 | B | 1 | 0 | 0 | 0 | 0 |
| 5 | C | 3 | 0 | 0 | 2 | 0 |
| 5 | D | 1 | 0 | 0 | 0 | 0 |
| 5 | E | 3 | 0 | 0 | 0 | 0 |
| 5 | F | 1 | 0 | 0 | 0 | 0 |
| 5 | G | 3 | 0 | 0 | 3 | 0 |
| 5 | H | 1 | 0 | 0 | 0 | 0 |
| 6 | A | 5 | 0 | 0 | 0 | 0 |
| 6 | C | 5 | 0 | 0 | 0 | 0 |
| 6 | E | 10 | 0 | 0 | 0 | 0 |
| 6 | G | 5 | 0 | 0 | 0 | 0 |
| 7 | A | 54 | 0 | 24 | 0 | 0 |
| 7 | C | 54 | 0 | 24 | 1 | 0 |
| 7 | E | 54 | 0 | 24 | 4 | 0 |
| 7 | G | 54 | 0 | 24 | 2 | 0 |
| 8 | A | 9 | 0 | 11 | 1 | 0 |
| 8 | C | 9 | 0 | 11 | 1 | 0 |
| 8 | E | 9 | 0 | 11 | 0 | 0 |
| 8 | G | 9 | 0 | 11 | 0 | 0 |
| 9 | A | 10 | 0 | 7 | 0 | 0 |
| 9 | B | 10 | 0 | 7 | 3 | 0 |
| 9 | C | 10 | 0 | 7 | 0 | 0 |
| 9 | D | 10 | 0 | 7 | 2 | 0 |
| 9 | E | 10 | 0 | 7 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | F | 10 | 0 | 7 | 3 | 0 |
| 9 | G | 10 | 0 | 7 | 0 | 0 |
| 9 | H | 10 | 0 | 7 | 2 | 0 |
| 10 | A | 9 | 0 | 20 | 0 | 0 |
| 10 | C | 9 | 0 | 20 | 1 | 0 |
| 10 | E | 9 | 0 | 20 | 2 | 0 |
| 10 | G | 9 | 0 | 20 | 0 | 0 |
| 11 | A | 699 | 0 | 0 | 14 | 0 |
| 11 | B | 231 | 0 | 0 | 4 | 0 |
| 11 | C | 706 | 0 | 0 | 19 | 0 |
| 11 | D | 250 | 0 | 0 | 5 | 0 |
| 11 | E | 754 | 0 | 0 | 23 | 0 |
| 11 | F | 231 | 0 | 0 | 4 | 0 |
| 11 | G | 622 | 0 | 0 | 20 | 0 |
| 11 | H | 173 | 0 | 0 | 4 | 0 |
| All | All | 48477 | 0 | 44656 | 1411 | 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 16.

All (1411) 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:E:808:VAL:HA | 1:E:811[B]:GLN:HE21 | 1.12 | 1.11 |
| 2:H:133:ILE:HD12 | 2:H:143:ALA:HB2 | 1.28 | 1.10 |
| 1:A:695:VAL:HG13 | 1:A:700:MET:HB3 | 1.36 | 1.08 |
| 1:C:695:VAL:HG11 | 1:C:701:ALA:HB2 | 1.38 | 1.04 |
| 2:H:187:GLU:HG2 | 2:H:215:ARG:HD2 | 1.35 | 1.03 |
| 1:G:784:GLN:H | 1:G:784:GLN:NE2 | 1.57 | 1.00 |
| 1:G:695:VAL:HG13 | 1:G:700:MET:HB3 | 1.44 | 0.99 |
| 1:C:1063:ILE:HD13 | 1:C:1068:MET:HG3 | 1.41 | 0.99 |
| 1:E:1002:GLN:HE22 | 1:E:1006[B]:LYS:NZ | 1.60 | 0.97 |
| 1:A:784:GLN:HE21 | 1:A:784:GLN:H | 0.98 | 0.96 |
| 1:A:784:GLN:H | 1:A:784:GLN:NE2 | 1.64 | 0.95 |
| 1:A:956[B]:ARG:HG2 | 1:A:956[B]:ARG:HH11 | 1.31 | 0.94 |
| 1:G:784:GLN:HE21 | 1:G:784:GLN:N | 1.64 | 0.94 |
| 2:B:187:GLU:HG2 | 2:B:215:ARG:HD2 | 1.47 | 0.93 |
| 1:A:38[A]:ARG:HG3 | 1:A:38[A]:ARG:HH11 | 1.34 | 0.93 |
| 1:E:696:THR:H | 1:E:700:MET:HE3 | 1.31 | 0.93 |
| 1:C:563:MET:HE3 | 1:C:635:PRO:HG3 | 1.51 | 0.92 |
| 1:C:38:ARG:HG3 | 1:C:38:ARG:HH11 | 1.35 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:D:228:VAL:HA | 2:D:231:MET:HE2 | 1.51 | 0.91 |
| 1:E:1002:GLN:HE22 | 1:E:1006[B]:LYS:HZ3 | 1.11 | 0.91 |
| 2:D:322:PRO:HB2 | 2:D:324:ASN:ND2 | 1.84 | 0.91 |
| 1:A:563:MET:HE3 | 1:A:635:PRO:HG3 | 1.53 | 0.90 |
| 1:G:1021:ARG:HG2 | 1:G:1021:ARG:HH11 | 1.38 | 0.89 |
| 1:C:1001:ILE:HD12 | 1:C:1002:GLN:N | 1.88 | 0.88 |
| 2:B:324:ASN:HD22 | 2:B:324:ASN:N | 1.70 | 0.88 |
| 1:E:808:VAL:HA | 1:E:811[B]:GLN:NE2 | 1.89 | 0.88 |
| 1:E:172:PHE:HB3 | 1:E:200:PRO:HG2 | 1.56 | 0.87 |
| 2:B:324:ASN:HD22 | 2:B:324:ASN:H | 1.18 | 0.87 |
| 1:C:994:VAL:HG13 | 1:C:1000:HIS:ND1 | 1.89 | 0.87 |
| 2:H:6:LEU:HD11 | 2:H:8:VAL:CG2 | 2.04 | 0.87 |
| 1:G:728:VAL:CG1 | 1:G:733:ASP:HB3 | 2.03 | 0.87 |
| 1:A:695:VAL:HG11 | 1:A:701:ALA:HB2 | 1.57 | 0.86 |
| 1:E:698:ILE:HG13 | 1:E:738:PHE:CD1 | 2.11 | 0.86 |
| 1:E:784:GLN:H | 1:E:784:GLN:NE2 | 1.73 | 0.86 |
| 1:C:687:LEU:CD1 | 1:C:812:GLN:HG2 | 2.05 | 0.85 |
| 1:G:563:MET:CE | 1:G:635:PRO:HG3 | 2.08 | 0.84 |
| 2:H:322:PRO:HB2 | 2:H:324:ASN:ND2 | 1.92 | 0.84 |
| 1:A:1001:ILE:HD12 | 1:A:1002:GLN:N | 1.90 | 0.84 |
| 2:B:285:LYS:HG3 | 2:B:314:PHE:CE1 | 2.12 | 0.84 |
| 1:E:784:GLN:H | 1:E:784:GLN:HE21 | 1.23 | 0.84 |
| 2:B:322:PRO:HB2 | 2:B:324:ASN:ND2 | 1.93 | 0.83 |
| 1:G:1063:ILE:HD13 | 1:G:1068:MET:HG3 | 1.59 | 0.83 |
| 1:C:670:ASP:HB3 | 1:C:677:ARG:HH21 | 1.43 | 0.83 |
| 2:F:228:VAL:HA | 2:F:231:MET:CE | 2.09 | 0.83 |
| 2:B:57:TYR:CD1 | 2:B:58:PRO:HD2 | 2.14 | 0.82 |
| 1:C:563:MET:CE | 1:C:635:PRO:HG3 | 2.09 | 0.82 |
| 1:C:4:ARG:HD3 | 1:C:7:ILE:HD12 | 1.59 | 0.82 |
| 2:F:322:PRO:HB2 | 2:F:324:ASN:ND2 | 1.94 | 0.82 |
| 2:H:6:LEU:HD11 | 2:H:8:VAL:HG23 | 1.62 | 0.82 |
| 2:D:241:GLY:O | 9:D:4034:GLN:HG3 | 1.80 | 0.81 |
| 2:H:187:GLU:HG2 | 2:H:215:ARG:CD | 2.10 | 0.81 |
| 1:G:663:GLY:HA3 | 1:G:869:MET:HE3 | 1.63 | 0.81 |
| 2:F:201:ALA:HB2 | 2:F:239:SER:CB | 2.10 | 0.81 |
| 1:C:670:ASP:HB3 | 1:C:677:ARG:NH2 | 1.97 | 0.80 |
| 1:A:734:LEU:HD12 | 1:A:734:LEU:O | 1.82 | 0.80 |
| 1:C:1001:ILE:HD12 | 1:C:1002:GLN:H | 1.44 | 0.80 |
| 1:A:38[B]:ARG:HG2 | 1:A:38[B]:ARG:HH11 | 1.43 | 0.80 |
| 1:A:313:LYS:HE2 | 1:A:608:THR:O | 1.82 | 0.80 |
| 2:D:322:PRO:HB2 | 2:D:324:ASN:HD21 | 1.45 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:B:324:ASN:H | 2:B:324:ASN:ND2 | 1.80 | 0.79 |
| 1:E:1002:GLN:NE2 | 1:E:1006[B]:LYS:NZ | 2.31 | 0.79 |
| 1:C:74:VAL:HG11 | 1:C:102:LEU:HD11 | 1.64 | 0.79 |
| 1:G:714:VAL:HG13 | 1:G:752:LEU:HD11 | 1.64 | 0.79 |
| 2:F:241:GLY:O | 9:F:4056:GLN:HG3 | 1.82 | 0.79 |
| 1:C:172:PHE:HB3 | 1:C:200:PRO:HG2 | 1.65 | 0.79 |
| 1:E:695:VAL:HG21 | 1:E:701:ALA:HA | 1.65 | 0.79 |
| 1:C:687:LEU:HD13 | 1:C:812:GLN:HG2 | 1.62 | 0.79 |
| 1:C:695:VAL:HG11 | 1:C:701:ALA:CB | 2.11 | 0.78 |
| 2:F:57:TYR:CD1 | 2:F:58:PRO:HD2 | 2.18 | 0.78 |
| 1:E:1:MET:HB2 | 1:E:224:LYS:NZ | 1.97 | 0.78 |
| 1:E:670:ASP:HB3 | 1:E:677:ARG:HH21 | 1.46 | 0.78 |
| 1:A:695:VAL:CG1 | 1:A:700:MET:HB3 | 2.14 | 0.77 |
| 1:E:151:THR:HB | 1:E:153[B]:GLU:OE2 | 1.85 | 0.77 |
| 1:C:1:MET:HB2 | 1:C:224:LYS:NZ | 1.99 | 0.77 |
| 1:G:181:ILE:HD11 | 1:G:376:THR:HG23 | 1.65 | 0.77 |
| 1:E:563:MET:HE3 | 1:E:635:PRO:HG3 | 1.66 | 0.77 |
| 1:E:1:MET:HB2 | 1:E:224:LYS:HZ2 | 1.47 | 0.77 |
| 1:G:64:THR:O | 1:G:1065:VAL:HG23 | 1.85 | 0.77 |
| 1:G:693:ALA:HB2 | 1:G:708:ILE:HD11 | 1.66 | 0.77 |
| 2:H:57:TYR:CD1 | 2:H:58:PRO:HD2 | 2.20 | 0.77 |
| 1:G:704:LYS:O | 1:G:708:ILE:HD12 | 1.85 | 0.77 |
| 2:F:201:ALA:HB2 | 2:F:239:SER:HB2 | 1.65 | 0.76 |
| 1:E:808:VAL:CA | 1:E:811[B]:GLN:HE21 | 1.94 | 0.76 |
| 1:G:903:VAL:HG13 | 11:G:3404:HOH:O | 1.86 | 0.76 |
| 2:H:195:VAL:HG23 | 2:H:233:PRO:HB3 | 1.67 | 0.76 |
| 2:D:228:VAL:HA | 2:D:231:MET:CE | 2.14 | 0.76 |
| 2:H:299:ASP:OD1 | 2:H:302:LYS:HD3 | 1.85 | 0.76 |
| 2:B:226:GLU:O | 2:B:230:LYS:HG3 | 1.86 | 0.76 |
| 2:D:324:ASN:H | 2:D:324:ASN:HD22 | 1.31 | 0.76 |
| 1:G:1026:SER:HB2 | 1:G:1030:ARG:HH12 | 1.50 | 0.76 |
| 1:C:363:ASN:HA | 1:C:365:GLU:OE2 | 1.86 | 0.76 |
| 1:G:858:GLY:HA2 | 1:G:1069:HIS:CE1 | 2.20 | 0.76 |
| 1:A:784:GLN:HE21 | 1:A:784:GLN:N | 1.80 | 0.76 |
| 1:G:528:ARG:HG2 | 1:G:543:MET:HG2 | 1.68 | 0.75 |
| 1:C:973:ALA:O | 1:C:991[A]:VAL:HG12 | 1.85 | 0.75 |
| 1:G:385:MET:HG2 | 1:G:618:PHE:CE1 | 2.21 | 0.75 |
| 2:H:324:ASN:HD22 | 2:H:324:ASN:H | 1.35 | 0.75 |
| 1:C:967:GLN:HG3 | 1:C:1054:LEU:HD13 | 1.69 | 0.75 |
| 1:E:153[A]:GLU:HG2 | 11:E:4283:HOH:O | 1.85 | 0.75 |
| 1:E:698:ILE:O | 1:E:702:VAL:HG23 | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:C:509:ARG:HD3 | 11:C:4652:HOH:O | 1.87 | 0.74 |
| 1:G:865:ALA:O | 1:G:869:MET:HG3 | 1.86 | 0.74 |
| 1:A:728:VAL:CG1 | 1:A:733:ASP:HB3 | 2.17 | 0.74 |
| 1:C:1:MET:HB2 | 1:C:224:LYS:HZ2 | 1.51 | 0.74 |
| 1:C:728:VAL:HG12 | 1:C:733:ASP:HB3 | 1.68 | 0.74 |
| 1:G:728:VAL:HG12 | 1:G:733:ASP:HB3 | 1.70 | 0.74 |
| 2:D:133:ILE:HD12 | 2:D:143:ALA:HB2 | 1.67 | 0.74 |
| 1:G:714:VAL:HG13 | 1:G:752:LEU:CD1 | 2.18 | 0.74 |
| 2:H:54:THR:HG21 | 2:H:118:LEU:HD23 | 1.70 | 0.74 |
| 2:F:150:PHE:CD2 | 2:F:151:PRO:HD2 | 2.23 | 0.73 |
| 2:H:71:GLU:O | 2:H:203:ARG:HG3 | 1.87 | 0.73 |
| 1:A:681:ALA:O | 1:A:685:LEU:HG | 1.88 | 0.73 |
| 2:B:71:GLU:O | 2:B:203:ARG:HG3 | 1.87 | 0.73 |
| 1:C:38:ARG:HG3 | 1:C:38:ARG:NH1 | 2.02 | 0.73 |
| 1:G:954:LYS:O | 1:G:957:VAL:HG12 | 1.88 | 0.73 |
| 1:E:682:VAL:HG13 | 1:E:687:LEU:HB2 | 1.70 | 0.73 |
| 1:A:772:MET:SD | 1:A:880:THR:HG22 | 2.29 | 0.73 |
| 1:G:905:PRO:HB2 | 1:G:1040:TYR:OH | 1.89 | 0.73 |
| 1:C:802:SER:O | 1:C:806:GLN:HG3 | 1.89 | 0.73 |
| 2:H:324:ASN:HD22 | 2:H:324:ASN:N | 1.87 | 0.73 |
| 1:A:973:ALA:O | 1:A:991:VAL:HG12 | 1.88 | 0.73 |
| 1:A:930:LYS:HE3 | 11:A:4162:HOH:O | 1.89 | 0.73 |
| 1:C:358:LYS:HE3 | 11:C:4153:HOH:O | 1.89 | 0.72 |
| 1:A:1017:THR:HG21 | 1:A:1023:ILE:HA | 1.71 | 0.72 |
| 1:C:400:ARG:HD3 | 11:C:4391:HOH:O | 1.88 | 0.72 |
| 1:G:873:SER:O | 1:G:877:GLN:HG3 | 1.89 | 0.72 |
| 2:H:228:VAL:HA | 2:H:231:MET:CE | 2.18 | 0.72 |
| 1:A:772:MET:HE2 | 1:A:880:THR:HA | 1.72 | 0.72 |
| 1:A:698:ILE:HD12 | 1:A:698:ILE:H | 1.54 | 0.72 |
| 1:E:863:LYS:O | 1:E:867:ARG:HG3 | 1.89 | 0.72 |
| 2:B:322:PRO:HB2 | 2:B:324:ASN:HD21 | 1.54 | 0.72 |
| 1:G:181:ILE:CD1 | 1:G:376:THR:HG23 | 2.20 | 0.72 |
| 2:F:251:ALA:O | 2:F:255:ILE:HD12 | 1.88 | 0.72 |
| 1:G:57:ASP:HB3 | 1:G:59:GLU:OE2 | 1.89 | 0.72 |
| 2:F:228:VAL:HA | 2:F:231:MET:HE2 | 1.72 | 0.72 |
| 1:A:318:PRO:HG3 | 1:A:610:TYR:OH | 1.88 | 0.72 |
| 2:D:187:GLU:HG2 | 2:D:215:ARG:HD2 | 1.72 | 0.72 |
| 1:E:1004:ARG:HD3 | 1:E:1009[B]:GLU:OE2 | 1.90 | 0.71 |
| 1:E:417:ASP:HB3 | 1:E:420:ALA:HB2 | 1.72 | 0.71 |
| 1:G:693:ALA:CB | 1:G:708:ILE:HD11 | 2.20 | 0.71 |
| 1:A:997:GLY:O | 1:A:998:ARG:HG3 | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:E:674:ASP:HB3 | 1:E:677:ARG:HG3 | 1.73 | 0.71 |
| 1:G:663:GLY:HA3 | 1:G:869:MET:CE | 2.21 | 0.71 |
| 1:G:734:LEU:HD12 | 1:G:734:LEU:O | 1.89 | 0.71 |
| 2:B:117:LYS:HE3 | 11:B:4071:HOH:O | 1.89 | 0.71 |
| 1:G:58:PRO:HD2 | 1:G:59:GLU:OE2 | 1.90 | 0.71 |
| 1:G:670:ASP:HB3 | 1:G:677:ARG:HH21 | 1.54 | 0.71 |
| 1:A:728:VAL:HG13 | 1:A:733:ASP:HB3 | 1.73 | 0.71 |
| 2:F:324:ASN:O | 2:F:342:ARG:HD2 | 1.91 | 0.70 |
| 2:D:246:ALA:HB3 | 2:D:247:PRO:HD3 | 1.73 | 0.70 |
| 2:D:259:LEU:HD13 | 2:D:342:ARG:NH1 | 2.06 | 0.70 |
| 1:G:998:ARG:HA | 1:G:999:PRO:C | 2.12 | 0.70 |
| 1:A:873:SER:O | 1:A:877:GLN:HG3 | 1.92 | 0.70 |
| 1:E:213:TRP:CZ3 | 1:E:296:ILE:HD12 | 2.27 | 0.70 |
| 1:A:38[A]:ARG:HG3 | 1:A:38[A]:ARG:NH1 | 2.02 | 0.70 |
| 2:H:133:ILE:CD1 | 2:H:143:ALA:HB2 | 2.16 | 0.70 |
| 1:C:726:GLU:HG3 | 1:C:727:ILE:H | 1.55 | 0.70 |
| 2:H:218:ILE:N | 2:H:218:ILE:HD13 | 2.07 | 0.69 |
| 1:G:548:GLU:HG2 | 2:H:114:ASP:CG | 2.12 | 0.69 |
| 1:E:126:ALA:HB3 | 1:E:302:PRO:HG3 | 1.73 | 0.69 |
| 1:C:998:ARG:HG2 | 1:C:999:PRO:HA | 1.73 | 0.69 |
| 2:D:57:TYR:CD1 | 2:D:58:PRO:HD2 | 2.27 | 0.69 |
| 1:E:3:LYS:HB3 | 1:E:330:TYR:CE1 | 2.27 | 0.69 |
| 2:F:324:ASN:H | 2:F:324:ASN:HD22 | 1.40 | 0.69 |
| 2:H:322:PRO:HB2 | 2:H:324:ASN:HD21 | 1.57 | 0.69 |
| 1:G:563:MET:HE3 | 1:G:635:PRO:HG3 | 1.75 | 0.69 |
| 1:A:172:PHE:HB3 | 1:A:200:PRO:HG2 | 1.74 | 0.69 |
| 1:E:1001:ILE:HD12 | 1:E:1002:GLN:N | 2.07 | 0.69 |
| 1:G:648:LEU:HD22 | 1:G:845:ARG:HD3 | 1.75 | 0.69 |
| 1:A:974:THR:HG21 | 1:A:993[B]:LYS:HD3 | 1.74 | 0.69 |
| 1:E:1:MET:N | 1:E:224:LYS:HE3 | 2.07 | 0.69 |
| 1:E:166:CYS:C | 1:E:167:ILE:HD12 | 2.13 | 0.69 |
| 2:F:187:GLU:HG2 | 2:F:215:ARG:HD2 | 1.73 | 0.69 |
| 2:H:6:LEU:HD12 | 2:H:7:LEU:N | 2.08 | 0.69 |
| 2:H:34:THR:HA | 2:H:56:THR:OG1 | 1.92 | 0.68 |
| 1:G:784:GLN:H | 1:G:784:GLN:HE21 | 0.79 | 0.68 |
| 2:H:286:MET:CE | 2:H:289:GLY:HA2 | 2.23 | 0.68 |
| 1:G:79:GLU:HG2 | 1:G:111:PHE:CE2 | 2.29 | 0.68 |
| 2:H:195:VAL:CG2 | 2:H:233:PRO:HB3 | 2.23 | 0.68 |
| 1:E:103:GLU:HG3 | 1:E:104:ARG:N | 2.06 | 0.68 |
| 1:C:659:VAL:HG13 | 1:C:660:PRO:HD2 | 1.74 | 0.68 |
| 1:C:726:GLU:HG3 | 1:C:727:ILE:N | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:734:LEU:HD11 | 1:A:738:PHE:CE2 | 2.29 | 0.68 |
| 1:C:883:VAL:O | 1:C:884:ILE:HD13 | 1.94 | 0.68 |
| 1:E:224:LYS:HE2 | 1:E:329:GLY:O | 1.94 | 0.68 |
| 1:G:563:MET:HE1 | 1:G:635:PRO:HG3 | 1.73 | 0.68 |
| 1:E:43:ARG:NH2 | 1:E:81:GLU:OE2 | 2.27 | 0.68 |
| 1:E:670:ASP:HB3 | 1:E:677:ARG:NH2 | 2.08 | 0.68 |
| 1:G:728:VAL:HG13 | 1:G:733:ASP:HB3 | 1.74 | 0.68 |
| 2:B:324:ASN:O | 2:B:342:ARG:HD2 | 1.94 | 0.67 |
| 1:C:1063:ILE:CD1 | 1:C:1068:MET:HG3 | 2.22 | 0.67 |
| 1:G:1001:ILE:HD12 | 1:G:1002:GLN:H | 1.60 | 0.67 |
| 1:E:1:MET:N | 11:E:4680:HOH:O | 2.25 | 0.67 |
| 1:E:1021:ARG:HG2 | 1:E:1021:ARG:HH11 | 1.57 | 0.67 |
| 1:G:734:LEU:HD11 | 1:G:738:PHE:CE2 | 2.29 | 0.67 |
| 2:B:187:GLU:HG2 | 2:B:215:ARG:CD | 2.22 | 0.67 |
| 1:E:696:THR:N | 1:E:700:MET:HE3 | 2.07 | 0.67 |
| 1:G:695:VAL:HG11 | 1:G:701:ALA:HB2 | 1.74 | 0.67 |
| 1:G:273:ARG:HD2 | 11:G:3191:HOH:O | 1.95 | 0.67 |
| 2:F:139:ASP:OD2 | 2:F:142:LEU:HB2 | 1.94 | 0.67 |
| 2:H:6:LEU:HD11 | 2:H:8:VAL:HG22 | 1.77 | 0.67 |
| 2:H:228:VAL:HA | 2:H:231:MET:HE2 | 1.76 | 0.67 |
| 1:G:4:ARG:HD3 | 1:G:7:ILE:HD12 | 1.76 | 0.67 |
| 1:G:475:LYS:O | 1:G:479:VAL:HG13 | 1.95 | 0.67 |
| 1:A:698:ILE:O | 1:A:701:ALA:HB3 | 1.95 | 0.66 |
| 2:H:55:LEU:HD13 | 2:H:60:ILE:HD12 | 1.77 | 0.66 |
| 1:A:563:MET:CE | 1:A:635:PRO:HG3 | 2.24 | 0.66 |
| 1:C:698:ILE:HD12 | 1:C:698:ILE:H | 1.61 | 0.66 |
| 1:G:166:CYS:C | 1:G:167:ILE:HD12 | 2.15 | 0.66 |
| 1:C:224:LYS:HE2 | 1:C:329:GLY:O | 1.95 | 0.66 |
| 1:A:772:MET:CE | 1:A:880:THR:HG22 | 2.26 | 0.66 |
| 1:C:695:VAL:HG13 | 1:C:700:MET:HB3 | 1.76 | 0.66 |
| 1:G:1:MET:HB2 | 1:G:224:LYS:NZ | 2.11 | 0.66 |
| 1:C:32:GLN:OE1 | 1:C:320:ALA:HB3 | 1.95 | 0.65 |
| 2:H:27:VAL:HG22 | 2:H:131:CYS:HB2 | 1.77 | 0.65 |
| 2:H:58:PRO:HA | 2:H:83:ARG:HB3 | 1.77 | 0.65 |
| 1:G:936:ASN:HB2 | 11:G:2917:HOH:O | 1.97 | 0.65 |
| 1:G:1030:ARG:NH1 | 1:G:1030:ARG:HG3 | 2.10 | 0.65 |
| 1:A:695:VAL:HG11 | 1:A:701:ALA:CB | 2.27 | 0.65 |
| 2:B:218:ILE:HD13 | 2:B:218:ILE:N | 2.12 | 0.65 |
| 2:D:64:GLY:HA3 | 2:D:94:ASN:OD1 | 1.97 | 0.65 |
| 1:G:695:VAL:CG1 | 1:G:700:MET:HB3 | 2.21 | 0.65 |
| 2:B:279:SER:O | 2:B:322:PRO:HG3 | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:954:LYS:O | 1:E:980:VAL:HG11 | 1.96 | 0.65 |
| 2:H:205:ILE:HG13 | 2:H:355:GLU:HG3 | 1.79 | 0.65 |
| 1:A:726:GLU:HG3 | 1:A:727:ILE:H | 1.62 | 0.65 |
| 1:C:708:ILE:HG21 | 1:C:712:LEU:HD11 | 1.79 | 0.65 |
| 2:F:8:VAL:HG22 | 2:F:14:GLN:HG2 | 1.78 | 0.65 |
| 2:F:232:ASN:N | 2:F:233:PRO:HD3 | 2.11 | 0.65 |
| 2:H:324:ASN:O | 2:H:342:ARG:HD2 | 1.97 | 0.65 |
| 1:C:652:ARG:NH1 | 1:C:670:ASP:OD2 | 2.30 | 0.64 |
| 2:D:205:ILE:HG13 | 2:D:355:GLU:HG3 | 1.79 | 0.64 |
| 1:G:772:MET:SD | 1:G:880:THR:HG22 | 2.37 | 0.64 |
| 1:C:154:GLU:OE1 | 11:C:4246:HOH:O | 2.15 | 0.64 |
| 1:C:1000:HIS:HD2 | 1:C:1003:ASP:H | 1.43 | 0.64 |
| 1:E:515:LYS:O | 1:E:515:LYS:HD3 | 1.98 | 0.64 |
| 1:E:343:ARG:NH2 | 11:E:4720:HOH:O | 2.30 | 0.64 |
| 2:F:218:ILE:HD13 | 2:F:218:ILE:N | 2.12 | 0.64 |
| 1:A:358:LYS:HE3 | 11:A:4129:HOH:O | 1.97 | 0.64 |
| 1:C:734:LEU:O | 1:C:734:LEU:HD12 | 1.97 | 0.64 |
| 1:A:67:GLU:HB3 | 1:A:68:PRO:HD2 | 1.79 | 0.64 |
| 2:B:249:ASP:OD2 | 2:B:250:TYR:N | 2.31 | 0.64 |
| 1:C:994:VAL:HG13 | 1:C:1000:HIS:CE1 | 2.31 | 0.64 |
| 2:H:286:MET:HE2 | 2:H:289:GLY:HA2 | 1.79 | 0.64 |
| 2:B:272:HIS:ND1 | 2:B:349:SER:OG | 2.30 | 0.64 |
| 1:E:947:LEU:HG | 1:E:1014:ILE:CG2 | 2.28 | 0.64 |
| 1:A:698:ILE:H | 1:A:698:ILE:CD1 | 2.11 | 0.64 |
| 2:F:186:LYS:O | 2:F:189:GLU:HB2 | 1.97 | 0.64 |
| 1:E:646:THR:HB | 1:E:647:PRO:HD3 | 1.80 | 0.64 |
| 1:G:1030:ARG:HG3 | 1:G:1030:ARG:HH11 | 1.63 | 0.64 |
| 1:A:1000:HIS:HD2 | 1:A:1003:ASP:H | 1.44 | 0.63 |
| 1:E:998:ARG:HG2 | 1:E:999:PRO:HA | 1.80 | 0.63 |
| 1:G:901:PRO:HD2 | 5:G:4084:CL:CL | 2.36 | 0.63 |
| 1:E:6:ASP:OD2 | 1:E:6:ASP:N | 2.29 | 0.63 |
| 1:A:259:LYS:HD3 | 2:B:175:TRP:CE3 | 2.34 | 0.63 |
| 1:A:648:LEU:HD22 | 1:A:845:ARG:HD3 | 1.79 | 0.63 |
| 1:G:981:LEU:HD12 | 1:G:988:PRO:HG3 | 1.79 | 0.63 |
| 1:A:38[B]:ARG:HG2 | 1:A:38[B]:ARG:NH1 | 2.04 | 0.63 |
| 1:C:695:VAL:CG1 | 1:C:701:ALA:HB2 | 2.24 | 0.63 |
| 1:E:728:VAL:HG13 | 1:E:733:ASP:HB3 | 1.80 | 0.63 |
| 1:A:956[B]:ARG:HG2 | 1:A:956[B]:ARG:NH1 | 2.03 | 0.63 |
| 1:A:976:GLY:O | 1:A:980:VAL:HG23 | 1.99 | 0.63 |
| 1:C:905:PRO:HB2 | 1:C:1040:TYR:OH | 1.98 | 0.63 |
| 1:G:698:ILE:HD12 | 1:G:698:ILE:H | 1.62 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:636:LYS:NZ | 11:A:4560:HOH:O | 2.30 | 0.63 |
| 2:D:212:ARG:HG3 | 2:D:212:ARG:HH11 | 1.63 | 0.63 |
| 1:E:151:THR:OG1 | 1:E:153[B]:GLU:HG2 | 1.99 | 0.63 |
| 1:G:817:ALA:HB2 | 1:G:826:MET:SD | 2.39 | 0.63 |
| 2:H:269:SER:HB3 | 9:H:4079:GLN:OE1 | 1.99 | 0.63 |
| 1:A:150:HIS:N | 1:A:154:GLU:OE2 | 2.32 | 0.62 |
| 1:C:890:VAL:HG23 | 1:C:927:ALA:HB1 | 1.79 | 0.62 |
| 2:F:225:ALA:O | 2:F:229:LEU:HG | 1.99 | 0.62 |
| 1:A:905:PRO:HB2 | 1:A:1040:TYR:OH | 2.00 | 0.62 |
| 1:C:734:LEU:HD11 | 1:C:738:PHE:CE2 | 2.34 | 0.62 |
| 1:C:1000:HIS:CD2 | 1:C:1003:ASP:H | 2.18 | 0.62 |
| 1:A:659:VAL:HG13 | 1:A:660:PRO:HD2 | 1.81 | 0.62 |
| 1:A:698:ILE:HD12 | 1:A:698:ILE:N | 2.13 | 0.62 |
| 2:F:322:PRO:HB2 | 2:F:324:ASN:HD21 | 1.64 | 0.62 |
| 1:C:947:LEU:N | 1:C:947:LEU:HD12 | 2.13 | 0.62 |
| 1:G:167:ILE:HD12 | 1:G:167:ILE:N | 2.15 | 0.62 |
| 1:A:4:ARG:HD3 | 1:A:7:ILE:HD12 | 1.82 | 0.62 |
| 1:A:726:GLU:HG3 | 1:A:727:ILE:N | 2.15 | 0.62 |
| 1:A:992:ASN:ND2 | 1:G:975:HIS:NE2 | 2.48 | 0.62 |
| 1:C:687:LEU:HD11 | 1:C:812:GLN:HG2 | 1.80 | 0.61 |
| 1:E:4:ARG:HA | 11:E:4160:HOH:O | 1.99 | 0.61 |
| 1:E:734:LEU:HD12 | 1:E:734:LEU:O | 2.00 | 0.61 |
| 1:G:757[B]:ASP:OD1 | 1:G:833:LYS:NZ | 2.33 | 0.61 |
| 2:H:328:THR:HG21 | 11:H:3665:HOH:O | 1.99 | 0.61 |
| 2:H:5:ALA:HB3 | 2:H:110:ILE:HG13 | 1.81 | 0.61 |
| 2:H:187:GLU:CG | 2:H:215:ARG:HD2 | 2.21 | 0.61 |
| 1:A:907:LEU:HD11 | 8:A:4011:ORN:HD3 | 1.82 | 0.61 |
| 1:A:858:GLY:HA2 | 1:A:1069:HIS:CE1 | 2.35 | 0.61 |
| 1:C:784:GLN:H | 1:C:784:GLN:HE21 | 1.49 | 0.61 |
| 1:E:167:ILE:HD12 | 1:E:167:ILE:N | 2.15 | 0.61 |
| 1:C:698:ILE:HD12 | 1:C:698:ILE:N | 2.16 | 0.61 |
| 1:E:1021:ARG:HH11 | 1:E:1021:ARG:CG | 2.14 | 0.61 |
| 2:H:244:ASP:OD2 | 2:H:245:PRO:HD2 | 2.00 | 0.61 |
| 1:A:1021:ARG:HH11 | 1:A:1021:ARG:CG | 2.13 | 0.61 |
| 1:G:805:ILE:HD12 | 1:G:832:VAL:HG11 | 1.83 | 0.61 |
| 1:C:416:ASP:O | 1:C:418:PRO:HD3 | 2.01 | 0.61 |
| 2:D:195:VAL:HG11 | 2:D:231:MET:HE1 | 1.81 | 0.61 |
| 1:C:728:VAL:HG11 | 1:C:734:LEU:HA | 1.83 | 0.61 |
| 2:H:284:VAL:O | 2:H:315:ALA:N | 2.33 | 0.61 |
| 1:C:812:GLN:NE2 | 11:C:4684:HOH:O | 2.06 | 0.60 |
| 1:A:375:THR:HG23 | 1:A:377:GLN:H | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:C:675:ARG:H | 1:C:675:ARG:CD | 2.11 | 0.60 |
| 2:F:170:TRP:HB3 | 2:F:216:LEU:HB2 | 1.82 | 0.60 |
| 1:G:1063:ILE:HD13 | 1:G:1068:MET:CG | 2.30 | 0.60 |
| 2:B:298:LYS:HE2 | 2:B:303:ASN:OD1 | 2.01 | 0.60 |
| 1:C:981:LEU:HD12 | 1:C:988:PRO:HG3 | 1.83 | 0.60 |
| 1:C:1017:THR:HG21 | 1:C:1023:ILE:HA | 1.84 | 0.60 |
| 1:G:10:ILE:HD12 | 1:G:42:TYR:HB3 | 1.83 | 0.60 |
| 1:A:956[A]:ARG:HD3 | 11:A:4668:HOH:O | 2.01 | 0.60 |
| 1:C:698:ILE:H | 1:C:698:ILE:CD1 | 2.15 | 0.60 |
| 1:C:951:GLU:HA | 1:C:954:LYS:HD2 | 1.82 | 0.60 |
| 1:G:1001:ILE:CD1 | 1:G:1002:GLN:N | 2.65 | 0.60 |
| 1:A:757:ASP:O | 1:A:833:LYS:NZ | 2.32 | 0.60 |
| 1:E:702:VAL:HG11 | 1:E:735:ARG:NH2 | 2.15 | 0.60 |
| 1:E:956[A]:ARG:HB3 | 1:E:1044:LEU:CD2 | 2.31 | 0.60 |
| 1:G:1:MET:HB2 | 1:G:224:LYS:HZ2 | 1.66 | 0.60 |
| 1:C:822:VAL:O | 1:C:823:ARG:HD3 | 2.01 | 0.60 |
| 1:C:1021:ARG:HH11 | 1:C:1021:ARG:HG3 | 1.65 | 0.60 |
| 2:F:228:VAL:HA | 2:F:231:MET:HE3 | 1.80 | 0.60 |
| 2:F:324:ASN:HD22 | 2:F:324:ASN:N | 1.99 | 0.60 |
| 2:H:158:LEU:CB | 2:H:242:PRO:HB2 | 2.31 | 0.60 |
| 1:A:1020:ARG:NH2 | 1:A:1023:ILE:HG21 | 2.17 | 0.60 |
| 1:C:890:VAL:HG23 | 1:C:927:ALA:CB | 2.31 | 0.60 |
| 1:E:812:GLN:NE2 | 11:E:4800:HOH:O | 2.35 | 0.60 |
| 2:H:33:ASN:HA | 2:H:291:HIS:O | 2.02 | 0.60 |
| 2:H:344:ASP:OD2 | 2:H:344:ASP:N | 2.34 | 0.60 |
| 2:B:186:LYS:O | 2:B:189:GLU:HB2 | 2.02 | 0.59 |
| 2:B:370:PHE:O | 2:B:374:ILE:HG13 | 2.02 | 0.59 |
| 1:G:676:GLU:O | 1:G:680:HIS:ND1 | 2.35 | 0.59 |
| 1:C:784:GLN:H | 1:C:784:GLN:NE2 | 1.99 | 0.59 |
| 1:E:563:MET:CE | 1:E:635:PRO:HG3 | 2.32 | 0.59 |
| 1:C:708:ILE:CG2 | 1:C:712:LEU:HD11 | 2.31 | 0.59 |
| 1:G:282:SER:N | 11:G:3572:HOH:O | 2.35 | 0.59 |
| 1:G:343:ARG:NH1 | 11:G:3545:HOH:O | 2.34 | 0.59 |
| 1:A:646:THR:HB | 1:A:647:PRO:HD3 | 1.83 | 0.59 |
| 1:A:954:LYS:O | 1:A:957:VAL:HG12 | 2.02 | 0.59 |
| 1:C:313:LYS:HE2 | 1:C:608:THR:O | 2.02 | 0.59 |
| 2:D:273:GLN:HE21 | 2:D:351:GLN:HE22 | 1.50 | 0.59 |
| 1:A:674:ASP:HB3 | 1:A:677:ARG:HG3 | 1.85 | 0.59 |
| 1:G:728:VAL:HG11 | 1:G:734:LEU:HA | 1.83 | 0.59 |
| 1:G:1000:HIS:HD2 | 1:G:1003:ASP:H | 1.50 | 0.59 |
| 2:B:246:ALA:HB3 | 2:B:247:PRO:HD3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:509:ARG:HH11 | 1:G:509:ARG:HB2 | 1.66 | 0.59 |
| 2:H:55:LEU:CD1 | 2:H:60:ILE:HD12 | 2.32 | 0.59 |
| 2:D:174:SER:O | 2:D:182:PRO:HD3 | 2.03 | 0.59 |
| 1:A:675:ARG:CD | 1:A:675:ARG:H | 2.15 | 0.59 |
| 1:A:906:LEU:O | 1:A:912:ARG:NH2 | 2.30 | 0.59 |
| 1:A:992:ASN:ND2 | 1:A:996:GLU:HB3 | 2.17 | 0.59 |
| 2:D:26:ALA:O | 2:D:131:CYS:HA | 2.03 | 0.59 |
| 1:C:509:ARG:NH1 | 1:C:512:GLU:OE1 | 2.35 | 0.59 |
| 1:C:954:LYS:O | 1:C:957:VAL:HG12 | 2.02 | 0.59 |
| 2:F:379:LYS:HZ3 | 2:F:379:LYS:HB2 | 1.67 | 0.59 |
| 1:E:1020:ARG:O | 1:E:1024:GLU:HG3 | 2.03 | 0.59 |
| 1:G:850:VAL:HB | 1:G:851:PRO:HD3 | 1.84 | 0.59 |
| 2:B:187:GLU:CG | 2:B:215:ARG:HD2 | 2.26 | 0.58 |
| 1:C:146:SER:HB2 | 1:C:205:LEU:HD11 | 1.85 | 0.58 |
| 1:A:315:THR:O | 1:A:531:THR:HG22 | 2.03 | 0.58 |
| 1:C:975:HIS:HE2 | 1:E:992:ASN:ND2 | 2.01 | 0.58 |
| 2:H:46:PRO:O | 2:H:242:PRO:HG3 | 2.03 | 0.58 |
| 1:C:133:ASP:OD2 | 11:C:4117:HOH:O | 2.17 | 0.58 |
| 2:H:324:ASN:ND2 | 2:H:324:ASN:H | 2.00 | 0.58 |
| 1:E:318:PRO:HG3 | 1:E:610:TYR:OH | 2.03 | 0.58 |
| 1:G:698:ILE:HD12 | 1:G:698:ILE:N | 2.18 | 0.58 |
| 2:B:46:PRO:HA | 2:B:76:HIS:CG | 2.37 | 0.58 |
| 1:C:447:LEU:HD23 | 1:G:446:GLY:O | 2.02 | 0.58 |
| 1:C:998:ARG:CG | 1:C:999:PRO:HA | 2.33 | 0.58 |
| 2:D:118:LEU:O | 2:D:118:LEU:HD12 | 2.04 | 0.58 |
| 1:E:805:ILE:CD1 | 1:E:837:VAL:HG23 | 2.33 | 0.58 |
| 2:H:363:ALA:C | 2:H:365:PRO:HD2 | 2.23 | 0.58 |
| 2:B:285:LYS:HG3 | 2:B:314:PHE:CD1 | 2.39 | 0.58 |
| 1:G:165:PRO:HA | 1:G:182:ALA:O | 2.04 | 0.58 |
| 1:C:980:VAL:HG13 | 11:C:4704:HOH:O | 2.03 | 0.58 |
| 1:C:1052:MET:HG2 | 11:C:4681:HOH:O | 2.04 | 0.58 |
| 2:F:269:SER:HB3 | 9:F:4056:GLN:OE1 | 2.04 | 0.58 |
| 1:G:1021:ARG:HH11 | 1:G:1021:ARG:CG | 2.12 | 0.58 |
| 1:C:728:VAL:CG1 | 1:C:733:ASP:HB3 | 2.33 | 0.58 |
| 1:G:667:ASP:CG | 1:G:677:ARG:HH22 | 2.07 | 0.58 |
| 1:A:272:LEU:HD11 | 1:A:282:SER:HB2 | 1.85 | 0.58 |
| 2:B:350:PHE:HB2 | 2:B:366:LEU:HD22 | 1.86 | 0.58 |
| 1:C:1063:ILE:HD13 | 1:C:1068:MET:CG | 2.26 | 0.58 |
| 1:A:863:LYS:HE2 | 11:A:4575:HOH:O | 2.03 | 0.57 |
| 2:D:350:PHE:HB2 | 2:D:366:LEU:HD22 | 1.86 | 0.57 |
| 1:G:809:MET:O | 1:G:813:VAL:HG23 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:166:CYS:C | 1:A:167:ILE:HD12 | 2.25 | 0.57 |
| 1:A:964:LEU:O | 1:A:969:PHE:HB2 | 2.03 | 0.57 |
| 2:B:313:GLY:HA3 | 11:B:4020:HOH:O | 2.04 | 0.57 |
| 1:C:103:GLU:HG3 | 1:C:104:ARG:N | 2.15 | 0.57 |
| 1:C:695:VAL:CG1 | 1:C:700:MET:HB3 | 2.34 | 0.57 |
| 2:D:6:LEU:HD13 | 2:D:16:HIS:CE1 | 2.39 | 0.57 |
| 1:C:479:VAL:CG2 | 1:C:483:GLY:HA3 | 2.34 | 0.57 |
| 1:E:1000:HIS:HD2 | 1:E:1003:ASP:H | 1.52 | 0.57 |
| 2:F:48:TYR:HA | 2:F:51:GLN:HE21 | 1.69 | 0.57 |
| 2:H:246:ALA:HB3 | 2:H:247:PRO:HD3 | 1.85 | 0.57 |
| 1:E:194:ARG:HD3 | 11:E:4114:HOH:O | 2.04 | 0.57 |
| 1:G:237:PHE:CE2 | 1:G:458:ILE:HD13 | 2.40 | 0.57 |
| 2:H:133:ILE:HG22 | 2:H:138:PRO:HB3 | 1.85 | 0.57 |
| 1:A:40:GLU:CG | 1:A:325:LYS:HE2 | 2.35 | 0.57 |
| 1:A:1011:THR:HG23 | 11:A:4539:HOH:O | 2.04 | 0.57 |
| 1:E:213:TRP:CE2 | 1:E:289:ASN:HB2 | 2.39 | 0.57 |
| 1:G:729:TYR:CE1 | 1:G:1019:GLY:HA2 | 2.39 | 0.57 |
| 1:G:560:GLU:OE1 | 1:G:636:LYS:HE3 | 2.05 | 0.57 |
| 2:H:78:GLN:HA | 2:H:78:GLN:NE2 | 2.19 | 0.57 |
| 1:E:1017:THR:HG22 | 1:E:1023:ILE:HG13 | 1.87 | 0.57 |
| 1:A:194:ARG:NH2 | 11:A:4602:HOH:O | 2.28 | 0.57 |
| 2:D:286:MET:CE | 2:D:312:HIS:ND1 | 2.67 | 0.57 |
| 1:E:691:ALA:HB3 | 1:E:708:ILE:HG23 | 1.86 | 0.57 |
| 2:B:195:VAL:HG23 | 2:B:233:PRO:HB3 | 1.86 | 0.57 |
| 1:C:419[B]:GLU:OE1 | 1:G:422:THR:HG21 | 2.05 | 0.57 |
| 1:C:559:ARG:HG3 | 1:C:559:ARG:HH11 | 1.69 | 0.57 |
| 1:E:344:THR:HB | 1:E:345:PRO:HD2 | 1.87 | 0.57 |
| 1:E:693:ALA:HB3 | 1:E:708:ILE:HD11 | 1.86 | 0.57 |
| 2:B:139:ASP:OD2 | 2:B:142:LEU:HB2 | 2.05 | 0.56 |
| 1:C:901:PRO:HD2 | 5:C:4039:CL:CL | 2.42 | 0.56 |
| 1:G:417:ASP:HB3 | 1:G:420:ALA:HB2 | 1.87 | 0.56 |
| 1:A:321:LYS:NZ | 1:A:611:ASP:OD1 | 2.36 | 0.56 |
| 1:A:562:ILE:HG21 | 1:A:589:LEU:CD1 | 2.35 | 0.56 |
| 2:F:253:THR:O | 2:F:256:GLN:HB2 | 2.05 | 0.56 |
| 1:A:344:THR:HB | 1:A:345:PRO:HD2 | 1.86 | 0.56 |
| 2:B:150:PHE:CD2 | 2:B:151:PRO:HD2 | 2.40 | 0.56 |
| 1:C:40:GLU:OE1 | 1:C:325:LYS:HE2 | 2.04 | 0.56 |
| 1:C:375:THR:HG23 | 1:C:377:GLN:H | 1.69 | 0.56 |
| 1:C:672:ALA:HB3 | 1:C:844:PRO:HG3 | 1.86 | 0.56 |
| 1:C:693:ALA:HB1 | 1:C:704:LYS:HG2 | 1.86 | 0.56 |
| 2:F:350:PHE:HB2 | 2:F:366:LEU:HD22 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:534:ALA:O | 2:H:123:ARG:HD3 | 2.05 | 0.56 |
| 1:A:672:ALA:HB3 | 1:A:844:PRO:HG3 | 1.87 | 0.56 |
| 1:A:973:ALA:C | 1:A:991:VAL:HG12 | 2.26 | 0.56 |
| 1:A:998:ARG:CB | 1:A:999:PRO:HA | 2.34 | 0.56 |
| 1:E:196:LEU:HG | 1:E:204:LEU:HD11 | 1.86 | 0.56 |
| 1:E:698:ILE:HG13 | 1:E:738:PHE:CG | 2.39 | 0.56 |
| 1:G:349:GLU:O | 2:H:294:ASN:HB2 | 2.04 | 0.56 |
| 1:G:954:LYS:O | 1:G:980:VAL:HG11 | 2.06 | 0.56 |
| 1:E:726:GLU:HG3 | 1:E:1020:ARG:NH2 | 2.21 | 0.56 |
| 1:E:1019:GLY:O | 1:E:1023:ILE:HD12 | 2.05 | 0.56 |
| 1:A:489:LEU:HD22 | 1:A:516:LEU:HD23 | 1.86 | 0.56 |
| 1:C:695:VAL:HG21 | 1:C:752:LEU:HD22 | 1.88 | 0.56 |
| 1:G:569:PRO:O | 1:G:571:ARG:HD2 | 2.06 | 0.56 |
| 1:C:3:LYS:HG2 | 11:C:4580:HOH:O | 2.04 | 0.56 |
| 2:D:286:MET:HE3 | 2:D:312:HIS:ND1 | 2.21 | 0.56 |
| 2:F:272:HIS:HA | 2:F:349:SER:HB2 | 1.88 | 0.56 |
| 2:H:248:CYS:O | 2:H:252:ILE:HG13 | 2.06 | 0.56 |
| 2:D:44:THR:O | 2:D:46:PRO:HD3 | 2.06 | 0.56 |
| 1:G:1001:ILE:HD12 | 1:G:1002:GLN:N | 2.20 | 0.56 |
| 2:H:139:ASP:OD2 | 2:H:142:LEU:HB2 | 2.06 | 0.56 |
| 1:A:682:VAL:HG11 | 1:A:689:GLN:HE21 | 1.71 | 0.56 |
| 1:E:757:ASP:O | 1:E:833:LYS:NZ | 2.27 | 0.56 |
| 1:G:964:LEU:O | 1:G:969:PHE:HB2 | 2.06 | 0.56 |
| 1:G:679:GLN:HG2 | 1:G:689:GLN:HE22 | 1.71 | 0.55 |
| 2:H:169:SER:HA | 2:H:216:LEU:O | 2.07 | 0.55 |
| 2:H:228:VAL:HA | 2:H:231:MET:HE3 | 1.86 | 0.55 |
| 1:A:700:MET:O | 1:A:704:LYS:HB2 | 2.06 | 0.55 |
| 1:A:1020:ARG:HH21 | 1:A:1023:ILE:HG21 | 1.70 | 0.55 |
| 2:B:172:GLN:O | 2:B:207:ARG:HA | 2.06 | 0.55 |
| 2:B:259:LEU:O | 2:B:345:LYS:HE3 | 2.07 | 0.55 |
| 1:C:1048:PHE:O | 1:C:1052:MET:HG3 | 2.07 | 0.55 |
| 1:G:548:GLU:HG2 | 2:H:114:ASP:OD1 | 2.05 | 0.55 |
| 1:C:858:GLY:HA2 | 1:C:1069:HIS:NE2 | 2.21 | 0.55 |
| 1:C:1068:MET:O | 1:C:1071:GLN:HB2 | 2.07 | 0.55 |
| 1:G:956:ARG:HB3 | 1:G:1044:LEU:CD2 | 2.36 | 0.55 |
| 1:A:103:GLU:HG2 | 1:A:108:LEU:HD12 | 1.89 | 0.55 |
| 1:A:948:SER:O | 1:A:1015:ASN:HA | 2.06 | 0.55 |
| 2:B:46:PRO:HA | 2:B:76:HIS:CB | 2.37 | 0.55 |
| 1:C:735:ARG:O | 1:C:738:PHE:HB2 | 2.07 | 0.55 |
| 2:D:178:THR:HB | 11:D:1596:HOH:O | 2.06 | 0.55 |
| 1:E:998:ARG:HA | 1:E:999:PRO:C | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:668:ALA:O | 1:G:671:ARG:HB2 | 2.07 | 0.55 |
| 1:C:761:GLU:HG2 | 1:C:781:HIS:CE1 | 2.41 | 0.55 |
| 1:E:950:ARG:HD3 | 11:E:4812:HOH:O | 2.06 | 0.55 |
| 1:A:88:PRO:HB3 | 1:A:99:ALA:HB2 | 1.88 | 0.55 |
| 1:A:695:VAL:HG11 | 1:A:701:ALA:CA | 2.37 | 0.55 |
| 1:A:947:LEU:N | 1:A:947:LEU:HD12 | 2.21 | 0.55 |
| 1:C:222:ARG:NH1 | 1:C:273:ARG:HA | 2.21 | 0.55 |
| 1:C:735:ARG:O | 1:C:738:PHE:N | 2.39 | 0.55 |
| 2:D:206:LEU:O | 2:D:210:VAL:HG23 | 2.07 | 0.55 |
| 1:E:1:MET:H2 | 1:E:224:LYS:HE3 | 1.70 | 0.55 |
| 1:G:556:SER:HB2 | 1:G:558:ASP:HB2 | 1.88 | 0.55 |
| 2:B:350:PHE:HB2 | 2:B:366:LEU:CD2 | 2.37 | 0.55 |
| 2:B:364:ALA:N | 2:B:365:PRO:HD2 | 2.22 | 0.55 |
| 2:D:240:ASN:HB2 | 9:D:4034:GLN:OE1 | 2.06 | 0.55 |
| 1:A:167:ILE:HD12 | 1:A:167:ILE:N | 2.22 | 0.54 |
| 2:D:46:PRO:HA | 2:D:76:HIS:CG | 2.41 | 0.54 |
| 1:E:652:ARG:NH2 | 1:E:667:ASP:OD2 | 2.40 | 0.54 |
| 1:E:695:VAL:HG11 | 1:E:701:ALA:HB2 | 1.88 | 0.54 |
| 2:F:259:LEU:HD13 | 2:F:342:ARG:NH1 | 2.22 | 0.54 |
| 2:B:46:PRO:O | 2:B:242:PRO:HG3 | 2.06 | 0.54 |
| 2:D:285:LYS:HG3 | 2:D:314:PHE:CE1 | 2.42 | 0.54 |
| 1:A:28:TYR:O | 1:A:32:GLN:HG3 | 2.07 | 0.54 |
| 1:C:992:ASN:ND2 | 1:C:996:GLU:HB3 | 2.23 | 0.54 |
| 1:E:897:PHE:HB3 | 11:E:4620:HOH:O | 2.08 | 0.54 |
| 1:G:674:ASP:HB3 | 1:G:677:ARG:HG3 | 1.88 | 0.54 |
| 2:H:173:GLY:O | 2:H:207:ARG:HG2 | 2.08 | 0.54 |
| 1:C:702:VAL:HG11 | 1:C:735:ARG:NH2 | 2.21 | 0.54 |
| 1:G:701:ALA:O | 1:G:705:ALA:N | 2.30 | 0.54 |
| 1:C:695:VAL:HG21 | 1:C:701:ALA:HA | 1.87 | 0.54 |
| 1:E:185:ARG:HG2 | 1:E:189:GLU:OE2 | 2.07 | 0.54 |
| 2:F:78:GLN:NE2 | 11:F:2502:HOH:O | 2.33 | 0.54 |
| 1:G:540:THR:HG22 | 1:G:541:ALA:N | 2.23 | 0.54 |
| 1:A:79:GLU:HB2 | 1:A:111:PHE:CZ | 2.42 | 0.54 |
| 1:A:695:VAL:HG21 | 1:A:701:ALA:HA | 1.90 | 0.54 |
| 1:C:353:ASP:OD1 | 2:D:116:ARG:HD2 | 2.08 | 0.54 |
| 1:E:196:LEU:HG | 1:E:204:LEU:CD1 | 2.37 | 0.54 |
| 1:E:703:GLU:O | 1:E:706:LYS:HB2 | 2.07 | 0.54 |
| 1:E:726:GLU:HG3 | 1:E:1020:ARG:HH21 | 1.72 | 0.54 |
| 1:G:181:ILE:HD11 | 1:G:376:THR:CG2 | 2.35 | 0.54 |
| 1:G:947:LEU:HA | 1:G:1014:ILE:HG23 | 1.89 | 0.54 |
| 1:E:730:ASP:O | 1:E:733:ASP:HB2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:E:956[B]:ARG:HB3 | 1:E:1044:LEU:CD2 | 2.37 | 0.54 |
| 1:G:671:ARG:NH2 | 1:G:819:GLU:O | 2.40 | 0.54 |
| 1:C:257:THR:HG23 | 2:D:91:ASN:ND2 | 2.23 | 0.54 |
| 1:C:670:ASP:CB | 1:C:677:ARG:HH21 | 2.18 | 0.54 |
| 2:H:186:LYS:O | 2:H:189:GLU:HB2 | 2.08 | 0.54 |
| 1:A:17:PRO:HG3 | 1:A:917:VAL:CG1 | 2.38 | 0.54 |
| 1:A:998:ARG:HG2 | 1:A:999:PRO:HA | 1.90 | 0.54 |
| 2:D:244:ASP:OD2 | 2:D:245:PRO:HD2 | 2.08 | 0.54 |
| 1:E:289:ASN:OD1 | 1:E:290:PRO:HD2 | 2.08 | 0.54 |
| 1:E:710:TYR:HB3 | 1:E:729:TYR:O | 2.08 | 0.54 |
| 1:E:802:SER:OG | 1:E:805:ILE:HB | 2.08 | 0.54 |
| 1:E:808:VAL:HA | 1:E:811[B]:GLN:HG3 | 1.90 | 0.54 |
| 1:G:148:ILE:HG22 | 1:G:149:ALA:N | 2.22 | 0.54 |
| 1:C:761:GLU:HB3 | 1:C:781:HIS:ND1 | 2.23 | 0.53 |
| 1:G:922:ARG:NH2 | 1:G:1060:GLU:OE2 | 2.41 | 0.53 |
| 2:H:299:ASP:HA | 2:H:329:HIS:CD2 | 2.42 | 0.53 |
| 1:C:237:PHE:HB3 | 1:C:248:ILE:O | 2.07 | 0.53 |
| 1:G:475:LYS:HD3 | 1:G:488:PHE:CZ | 2.43 | 0.53 |
| 2:D:355:GLU:OE2 | 2:D:355:GLU:N | 2.37 | 0.53 |
| 1:G:172:PHE:HB3 | 1:G:200:PRO:HG2 | 1.90 | 0.53 |
| 1:A:289:ASN:OD1 | 1:A:290:PRO:HD2 | 2.07 | 0.53 |
| 1:A:362:PHE:CE1 | 1:A:380:SER:HB3 | 2.43 | 0.53 |
| 1:E:682:VAL:CG1 | 1:E:687:LEU:HB2 | 2.38 | 0.53 |
| 1:E:905:PRO:HB2 | 1:E:1040:TYR:OH | 2.09 | 0.53 |
| 1:G:1017:THR:HG21 | 1:G:1023:ILE:HA | 1.89 | 0.53 |
| 2:H:193:HIS:O | 2:H:234:ASP:HB2 | 2.08 | 0.53 |
| 2:H:352:GLY:O | 2:H:354:PRO:HD3 | 2.08 | 0.53 |
| 2:H:365:PRO:HA | 2:H:368:ASP:OD1 | 2.08 | 0.53 |
| 1:E:1002:GLN:NE2 | 1:E:1006[B]:LYS:HZ2 | 2.05 | 0.53 |
| 2:F:272:HIS:HA | 2:F:349:SER:CB | 2.39 | 0.53 |
| 1:G:1000:HIS:CD2 | 1:G:1003:ASP:H | 2.25 | 0.53 |
| 1:A:481:ILE:HG22 | 11:A:4626:HOH:O | 2.08 | 0.53 |
| 1:A:695:VAL:HG11 | 1:A:701:ALA:N | 2.23 | 0.53 |
| 2:B:105:HIS:ND1 | 11:B:4218:HOH:O | 2.34 | 0.53 |
| 1:C:252:PRO:HD3 | 1:C:352:ILE:HD11 | 1.90 | 0.53 |
| 1:C:956:ARG:HB3 | 1:C:1044:LEU:CD2 | 2.38 | 0.53 |
| 1:E:695:VAL:HG13 | 1:E:700:MET:HB3 | 1.89 | 0.53 |
| 1:E:930:LYS:HE3 | 11:E:4218:HOH:O | 2.09 | 0.53 |
| 1:G:475:LYS:NZ | 11:G:3293:HOH:O | 2.33 | 0.53 |
| 1:A:4:ARG:CD | 1:A:7:ILE:HD12 | 2.39 | 0.53 |
| 1:A:687:LEU:HD22 | 1:A:812:GLN:HG2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:713:VAL:HG12 | 1:A:713:VAL:O | 2.08 | 0.53 |
| 1:E:947:LEU:HD12 | 1:E:947:LEU:N | 2.24 | 0.53 |
| 1:A:1023:ILE:HG22 | 1:A:1024:GLU:N | 2.23 | 0.53 |
| 1:E:1:MET:H3 | 1:E:224:LYS:HE3 | 1.73 | 0.53 |
| 1:G:340:THR:O | 1:G:343:ARG:HB2 | 2.09 | 0.53 |
| 2:H:29:GLU:OE1 | 2:H:285:LYS:NZ | 2.31 | 0.53 |
| 2:H:46:PRO:HA | 2:H:76:HIS:CG | 2.43 | 0.53 |
| 1:A:1000:HIS:CD2 | 1:A:1003:ASP:H | 2.24 | 0.53 |
| 1:C:695:VAL:HG11 | 1:C:701:ALA:N | 2.23 | 0.53 |
| 1:C:695:VAL:HG11 | 1:C:701:ALA:CA | 2.38 | 0.53 |
| 1:A:331:THR:O | 1:A:334:GLU:HB2 | 2.09 | 0.53 |
| 1:A:734:LEU:HD12 | 1:A:734:LEU:C | 2.25 | 0.53 |
| 2:B:354:PRO:HB2 | 2:B:367:PHE:CE2 | 2.44 | 0.53 |
| 1:C:676:GLU:O | 1:C:680:HIS:ND1 | 2.42 | 0.53 |
| 2:H:156:MET:HG2 | 2:H:158:LEU:HG | 1.91 | 0.53 |
| 1:G:1001:ILE:O | 1:G:1005:ILE:HG13 | 2.08 | 0.52 |
| 2:H:133:ILE:HD12 | 2:H:143:ALA:CB | 2.19 | 0.52 |
| 2:B:41:GLU:OE2 | 2:B:41:GLU:N | 2.36 | 0.52 |
| 1:C:762:VAL:HG13 | 1:C:779:MET:O | 2.08 | 0.52 |
| 2:D:286:MET:HE2 | 2:D:314:PHE:C | 2.30 | 0.52 |
| 1:E:103:GLU:HG2 | 11:E:4778:HOH:O | 2.09 | 0.52 |
| 1:E:701:ALA:O | 1:E:705:ALA:N | 2.28 | 0.52 |
| 1:E:734:LEU:HD12 | 1:E:734:LEU:C | 2.27 | 0.52 |
| 2:F:197:TYR:HB3 | 2:F:199:PHE:CZ | 2.44 | 0.52 |
| 1:G:40:GLU:CG | 1:G:325:LYS:HE2 | 2.39 | 0.52 |
| 1:G:761:GLU:HG2 | 1:G:781:HIS:CE1 | 2.44 | 0.52 |
| 1:E:213:TRP:HZ3 | 1:E:296:ILE:HD12 | 1.74 | 0.52 |
| 1:G:151:THR:HG21 | 11:G:3075:HOH:O | 2.09 | 0.52 |
| 1:A:659:VAL:CG1 | 1:A:660:PRO:HD2 | 2.39 | 0.52 |
| 1:G:695:VAL:HG21 | 1:G:701:ALA:HA | 1.90 | 0.52 |
| 1:C:805:ILE:HD13 | 1:C:837:VAL:CG2 | 2.40 | 0.52 |
| 2:D:266:PHE:HB2 | 2:D:370:PHE:CD1 | 2.44 | 0.52 |
| 2:F:259:LEU:HD13 | 2:F:342:ARG:HH12 | 1.75 | 0.52 |
| 2:F:324:ASN:HA | 2:F:343:THR:OG1 | 2.10 | 0.52 |
| 1:G:993:LYS:NZ | 11:G:3612:HOH:O | 2.29 | 0.52 |
| 1:A:419:GLU:HG3 | 11:E:4704:HOH:O | 2.10 | 0.52 |
| 1:C:110:GLU:HG2 | 1:C:111:PHE:CE1 | 2.44 | 0.52 |
| 2:D:156:MET:HA | 11:D:1820:HOH:O | 2.10 | 0.52 |
| 2:F:197:TYR:O | 2:F:239:SER:HB3 | 2.10 | 0.52 |
| 1:G:158:VAL:O | 1:G:161:ASP:HB3 | 2.10 | 0.52 |
| 1:G:361:ARG:CZ | 1:G:571:ARG:HG2 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:G:1036:TYR:C | 1:G:1037:LYS:HG2 | 2.28 | 0.52 |
| 2:H:193:HIS:NE2 | 2:H:217:THR:OG1 | 2.27 | 0.52 |
| 2:B:322:PRO:CB | 2:B:324:ASN:HD21 | 2.22 | 0.52 |
| 2:F:205:ILE:HG12 | 2:F:355:GLU:CG | 2.40 | 0.52 |
| 1:G:489:LEU:HD13 | 1:G:522:LEU:HD23 | 1.92 | 0.52 |
| 1:A:556:SER:HB2 | 1:A:558:ASP:HB2 | 1.92 | 0.52 |
| 1:A:986:ILE:O | 1:A:988:PRO:HD3 | 2.10 | 0.52 |
| 2:D:272:HIS:HA | 2:D:349:SER:HB2 | 1.90 | 0.52 |
| 2:H:168:TYR:CE2 | 2:H:218:ILE:HG12 | 2.44 | 0.52 |
| 2:H:264:PRO:HB3 | 2:H:373:LEU:HB3 | 1.91 | 0.52 |
| 2:D:246:ALA:HB3 | 2:D:247:PRO:CD | 2.39 | 0.52 |
| 1:E:784:GLN:HE21 | 1:E:784:GLN:N | 2.00 | 0.52 |
| 1:E:956[A]:ARG:HB3 | 1:E:1044:LEU:HD21 | 1.91 | 0.52 |
| 1:A:975:HIS:HE2 | 1:G:992:ASN:HD21 | 1.58 | 0.52 |
| 1:A:975:HIS:HE2 | 1:G:992:ASN:ND2 | 2.08 | 0.52 |
| 1:C:321:LYS:NZ | 1:C:611:ASP:OD1 | 2.39 | 0.52 |
| 2:D:272:HIS:HA | 2:D:349:SER:CB | 2.40 | 0.52 |
| 1:E:28:TYR:CZ | 1:E:313:LYS:HE3 | 2.45 | 0.52 |
| 1:G:79:GLU:HG2 | 1:G:111:PHE:CZ | 2.45 | 0.52 |
| 1:G:868:VAL:HG23 | 1:G:877:GLN:NE2 | 2.25 | 0.52 |
| 1:A:349:GLU:O | 2:B:294:ASN:HB2 | 2.10 | 0.51 |
| 1:C:695:VAL:CG2 | 1:C:752:LEU:HD22 | 2.40 | 0.51 |
| 2:B:27:VAL:O | 2:B:78:GLN:HG2 | 2.10 | 0.51 |
| 1:E:1061:LYS:HE2 | 11:E:4658:HOH:O | 2.09 | 0.51 |
| 1:G:950:ARG:HD3 | 11:G:3654:HOH:O | 2.10 | 0.51 |
| 1:A:101:GLU:OE2 | 1:A:101:GLU:HA | 2.11 | 0.51 |
| 1:C:997:GLY:O | 1:C:998:ARG:HG3 | 2.10 | 0.51 |
| 1:G:1030:ARG:HH11 | 1:G:1030:ARG:CG | 2.23 | 0.51 |
| 2:D:279:SER:O | 2:D:322:PRO:HG3 | 2.09 | 0.51 |
| 2:F:279:SER:O | 2:F:322:PRO:HG3 | 2.10 | 0.51 |
| 1:G:1:MET:N | 1:G:224:LYS:HE3 | 2.25 | 0.51 |
| 1:G:18:ILE:HG23 | 1:G:23:ALA:HA | 1.91 | 0.51 |
| 1:G:47:VAL:HG13 | 1:G:47:VAL:O | 2.10 | 0.51 |
| 1:G:796:LEU:C | 1:G:796:LEU:HD23 | 2.31 | 0.51 |
| 2:H:174:SER:HB2 | 2:H:211:ASP:OD2 | 2.10 | 0.51 |
| 1:C:673:GLU:O | 1:C:675:ARG:NH1 | 2.43 | 0.51 |
| 2:D:48:TYR:HA | 2:D:51:GLN:HE21 | 1.75 | 0.51 |
| 1:E:966:LYS:O | 1:E:966:LYS:HG3 | 2.10 | 0.51 |
| 2:B:249:ASP:HB3 | 11:B:4178:HOH:O | 2.10 | 0.51 |
| 2:B:364:ALA:N | 2:B:365:PRO:CD | 2.73 | 0.51 |
| 1:E:258:ASP:O | 1:E:262:GLN:HG2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:858:GLY:HA2 | 1:E:1069:HIS:CE1 | 2.45 | 0.51 |
| 1:G:292:ASN:OD1 | 1:G:294:ARG:HB2 | 2.10 | 0.51 |
| 1:A:222:ARG:CZ | 1:A:273:ARG:HG2 | 2.41 | 0.51 |
| 1:C:740:THR:O | 1:C:741:ALA:O | 2.29 | 0.51 |
| 1:E:3:LYS:HB2 | 1:E:42:TYR:OH | 2.10 | 0.51 |
| 1:E:1001:ILE:O | 1:E:1005:ILE:HG13 | 2.11 | 0.51 |
| 2:F:257:LYS:O | 2:F:260:GLU:HB2 | 2.11 | 0.51 |
| 1:C:539:ASP:HB2 | 11:C:4614:HOH:O | 2.09 | 0.51 |
| 1:E:1048:PHE:O | 1:E:1052:MET:HG3 | 2.11 | 0.51 |
| 1:G:339:ILE:HD12 | 1:G:530:ASP:HA | 1.93 | 0.51 |
| 1:G:713:VAL:HG23 | 1:G:755:PHE:HB2 | 1.91 | 0.51 |
| 1:G:734:LEU:CD1 | 1:G:738:PHE:CE2 | 2.94 | 0.51 |
| 1:A:527:LYS:HB2 | 1:A:544:TYR:CZ | 2.46 | 0.51 |
| 1:C:127:GLU:HB2 | 1:C:172:PHE:CZ | 2.45 | 0.51 |
| 1:C:344:THR:HB | 1:C:345:PRO:HD2 | 1.93 | 0.51 |
| 1:E:998:ARG:CG | 1:E:999:PRO:HA | 2.40 | 0.51 |
| 1:E:817:ALA:HB2 | 1:E:826:MET:SD | 2.50 | 0.51 |
| 1:G:28:TYR:CZ | 1:G:313:LYS:HE3 | 2.45 | 0.51 |
| 1:G:692:ASN:HA | 1:G:752:LEU:O | 2.11 | 0.51 |
| 2:H:158:LEU:HB3 | 2:H:242:PRO:HB2 | 1.92 | 0.51 |
| 2:B:66:ASN:HB3 | 2:B:93:ARG:O | 2.12 | 0.50 |
| 1:C:669:ILE:HA | 1:C:844:PRO:HG2 | 1.92 | 0.50 |
| 2:D:353:HIS:CE1 | 11:D:1634:HOH:O | 2.64 | 0.50 |
| 1:E:62:ASP:OD2 | 11:E:4634:HOH:O | 2.18 | 0.50 |
| 1:E:1000:HIS:CD2 | 1:E:1003:ASP:H | 2.29 | 0.50 |
| 1:G:150:HIS:CD2 | 1:G:203:GLU:HB2 | 2.46 | 0.50 |
| 1:G:730:ASP:H | 1:G:733:ASP:HB2 | 1.76 | 0.50 |
| 2:H:158:LEU:HB2 | 2:H:242:PRO:HB2 | 1.92 | 0.50 |
| 2:D:218:ILE:HD13 | 2:D:218:ILE:N | 2.27 | 0.50 |
| 2:D:286:MET:CE | 2:D:315:ALA:HB2 | 2.40 | 0.50 |
| 2:D:327:VAL:HG13 | 2:D:337:LEU:CD1 | 2.41 | 0.50 |
| 1:G:1000:HIS:NE2 | 1:G:1002:GLN:HB3 | 2.27 | 0.50 |
| 2:H:48:TYR:HA | 2:H:51:GLN:HE21 | 1.75 | 0.50 |
| 2:H:81:VAL:CG1 | 2:H:113:ILE:HD11 | 2.42 | 0.50 |
| 1:A:333:ASP:OD1 | 1:A:333:ASP:N | 2.44 | 0.50 |
| 1:A:526:TYR:CE1 | 1:A:545:SER:HB3 | 2.46 | 0.50 |
| 1:C:858:GLY:HA2 | 1:C:1069:HIS:CE1 | 2.46 | 0.50 |
| 1:E:126:ALA:CB | 1:E:302:PRO:HG3 | 2.39 | 0.50 |
| 1:G:361:ARG:NH2 | 1:G:571:ARG:HG2 | 2.27 | 0.50 |
| 2:H:6:LEU:HD12 | 2:H:7:LEU:H | 1.76 | 0.50 |
| 2:H:250:TYR:CD2 | 2:H:250:TYR:N | 2.79 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:470:VAL:O | 1:A:474:GLU:HG3 | 2.11 | 0.50 |
| 1:A:672:ALA:CB | 1:A:844:PRO:HG3 | 2.41 | 0.50 |
| 1:C:289:ASN:HB3 | 1:C:292:ASN:OD1 | 2.11 | 0.50 |
| 1:C:726:GLU:CG | 1:C:727:ILE:N | 2.74 | 0.50 |
| 1:A:728:VAL:HG12 | 1:A:733:ASP:HB3 | 1.92 | 0.50 |
| 1:G:698:ILE:O | 1:G:701:ALA:HB3 | 2.12 | 0.50 |
| 1:G:729:TYR:HE1 | 1:G:1019:GLY:HA2 | 1.76 | 0.50 |
| 1:A:11:LEU:HA | 1:A:45:ILE:O | 2.11 | 0.50 |
| 1:A:950:ARG:HD3 | 11:A:4711:HOH:O | 2.11 | 0.50 |
| 1:C:11:LEU:HA | 1:C:45:ILE:O | 2.12 | 0.50 |
| 2:D:354:PRO:HB2 | 2:D:367:PHE:CE2 | 2.46 | 0.50 |
| 1:E:234:ILE:HG23 | 1:E:250:VAL:O | 2.11 | 0.50 |
| 1:E:693:ALA:CB | 1:E:708:ILE:HD11 | 2.42 | 0.50 |
| 1:C:562:ILE:HG21 | 1:C:589:LEU:CD1 | 2.42 | 0.50 |
| 1:E:393:GLU:HA | 1:E:496:GLY:HA3 | 1.94 | 0.50 |
| 1:G:947:LEU:HG | 1:G:1014:ILE:CG2 | 2.41 | 0.50 |
| 2:D:232:ASN:N | 2:D:233:PRO:HD3 | 2.27 | 0.50 |
| 1:A:710:TYR:HB3 | 1:A:729:TYR:O | 2.11 | 0.50 |
| 2:B:290:HIS:HB2 | 2:B:312:HIS:NE2 | 2.27 | 0.50 |
| 1:C:527:LYS:HB2 | 1:C:544:TYR:CZ | 2.47 | 0.50 |
| 2:D:174:SER:HB2 | 2:D:211:ASP:OD2 | 2.12 | 0.50 |
| 2:D:237:PHE:CZ | 2:D:268:ILE:HD12 | 2.47 | 0.50 |
| 1:E:808:VAL:O | 1:E:811[B]:GLN:HG3 | 2.11 | 0.50 |
| 1:G:126:ALA:HB3 | 1:G:302:PRO:HG3 | 1.93 | 0.50 |
| 1:G:294:ARG:HD2 | 5:G:4083:CL:CL | 2.49 | 0.50 |
| 2:H:324:ASN:ND2 | 2:H:324:ASN:N | 2.58 | 0.50 |
| 1:A:417:ASP:OD1 | 1:A:423:LYS:NZ | 2.35 | 0.49 |
| 1:A:704:LYS:O | 1:A:707:GLU:HB2 | 2.11 | 0.49 |
| 1:A:1001:ILE:O | 1:A:1005:ILE:HG13 | 2.12 | 0.49 |
| 2:D:370:PHE:O | 2:D:374:ILE:HG13 | 2.12 | 0.49 |
| 1:E:358:LYS:HG2 | 1:E:359:ILE:N | 2.26 | 0.49 |
| 2:F:32:PHE:O | 2:F:291:HIS:HB2 | 2.11 | 0.49 |
| 2:H:16:HIS:O | 2:H:113:ILE:HG22 | 2.12 | 0.49 |
| 2:B:290:HIS:HB2 | 2:B:312:HIS:CD2 | 2.47 | 0.49 |
| 1:C:288:VAL:O | 1:C:290:PRO:HD3 | 2.12 | 0.49 |
| 1:C:713:VAL:HG12 | 1:C:713:VAL:O | 2.12 | 0.49 |
| 2:D:324:ASN:ND2 | 2:D:324:ASN:H | 2.06 | 0.49 |
| 1:E:67:GLU:HB3 | 1:E:68:PRO:HD2 | 1.94 | 0.49 |
| 1:G:103:GLU:HG3 | 1:G:104:ARG:N | 2.19 | 0.49 |
| 1:G:636:LYS:HD3 | 11:G:3354:HOH:O | 2.11 | 0.49 |
| 1:A:947:LEU:N | 1:A:947:LEU:CD1 | 2.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:F:174:SER:HB2 | 2:F:211:ASP:OD2 | 2.12 | 0.49 |
| 2:F:322:PRO:HD2 | 2:F:325:LEU:HD12 | 1.93 | 0.49 |
| 1:G:167:ILE:N | 1:G:167:ILE:CD1 | 2.75 | 0.49 |
| 2:F:376:GLN:O | 2:F:376:GLN:HG2 | 2.08 | 0.49 |
| 1:A:150:HIS:CD2 | 1:A:203:GLU:HG3 | 2.47 | 0.49 |
| 1:C:972:ASP:OD2 | 1:C:991[B]:VAL:HG21 | 2.12 | 0.49 |
| 2:B:270:LEU:HA | 2:B:273:GLN:OE1 | 2.13 | 0.49 |
| 2:F:39:TYR:CZ | 2:F:61:GLY:HA2 | 2.47 | 0.49 |
| 2:F:249:ASP:OD2 | 2:F:250:TYR:N | 2.45 | 0.49 |
| 1:G:434:ASP:HB2 | 11:G:3231:HOH:O | 2.12 | 0.49 |
| 1:G:1005:ILE:HG21 | 1:G:1032:SER:HB3 | 1.93 | 0.49 |
| 1:G:1021:ARG:HG2 | 1:G:1021:ARG:NH1 | 2.16 | 0.49 |
| 1:A:278:GLU:HG2 | 11:A:4597:HOH:O | 2.13 | 0.49 |
| 2:B:245:PRO:HG3 | 2:B:273:GLN:OE1 | 2.13 | 0.49 |
| 1:C:802:SER:OG | 1:C:805:ILE:HB | 2.13 | 0.49 |
| 1:E:738:PHE:O | 1:E:741:ALA:HB3 | 2.12 | 0.49 |
| 2:F:269:SER:O | 2:F:272:HIS:HB3 | 2.13 | 0.49 |
| 1:G:56:THR:OG1 | 1:G:855:LYS:NZ | 2.34 | 0.49 |
| 1:C:130:ARG:HG3 | 1:C:148:ILE:HG13 | 1.95 | 0.49 |
| 1:E:1020:ARG:HA | 1:E:1020:ARG:HD3 | 1.46 | 0.49 |
| 1:G:441:ASP:OD2 | 1:G:444:ARG:NH1 | 2.44 | 0.49 |
| 1:A:106:GLY:HA2 | 11:A:4176:HOH:O | 2.13 | 0.49 |
| 1:A:981:LEU:CD1 | 1:A:988:PRO:HG3 | 2.43 | 0.49 |
| 1:C:110:GLU:HG2 | 1:C:111:PHE:CD1 | 2.48 | 0.49 |
| 1:C:534:ALA:HB2 | 2:D:116:ARG:NH1 | 2.27 | 0.49 |
| 2:H:153:LEU:HA | 2:H:156:MET:HE3 | 1.95 | 0.49 |
| 1:A:3:LYS:HB3 | 1:A:330:TYR:CE1 | 2.47 | 0.49 |
| 1:C:805:ILE:CD1 | 1:C:837:VAL:HG23 | 2.43 | 0.49 |
| 1:E:760:VAL:HG11 | 1:E:801:LEU:HD11 | 1.94 | 0.49 |
| 1:G:298:ILE:HG13 | 11:G:3128:HOH:O | 2.11 | 0.49 |
| 1:G:738:PHE:O | 1:G:741:ALA:HB3 | 2.13 | 0.49 |
| 1:G:951:GLU:HA | 1:G:954:LYS:HD2 | 1.94 | 0.49 |
| 1:G:967:GLN:HG3 | 1:G:1054:LEU:HD13 | 1.95 | 0.49 |
| 1:G:1017:THR:HG22 | 1:G:1018:SER:N | 2.28 | 0.49 |
| 2:D:212:ARG:HH11 | 2:D:212:ARG:CG | 2.25 | 0.48 |
| 2:H:48:TYR:O | 2:H:51:GLN:HB2 | 2.12 | 0.48 |
| 1:A:665:SER:O | 1:A:669:ILE:HG13 | 2.12 | 0.48 |
| 1:G:710:TYR:HB3 | 1:G:729:TYR:O | 2.12 | 0.48 |
| 1:E:493:LYS:HE2 | 1:E:517:ARG:HD3 | 1.95 | 0.48 |
| 1:A:562:ILE:HG21 | 1:A:589:LEU:HD12 | 1.94 | 0.48 |
| 1:A:726:GLU:CG | 1:A:727:ILE:N | 2.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:196:ALA:HB3 | 2:B:218:ILE:HD12 | 1.94 | 0.48 |
| 1:C:18:ILE:HG23 | 1:C:23:ALA:HA | 1.95 | 0.48 |
| 1:E:349:GLU:O | 2:F:294:ASN:HB2 | 2.13 | 0.48 |
| 2:F:275:LEU:HD23 | 2:F:349:SER:OG | 2.13 | 0.48 |
| 1:G:481:ILE:HD13 | 1:G:508:VAL:HG11 | 1.94 | 0.48 |
| 2:H:176:THR:O | 2:H:180:GLY:N | 2.40 | 0.48 |
| 1:A:558:ASP:HB3 | 1:A:559:ARG:H | 1.38 | 0.48 |
| 1:C:240:MET:HE2 | 1:C:287:ALA:HB2 | 1.96 | 0.48 |
| 2:F:48:TYR:HA | 2:F:51:GLN:NE2 | 2.28 | 0.48 |
| 1:G:67:GLU:HB3 | 1:G:68:PRO:HD2 | 1.94 | 0.48 |
| 1:G:734:LEU:HD12 | 1:G:734:LEU:C | 2.30 | 0.48 |
| 1:G:830:PHE:CE1 | 1:G:839:LEU:HD13 | 2.48 | 0.48 |
| 1:C:209:SER:OG | 1:C:211:ILE:HG13 | 2.14 | 0.48 |
| 1:E:347:SER:O | 2:F:296:PRO:HB3 | 2.14 | 0.48 |
| 2:F:125:LYS:NZ | 11:F:2862:HOH:O | 2.46 | 0.48 |
| 2:F:201:ALA:CB | 2:F:239:SER:HB2 | 2.38 | 0.48 |
| 1:A:954:LYS:O | 1:A:980:VAL:HG11 | 2.14 | 0.48 |
| 1:A:972:ASP:OD1 | 1:A:989:ARG:HB3 | 2.14 | 0.48 |
| 2:B:205:ILE:HG21 | 2:B:237:PHE:CZ | 2.48 | 0.48 |
| 1:E:671:ARG:NH2 | 1:E:819:GLU:O | 2.47 | 0.48 |
| 2:F:34:THR:HA | 2:F:56:THR:OG1 | 2.13 | 0.48 |
| 1:G:726:GLU:CG | 1:G:727:ILE:N | 2.77 | 0.48 |
| 2:H:285:LYS:HG3 | 2:H:314:PHE:CE1 | 2.49 | 0.48 |
| 1:A:167:ILE:N | 1:A:167:ILE:CD1 | 2.77 | 0.48 |
| 1:A:761:GLU:HB3 | 1:A:781:HIS:ND1 | 2.29 | 0.48 |
| 1:C:993:LYS:O | 1:C:1000:HIS:HB3 | 2.14 | 0.48 |
| 1:G:240:MET:HE3 | 7:G:4068:ADP:C4 | 2.49 | 0.48 |
| 1:G:579:ASP:OD1 | 1:G:605:THR:HB | 2.14 | 0.48 |
| 1:A:693:ALA:CB | 1:A:708:ILE:HD11 | 2.43 | 0.48 |
| 1:A:891:LYS:NZ | 11:A:4492:HOH:O | 2.47 | 0.48 |
| 1:C:698:ILE:O | 1:C:702:VAL:HG23 | 2.14 | 0.48 |
| 2:D:269:SER:O | 2:D:272:HIS:HB3 | 2.14 | 0.48 |
| 1:E:170:PRO:HA | 1:E:204:LEU:HD23 | 1.95 | 0.48 |
| 1:E:448:SER:O | 1:E:452:VAL:HG23 | 2.14 | 0.48 |
| 2:F:286:MET:HE1 | 2:F:312:HIS:O | 2.13 | 0.48 |
| 1:G:1:MET:H1 | 1:G:224:LYS:HE3 | 1.79 | 0.48 |
| 1:G:679:GLN:HG2 | 1:G:689:GLN:NE2 | 2.28 | 0.48 |
| 2:H:218:ILE:N | 2:H:218:ILE:CD1 | 2.75 | 0.48 |
| 1:A:467:GLU:O | 1:A:471:ARG:HG2 | 2.14 | 0.48 |
| 1:A:525:VAL:HG22 | 1:A:548:GLU:H | 1.79 | 0.48 |
| 1:C:4:ARG:CD | 1:C:7:ILE:HD12 | 2.37 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 2:D:7:LEU:HD23 | 2:D:15:PHE:CD2 | 2.49 | 0.48 |
| 2:D:85:LEU:HD12 | 2:D:86:PRO:HD2 | 1.95 | 0.48 |
| 2:D:87:LEU:HD12 | 2:D:87:LEU:HA | 1.50 | 0.48 |
| 1:E:804:GLU:O | 1:E:808:VAL:HG23 | 2.14 | 0.48 |
| 1:G:956:ARG:HB3 | 1:G:1044:LEU:HD21 | 1.96 | 0.48 |
| 1:A:89:THR:O | 1:A:304:VAL:HG22 | 2.14 | 0.47 |
| 2:B:173:GLY:O | 2:B:207:ARG:HG2 | 2.14 | 0.47 |
| 2:B:232:ASN:N | 2:B:233:PRO:HD3 | 2.30 | 0.47 |
| 1:E:726:GLU:CG | 1:E:727:ILE:N | 2.77 | 0.47 |
| 2:F:322:PRO:HB2 | 2:F:324:ASN:HD22 | 1.77 | 0.47 |
| 1:G:805:ILE:HD12 | 1:G:832:VAL:CG1 | 2.43 | 0.47 |
| 2:H:322:PRO:CB | 2:H:324:ASN:HD21 | 2.24 | 0.47 |
| 1:A:17:PRO:HG3 | 1:A:917:VAL:HG13 | 1.95 | 0.47 |
| 1:C:668:ALA:O | 1:C:671:ARG:HB2 | 2.15 | 0.47 |
| 1:C:703:GLU:HA | 1:C:703:GLU:OE2 | 2.14 | 0.47 |
| 1:C:973:ALA:C | 1:C:991[A]:VAL:HG12 | 2.33 | 0.47 |
| 1:G:738:PHE:HA | 1:G:741:ALA:HB3 | 1.96 | 0.47 |
| 1:A:1:MET:HB2 | 1:A:224:LYS:NZ | 2.29 | 0.47 |
| 1:A:730:ASP:H | 1:A:733:ASP:HB2 | 1.77 | 0.47 |
| 1:E:278:GLU:HG2 | 11:E:4235:HOH:O | 2.14 | 0.47 |
| 1:E:525:VAL:HG22 | 1:E:548:GLU:H | 1.78 | 0.47 |
| 2:H:39:TYR:CZ | 2:H:61:GLY:HA2 | 2.50 | 0.47 |
| 1:A:82:ARG:NH1 | 1:A:82:ARG:HG3 | 2.30 | 0.47 |
| 1:A:224:LYS:HE2 | 1:A:329:GLY:O | 2.14 | 0.47 |
| 1:E:383:GLU:OE2 | 1:E:604:GLU:OE1 | 2.32 | 0.47 |
| 2:F:106:ASN:ND2 | 11:F:2545:HOH:O | 2.47 | 0.47 |
| 2:F:164:THR:O | 2:F:220:PRO:HB3 | 2.15 | 0.47 |
| 1:G:423:LYS:HB3 | 11:G:3274:HOH:O | 2.14 | 0.47 |
| 1:A:951:GLU:HA | 1:A:954:LYS:HD2 | 1.96 | 0.47 |
| 1:A:998:ARG:HA | 1:A:999:PRO:C | 2.32 | 0.47 |
| 2:B:205:ILE:O | 2:B:209:LEU:HG | 2.15 | 0.47 |
| 2:B:222:GLN:HA | 2:B:250:TYR:CD1 | 2.50 | 0.47 |
| 1:C:865:ALA:O | 1:C:869:MET:HG3 | 2.13 | 0.47 |
| 1:C:992:ASN:O | 1:C:1000:HIS:HA | 2.14 | 0.47 |
| 1:G:906:LEU:O | 1:G:912:ARG:NH2 | 2.31 | 0.47 |
| 1:A:728:VAL:HG11 | 1:A:734:LEU:HA | 1.97 | 0.47 |
| 1:C:3:LYS:HB3 | 1:C:330:TYR:CE1 | 2.50 | 0.47 |
| 1:C:704:LYS:HD2 | 1:C:707:GLU:OE1 | 2.14 | 0.47 |
| 1:C:737:TYR:O | 1:C:741:ALA:HB2 | 2.15 | 0.47 |
| 1:C:1000:HIS:CD2 | 1:C:1000:HIS:H | 2.33 | 0.47 |
| 1:G:1000:HIS:CD2 | 1:G:1002:GLN:HB3 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:8:VAL:HG12 | 2:H:9:LEU:N | 2.29 | 0.47 |
| 1:A:693:ALA:HB2 | 1:A:708:ILE:HD11 | 1.96 | 0.47 |
| 1:A:734:LEU:CD1 | 1:A:738:PHE:CE2 | 2.98 | 0.47 |
| 1:C:167:ILE:HG13 | 1:C:181:ILE:HG12 | 1.96 | 0.47 |
| 1:E:698:ILE:CD1 | 1:E:698:ILE:N | 2.77 | 0.47 |
| 1:E:841:GLU:HB2 | 11:E:4625:HOH:O | 2.15 | 0.47 |
| 1:E:1017:THR:CG2 | 1:E:1023:ILE:HG13 | 2.43 | 0.47 |
| 2:F:236:ILE:O | 2:F:265:VAL:HA | 2.15 | 0.47 |
| 2:F:259:LEU:O | 2:F:345:LYS:HE2 | 2.15 | 0.47 |
| 1:G:224:LYS:HE2 | 1:G:329:GLY:O | 2.14 | 0.47 |
| 1:G:339:ILE:CD1 | 1:G:530:ASP:HA | 2.45 | 0.47 |
| 1:G:863:LYS:O | 1:G:867:ARG:HG3 | 2.14 | 0.47 |
| 1:G:1017:THR:CG2 | 1:G:1018:SER:N | 2.77 | 0.47 |
| 1:G:1026:SER:CB | 1:G:1030:ARG:HH12 | 2.22 | 0.47 |
| 2:H:272:HIS:HB2 | 2:H:349:SER:HB2 | 1.95 | 0.47 |
| 2:H:322:PRO:HD2 | 2:H:325:LEU:HD12 | 1.97 | 0.47 |
| 1:A:184:ASN:O | 1:A:188:PHE:HB2 | 2.15 | 0.47 |
| 1:A:772:MET:CE | 1:A:880:THR:HA | 2.44 | 0.47 |
| 1:C:64:THR:O | 1:C:1065:VAL:HG23 | 2.14 | 0.47 |
| 1:C:294:ARG:HD2 | 5:C:4038:CL:CL | 2.51 | 0.47 |
| 1:C:986:ILE:O | 1:C:988:PRO:HD3 | 2.14 | 0.47 |
| 2:F:244:ASP:OD2 | 2:F:245:PRO:HD2 | 2.14 | 0.47 |
| 1:A:361:ARG:CZ | 1:A:571:ARG:HG2 | 2.45 | 0.47 |
| 1:A:698:ILE:O | 1:A:702:VAL:HG23 | 2.15 | 0.47 |
| 1:C:130:ARG:HB2 | 1:C:148:ILE:HD12 | 1.95 | 0.47 |
| 1:E:500:ALA:O | 1:E:504:LYS:HG3 | 2.15 | 0.47 |
| 2:F:26:ALA:O | 2:F:131:CYS:HA | 2.15 | 0.47 |
| 1:A:1021:ARG:HH11 | 1:A:1021:ARG:HG2 | 1.80 | 0.47 |
| 1:C:74:VAL:CG1 | 1:C:102:LEU:HD11 | 2.42 | 0.47 |
| 1:C:808:VAL:HA | 1:C:811[B]:GLN:OE1 | 2.14 | 0.47 |
| 2:D:118:LEU:HD12 | 2:D:118:LEU:C | 2.36 | 0.47 |
| 1:E:904:ASP:O | 1:E:906:LEU:N | 2.45 | 0.47 |
| 2:F:83:ARG:O | 2:F:112:ASP:HA | 2.15 | 0.47 |
| 1:G:11:LEU:HA | 1:G:45:ILE:O | 2.14 | 0.47 |
| 1:A:24:CYS:SG | 1:A:576:ILE:HB | 2.55 | 0.46 |
| 2:D:133:ILE:CD1 | 2:D:143:ALA:HB2 | 2.39 | 0.46 |
| 1:E:458:ILE:O | 1:E:463:LEU:HD11 | 2.15 | 0.46 |
| 1:E:1017:THR:HG21 | 1:E:1023:ILE:HA | 1.97 | 0.46 |
| 1:G:670:ASP:HB3 | 1:G:677:ARG:NH2 | 2.28 | 0.46 |
| 2:H:40:GLN:HE21 | 2:H:70:GLU:HG2 | 1.80 | 0.46 |
| 2:H:332:LEU:HD12 | 2:H:332:LEU:HA | 1.53 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:383:GLU:OE2 | 1:A:604:GLU:OE1 | 2.34 | 0.46 |
| 2:B:42:ILE:HG23 | 2:B:48:TYR:CE2 | 2.51 | 0.46 |
| 1:C:318:PRO:HB2 | 1:C:321:LYS:HB2 | 1.97 | 0.46 |
| 1:E:1017:THR:HG22 | 1:E:1018:SER:N | 2.30 | 0.46 |
| 2:F:55:LEU:HD13 | 2:F:60:ILE:HD12 | 1.97 | 0.46 |
| 1:G:277:VAL:O | 1:G:277:VAL:HG12 | 2.15 | 0.46 |
| 2:H:45:ASP:HB3 | 2:H:48:TYR:HD2 | 1.80 | 0.46 |
| 1:A:9:SER:OG | 1:A:83:PRO:HA | 2.16 | 0.46 |
| 1:A:469:LEU:O | 1:A:473:GLU:HG3 | 2.15 | 0.46 |
| 2:D:173:GLY:O | 2:D:207:ARG:HG2 | 2.15 | 0.46 |
| 2:D:286:MET:HE1 | 2:D:315:ALA:HB2 | 1.97 | 0.46 |
| 1:E:678:PHE:O | 1:E:681:ALA:N | 2.48 | 0.46 |
| 1:G:148:ILE:CG2 | 1:G:149:ALA:N | 2.78 | 0.46 |
| 2:H:325:LEU:HD23 | 2:H:325:LEU:HA | 1.68 | 0.46 |
| 1:C:4:ARG:HD3 | 1:C:7:ILE:CD1 | 2.40 | 0.46 |
| 1:C:733:ASP:OD1 | 1:C:736:ARG:NH1 | 2.48 | 0.46 |
| 2:D:274:LEU:HD23 | 2:D:274:LEU:HA | 1.69 | 0.46 |
| 1:E:734:LEU:O | 1:E:737:TYR:HB3 | 2.14 | 0.46 |
| 2:H:144:LEU:HD12 | 2:H:144:LEU:O | 2.16 | 0.46 |
| 1:A:40:GLU:HG2 | 1:A:325:LYS:HE2 | 1.97 | 0.46 |
| 2:B:121:LEU:O | 2:B:121:LEU:HD12 | 2.15 | 0.46 |
| 1:C:3:LYS:HB2 | 1:C:42:TYR:OH | 2.16 | 0.46 |
| 1:C:51:PRO:HG3 | 1:C:918:MET:HB2 | 1.97 | 0.46 |
| 1:C:66:ILE:CG2 | 1:C:918:MET:HB3 | 2.45 | 0.46 |
| 1:C:166:CYS:C | 1:C:167:ILE:HD12 | 2.35 | 0.46 |
| 2:F:225:ALA:HA | 2:F:258:PHE:CZ | 2.49 | 0.46 |
| 1:G:702:VAL:O | 1:G:706:LYS:HD3 | 2.15 | 0.46 |
| 1:G:939:MET:HE1 | 1:G:1050:THR:HG21 | 1.97 | 0.46 |
| 1:C:885:PRO:HG2 | 11:C:4735:HOH:O | 2.16 | 0.46 |
| 1:C:990:LEU:HD13 | 1:E:990:LEU:HD22 | 1.98 | 0.46 |
| 10:C:4036:NET:H71 | 10:C:4036:NET:H23 | 1.62 | 0.46 |
| 2:D:45:ASP:HB3 | 2:D:48:TYR:HD2 | 1.80 | 0.46 |
| 2:D:201:ALA:HB2 | 2:D:239:SER:CB | 2.46 | 0.46 |
| 1:E:735:ARG:O | 1:E:738:PHE:HB2 | 2.16 | 0.46 |
| 1:G:598:MET:HG3 | 1:G:599:VAL:N | 2.31 | 0.46 |
| 1:G:874:LEU:HB3 | 1:G:879:VAL:O | 2.16 | 0.46 |
| 2:H:286:MET:HE2 | 2:H:286:MET:HB3 | 1.83 | 0.46 |
| 1:C:77:ILE:O | 1:C:81:GLU:N | 2.43 | 0.46 |
| 1:C:365:GLU:H | 1:C:365:GLU:HG3 | 1.04 | 0.46 |
| 1:E:412:LYS:HG2 | 1:E:438:TYR:CZ | 2.51 | 0.46 |
| 1:E:1017:THR:CG2 | 1:E:1018:SER:N | 2.78 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:F:46:PRO:HA | 2:F:76:HIS:CG | 2.50 | 0.46 |
| 2:H:249:ASP:HB3 | 11:H:3526:HOH:O | 2.14 | 0.46 |
| 2:H:300:VAL:HG22 | 2:H:328:THR:O | 2.16 | 0.46 |
| 2:F:332:LEU:HD12 | 2:F:332:LEU:HA | 1.60 | 0.46 |
| 1:G:53:THR:OG1 | 1:G:56:THR:HG23 | 2.16 | 0.46 |
| 1:G:648:LEU:CD2 | 1:G:845:ARG:HD3 | 2.45 | 0.46 |
| 1:A:840:ILE:O | 1:A:841:GLU:HB3 | 2.14 | 0.46 |
| 2:B:185:LYS:CD | 2:B:190:LEU:HD21 | 2.46 | 0.46 |
| 1:C:130:ARG:HB2 | 1:C:148:ILE:CD1 | 2.45 | 0.46 |
| 1:G:315:THR:O | 1:G:531:THR:HG22 | 2.15 | 0.46 |
| 1:G:1052:MET:O | 1:G:1055:ASN:HB2 | 2.16 | 0.46 |
| 1:A:38[B]:ARG:HH11 | 1:A:38[B]:ARG:CG | 2.20 | 0.46 |
| 1:A:764:VAL:HG11 | 1:A:813:VAL:HG21 | 1.97 | 0.46 |
| 1:A:814:GLN:NE2 | 11:A:4511:HOH:O | 2.48 | 0.46 |
| 2:B:241:GLY:N | 9:B:4012:GLN:OE1 | 2.39 | 0.46 |
| 1:C:710:TYR:HB3 | 1:C:729:TYR:O | 2.15 | 0.46 |
| 2:D:286:MET:HE1 | 2:D:312:HIS:CE1 | 2.51 | 0.46 |
| 1:G:615:ARG:NE | 1:G:633:GLU:OE1 | 2.45 | 0.46 |
| 2:H:222:GLN:HA | 2:H:250:TYR:CD1 | 2.51 | 0.46 |
| 1:C:118:ALA:HA | 11:C:4198:HOH:O | 2.16 | 0.45 |
| 1:C:186:GLU:N | 11:C:4608:HOH:O | 2.43 | 0.45 |
| 1:C:655:GLU:CD | 1:C:666:PRO:HG2 | 2.36 | 0.45 |
| 1:C:1021:ARG:HH11 | 1:C:1021:ARG:CG | 2.28 | 0.45 |
| 1:E:146:SER:HB3 | 1:E:207:ASP:OD1 | 2.15 | 0.45 |
| 1:A:336[A]:MET:HB3 | 1:A:342:GLY:HA2 | 1.98 | 0.45 |
| 2:B:6:LEU:HD23 | 2:B:138:PRO:HB2 | 1.97 | 0.45 |
| 2:B:266:PHE:HB2 | 2:B:370:PHE:CD1 | 2.50 | 0.45 |
| 1:C:479:VAL:HG23 | 1:C:480:GLY:O | 2.16 | 0.45 |
| 2:F:379:LYS:HB2 | 2:F:379:LYS:NZ | 2.31 | 0.45 |
| 1:G:250:VAL:HA | 1:G:356:VAL:O | 2.16 | 0.45 |
| 1:G:475:LYS:CE | 11:G:3293:HOH:O | 2.64 | 0.45 |
| 1:G:726:GLU:HG3 | 1:G:727:ILE:N | 2.30 | 0.45 |
| 2:H:208:MET:SD | 2:H:355:GLU:HA | 2.56 | 0.45 |
| 2:H:313:GLY:HA3 | 11:H:2933:HOH:O | 2.15 | 0.45 |
| 2:H:364:ALA:N | 2:H:365:PRO:CD | 2.80 | 0.45 |
| 1:A:32:GLN:OE1 | 1:A:320:ALA:HB3 | 2.16 | 0.45 |
| 1:E:400:ARG:HD3 | 11:E:4438:HOH:O | 2.17 | 0.45 |
| 1:E:679:GLN:O | 1:E:683:GLU:HB2 | 2.16 | 0.45 |
| 1:G:294:ARG:NH1 | 5:G:4083:CL:CL | 2.86 | 0.45 |
| 1:G:550:GLU:CD | 2:H:120:ARG:HH21 | 2.19 | 0.45 |
| 1:C:715:ARG:HB2 | 1:C:751:LEU:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:C:805:ILE:CD1 | 1:C:837:VAL:CG2 | 2.94 | 0.45 |
| 1:C:975:HIS:HE2 | 1:E:992:ASN:HD21 | 1.63 | 0.45 |
| 2:D:298:LYS:O | 2:D:329:HIS:HA | 2.17 | 0.45 |
| 2:F:169:SER:HA | 2:F:216:LEU:O | 2.16 | 0.45 |
| 1:G:540:THR:CG2 | 1:G:541:ALA:N | 2.78 | 0.45 |
| 1:G:559:ARG:HG3 | 1:G:559:ARG:HH11 | 1.81 | 0.45 |
| 1:G:833:LYS:O | 1:G:836:GLU:HB2 | 2.15 | 0.45 |
| 1:A:1:MET:HB2 | 1:A:224:LYS:HZ2 | 1.81 | 0.45 |
| 1:A:384:VAL:HG22 | 1:A:385:MET:N | 2.32 | 0.45 |
| 1:E:953:ASP:O | 1:E:955:GLU:N | 2.50 | 0.45 |
| 1:E:956[B]:ARG:HB3 | 1:E:1044:LEU:HD21 | 1.96 | 0.45 |
| 2:F:46:PRO:O | 2:F:242:PRO:HG3 | 2.16 | 0.45 |
| 1:A:82:ARG:HG3 | 1:A:82:ARG:HH11 | 1.82 | 0.45 |
| 1:A:671:ARG:HG2 | 1:A:677:ARG:NH1 | 2.32 | 0.45 |
| 2:B:142:LEU:O | 2:B:145:GLU:HB3 | 2.17 | 0.45 |
| 1:C:86:VAL:HG13 | 1:C:86:VAL:O | 2.15 | 0.45 |
| 1:C:186:GLU:HB2 | 11:C:4608:HOH:O | 2.16 | 0.45 |
| 1:C:698:ILE:N | 1:C:698:ILE:CD1 | 2.79 | 0.45 |
| 2:D:39:TYR:CZ | 2:D:61:GLY:HA2 | 2.51 | 0.45 |
| 2:D:298:LYS:HE2 | 2:D:303:ASN:OD1 | 2.16 | 0.45 |
| 1:E:669:ILE:HA | 1:E:844:PRO:HG2 | 1.98 | 0.45 |
| 2:H:350:PHE:HD2 | 2:H:354:PRO:HD3 | 1.81 | 0.45 |
| 1:A:37:LEU:HD23 | 1:A:37:LEU:HA | 1.69 | 0.45 |
| 1:A:301:ASN:HA | 1:A:302:PRO:HD3 | 1.82 | 0.45 |
| 1:A:633:GLU:O | 1:A:634:LYS:HB2 | 2.17 | 0.45 |
| 2:F:23:THR:HG23 | 2:F:134:ALA:O | 2.16 | 0.45 |
| 1:G:40:GLU:HG2 | 1:G:325:LYS:HE2 | 1.98 | 0.45 |
| 1:G:475:LYS:HE3 | 11:G:3293:HOH:O | 2.15 | 0.45 |
| 1:G:527:LYS:HB2 | 1:G:544:TYR:CZ | 2.52 | 0.45 |
| 2:B:324:ASN:N | 2:B:324:ASN:ND2 | 2.39 | 0.45 |
| 1:E:157:ALA:HA | 11:E:4288:HOH:O | 2.16 | 0.45 |
| 1:E:612:THR:HG22 | 1:E:612:THR:O | 2.16 | 0.45 |
| 2:F:53:VAL:O | 2:F:80:LEU:HD12 | 2.16 | 0.45 |
| 2:F:270:LEU:HB2 | 9:F:4056:GLN:HG2 | 1.98 | 0.45 |
| 1:A:250:VAL:HA | 1:A:356:VAL:O | 2.17 | 0.45 |
| 2:B:57:TYR:CE1 | 2:B:58:PRO:HD2 | 2.52 | 0.45 |
| 2:B:232:ASN:N | 2:B:233:PRO:CD | 2.80 | 0.45 |
| 2:D:165:ALA:HB3 | 11:D:1800:HOH:O | 2.17 | 0.45 |
| 1:E:167:ILE:N | 1:E:167:ILE:CD1 | 2.80 | 0.45 |
| 1:G:954:LYS:HB3 | 1:G:980:VAL:HG21 | 1.98 | 0.45 |
| 1:A:38[A]:ARG:HH11 | 1:A:38[A]:ARG:CG | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:998:ARG:CG | 1:A:999:PRO:HA | 2.46 | 0.45 |
| 2:B:321:LEU:HD21 | 2:B:337:LEU:HD21 | 1.99 | 0.45 |
| 2:B:367:PHE:O | 2:B:370:PHE:HB3 | 2.17 | 0.45 |
| 1:C:456:THR:O | 1:C:457:ASN:HB2 | 2.16 | 0.45 |
| 2:D:2:ILE:HD12 | 2:D:3:LYS:N | 2.32 | 0.45 |
| 2:D:2:ILE:HD12 | 2:D:3:LYS:H | 1.81 | 0.45 |
| 1:E:704:LYS:O | 1:E:707:GLU:HB2 | 2.17 | 0.45 |
| 1:E:995:HIS:CD2 | 1:E:995:HIS:H | 2.33 | 0.45 |
| 1:G:301:ASN:HA | 1:G:302:PRO:HD3 | 1.87 | 0.45 |
| 1:G:820:LEU:O | 1:G:821:GLN:HB2 | 2.17 | 0.45 |
| 2:H:202:LYS:NZ | 2:H:355:GLU:OE1 | 2.30 | 0.45 |
| 2:H:275:LEU:HD12 | 2:H:275:LEU:O | 2.17 | 0.45 |
| 1:A:509:ARG:O | 1:A:512:GLU:HB2 | 2.16 | 0.44 |
| 1:C:213:TRP:HH2 | 1:C:294:ARG:HD3 | 1.82 | 0.44 |
| 1:C:325:LYS:O | 1:C:330:TYR:HB2 | 2.16 | 0.44 |
| 1:E:1:MET:HB2 | 1:E:224:LYS:HZ1 | 1.81 | 0.44 |
| 1:E:215:GLU:OE1 | 7:E:4045:ADP:O3' | 2.31 | 0.44 |
| 2:F:185:LYS:HD2 | 2:F:190:LEU:HD21 | 1.99 | 0.44 |
| 1:G:473[B]:GLU:OE1 | 1:G:501:ARG:NH2 | 2.43 | 0.44 |
| 1:G:698:ILE:H | 1:G:698:ILE:CD1 | 2.29 | 0.44 |
| 2:H:240:ASN:HB2 | 9:H:4079:GLN:OE1 | 2.16 | 0.44 |
| 2:D:286:MET:HE1 | 2:D:312:HIS:ND1 | 2.31 | 0.44 |
| 1:E:176:GLY:N | 7:E:4045:ADP:O2B | 2.43 | 0.44 |
| 1:E:503:ALA:HB1 | 1:E:508:VAL:O | 2.18 | 0.44 |
| 2:F:5:ALA:HB2 | 2:F:19:ALA:HB2 | 2.00 | 0.44 |
| 2:F:218:ILE:N | 2:F:218:ILE:CD1 | 2.79 | 0.44 |
| 2:H:253:THR:O | 2:H:256:GLN:HB2 | 2.17 | 0.44 |
| 2:B:344:ASP:OD2 | 2:B:344:ASP:N | 2.39 | 0.44 |
| 7:C:4029:ADP:H5'2 | 11:C:4571:HOH:O | 2.17 | 0.44 |
| 2:D:327:VAL:HG23 | 11:D:1624:HOH:O | 2.16 | 0.44 |
| 1:E:805:ILE:CD1 | 1:E:837:VAL:CG2 | 2.95 | 0.44 |
| 1:G:79:GLU:CG | 1:G:111:PHE:CZ | 3.00 | 0.44 |
| 1:G:87:LEU:HD12 | 1:G:87:LEU:HA | 1.66 | 0.44 |
| 1:G:254:GLN:NE2 | 2:H:57:TYR:OH | 2.50 | 0.44 |
| 1:G:632:ILE:HG13 | 1:G:633:GLU:N | 2.32 | 0.44 |
| 1:G:693:ALA:HB3 | 1:G:708:ILE:HD11 | 1.98 | 0.44 |
| 1:G:882:GLU:HB3 | 11:G:3372:HOH:O | 2.16 | 0.44 |
| 2:H:71:GLU:C | 2:H:203:ARG:HG3 | 2.37 | 0.44 |
| 2:H:196:ALA:HA | 2:H:237:PHE:O | 2.17 | 0.44 |
| 1:A:730:ASP:O | 1:A:733:ASP:HB2 | 2.18 | 0.44 |
| 1:A:1021:ARG:HH11 | 1:A:1021:ARG:HG3 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:948:SER:O | 1:C:1015:ASN:HA | 2.17 | 0.44 |
| 1:C:994:VAL:HG23 | 11:C:4748:HOH:O | 2.17 | 0.44 |
| 1:E:157:ALA:O | 1:E:160:ALA:HB3 | 2.18 | 0.44 |
| 1:E:384:VAL:HG22 | 1:E:385:MET:N | 2.32 | 0.44 |
| 1:E:417:ASP:OD2 | 1:E:418:PRO:HD2 | 2.16 | 0.44 |
| 1:E:750:VAL:O | 1:E:750:VAL:HG12 | 2.17 | 0.44 |
| 1:G:76:LYS:HD2 | 1:G:76:LYS:HA | 1.71 | 0.44 |
| 1:G:150:HIS:HD2 | 1:G:203:GLU:HB2 | 1.82 | 0.44 |
| 1:G:683:GLU:HA | 1:G:683:GLU:OE2 | 2.15 | 0.44 |
| 1:C:559:ARG:HG3 | 1:C:559:ARG:NH1 | 2.31 | 0.44 |
| 1:C:998:ARG:CB | 1:C:999:PRO:HA | 2.46 | 0.44 |
| 2:D:150:PHE:CD2 | 2:D:151:PRO:HD2 | 2.53 | 0.44 |
| 2:D:226:GLU:O | 2:D:230:LYS:HG3 | 2.17 | 0.44 |
| 1:G:675:ARG:CD | 1:G:675:ARG:H | 2.28 | 0.44 |
| 1:A:220:VAL:O | 1:A:281:GLY:HA2 | 2.17 | 0.44 |
| 1:E:283:ASN:HB2 | 11:E:4666:HOH:O | 2.17 | 0.44 |
| 1:G:695:VAL:HG11 | 1:G:701:ALA:CB | 2.43 | 0.44 |
| 1:G:784:GLN:NE2 | 1:G:784:GLN:N | 2.40 | 0.44 |
| 1:A:129:ARG:HB3 | 1:A:205:LEU:HD22 | 1.99 | 0.44 |
| 1:A:235:GLU:HB2 | 1:A:253:ALA:HA | 1.98 | 0.44 |
| 1:A:602:ASN:CG | 1:A:605:THR:HG23 | 2.38 | 0.44 |
| 2:B:102:LEU:HA | 2:B:102:LEU:HD23 | 1.74 | 0.44 |
| 2:B:334:ASP:CG | 2:B:336:THR:HG23 | 2.38 | 0.44 |
| 1:C:675:ARG:H | 1:C:675:ARG:HD3 | 1.83 | 0.44 |
| 1:C:831:ALA:HB2 | 1:C:840:ILE:HD11 | 1.99 | 0.44 |
| 1:G:654:LEU:HD22 | 1:G:659:VAL:HG21 | 1.98 | 0.44 |
| 1:G:726:GLU:HG3 | 1:G:727:ILE:H | 1.83 | 0.44 |
| 2:H:374:ILE:O | 2:H:377:TYR:HB3 | 2.18 | 0.44 |
| 1:A:675:ARG:HG3 | 1:A:751:LEU:HD21 | 1.98 | 0.44 |
| 2:B:48:TYR:HA | 2:B:51:GLN:HE21 | 1.82 | 0.44 |
| 1:C:358:LYS:HG2 | 1:C:359:ILE:N | 2.32 | 0.44 |
| 2:F:199:PHE:O | 2:F:241:GLY:HA3 | 2.18 | 0.44 |
| 2:B:13:THR:HG22 | 2:B:15:PHE:CE2 | 2.52 | 0.44 |
| 2:B:218:ILE:N | 2:B:218:ILE:CD1 | 2.80 | 0.44 |
| 1:C:158:VAL:HG11 | 1:C:206:ILE:HB | 1.99 | 0.44 |
| 1:C:666:PRO:O | 1:C:669:ILE:HB | 2.18 | 0.44 |
| 1:C:671:ARG:NH2 | 1:C:819:GLU:O | 2.51 | 0.44 |
| 1:C:686:LYS:O | 1:C:687:LEU:HD23 | 2.18 | 0.44 |
| 1:E:903:VAL:O | 1:E:905:PRO:HD3 | 2.18 | 0.44 |
| 1:G:563:MET:HB3 | 1:G:638:VAL:HG22 | 1.99 | 0.44 |
| 1:G:946:LEU:HB3 | 1:G:1013:ILE:HG12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:994:VAL:HG13 | 1:G:1000:HIS:CE1 | 2.53 | 0.44 |
| 2:B:198:ASP:HB2 | 2:B:218:ILE:CG2 | 2.48 | 0.43 |
| 2:B:199:PHE:O | 2:B:241:GLY:HA3 | 2.18 | 0.43 |
| 2:B:265:VAL:O | 2:B:347:ALA:HA | 2.18 | 0.43 |
| 1:C:772:MET:SD | 1:C:880:THR:HG22 | 2.57 | 0.43 |
| 1:C:775:ILE:HG13 | 1:C:810:ARG:HG2 | 2.00 | 0.43 |
| 1:E:57:ASP:HA | 1:E:58:PRO:HD3 | 1.79 | 0.43 |
| 1:E:148:ILE:CG2 | 1:E:149:ALA:N | 2.81 | 0.43 |
| 1:E:885:PRO:HA | 1:E:886:PRO:HD3 | 1.81 | 0.43 |
| 2:F:373:LEU:HA | 2:F:373:LEU:HD23 | 1.78 | 0.43 |
| 1:G:947:LEU:HD12 | 1:G:947:LEU:N | 2.33 | 0.43 |
| 1:A:101:GLU:OE2 | 1:A:104:ARG:NH2 | 2.45 | 0.43 |
| 1:A:158:VAL:HG11 | 1:A:206:ILE:HB | 1.99 | 0.43 |
| 1:A:612:THR:HG22 | 1:A:612:THR:O | 2.18 | 0.43 |
| 1:C:384:VAL:HB | 1:C:569:PRO:HG3 | 1.99 | 0.43 |
| 1:E:515:LYS:HD3 | 1:E:515:LYS:C | 2.38 | 0.43 |
| 1:E:686:LYS:C | 1:E:687:LEU:HD23 | 2.38 | 0.43 |
| 1:E:713:VAL:HG12 | 1:E:713:VAL:O | 2.17 | 0.43 |
| 1:E:808:VAL:HG13 | 1:E:811[B]:GLN:NE2 | 2.32 | 0.43 |
| 10:E:4058:NET:H31 | 10:E:4058:NET:H63 | 1.53 | 0.43 |
| 1:G:104:ARG:HB2 | 11:G:2906:HOH:O | 2.18 | 0.43 |
| 1:G:308:SER:HB3 | 11:G:3571:HOH:O | 2.17 | 0.43 |
| 1:G:1021:ARG:CG | 1:G:1021:ARG:NH1 | 2.78 | 0.43 |
| 2:H:279:SER:O | 2:H:322:PRO:HG3 | 2.18 | 0.43 |
| 2:H:321:LEU:HA | 2:H:321:LEU:HD12 | 1.78 | 0.43 |
| 1:C:920:VAL:O | 1:C:930:LYS:HD3 | 2.18 | 0.43 |
| 1:E:385:MET:HG2 | 1:E:386:ALA:N | 2.32 | 0.43 |
| 1:G:734:LEU:CD1 | 1:G:738:PHE:CD2 | 3.02 | 0.43 |
| 1:G:1001:ILE:HD13 | 1:G:1002:GLN:N | 2.32 | 0.43 |
| 2:H:5:ALA:HB2 | 2:H:19:ALA:HB2 | 1.99 | 0.43 |
| 2:B:325:LEU:HA | 2:B:325:LEU:HD23 | 1.51 | 0.43 |
| 1:C:765:ASP:OD2 | 1:C:827:ASN:HB2 | 2.18 | 0.43 |
| 1:C:1013:ILE:O | 1:C:1040:TYR:HA | 2.19 | 0.43 |
| 1:E:659:VAL:HG13 | 1:E:660:PRO:HD2 | 2.00 | 0.43 |
| 1:A:479:VAL:CG2 | 1:A:483:GLY:HA3 | 2.49 | 0.43 |
| 1:A:828:VAL:CG1 | 1:A:839:LEU:HD11 | 2.49 | 0.43 |
| 1:E:1:MET:CB | 1:E:224:LYS:NZ | 2.76 | 0.43 |
| 2:F:205:ILE:HG12 | 2:F:355:GLU:HG3 | 2.00 | 0.43 |
| 1:G:358:LYS:HG2 | 1:G:359:ILE:N | 2.31 | 0.43 |
| 1:G:456:THR:O | 1:G:457:ASN:HB2 | 2.18 | 0.43 |
| 1:G:965:LEU:HD23 | 1:G:965:LEU:HA | 1.87 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:255:ILE:HA | 2:B:258:PHE:HD2 | 1.84 | 0.43 |
| 1:C:895:LEU:HA | 1:C:896:PRO:HD3 | 1.83 | 0.43 |
| 1:C:956:ARG:HB3 | 1:C:1044:LEU:HD21 | 1.99 | 0.43 |
| 1:C:1063:ILE:CD1 | 1:C:1068:MET:CG | 2.93 | 0.43 |
| 1:E:472:LEU:O | 1:E:476:VAL:HG23 | 2.19 | 0.43 |
| 2:F:163:THR:OG1 | 2:F:164:THR:N | 2.50 | 0.43 |
| 1:G:24:CYS:HB2 | 1:G:604:GLU:HB3 | 2.00 | 0.43 |
| 1:G:385:MET:HG3 | 1:G:386:ALA:N | 2.34 | 0.43 |
| 2:H:17:GLY:HA3 | 2:H:110:ILE:HD11 | 2.01 | 0.43 |
| 1:A:671:ARG:CG | 1:A:677:ARG:NH1 | 2.81 | 0.43 |
| 1:A:793:ALA:HA | 1:A:891:LYS:O | 2.19 | 0.43 |
| 2:B:324:ASN:HA | 2:B:343:THR:OG1 | 2.18 | 0.43 |
| 2:B:350:PHE:CB | 2:B:366:LEU:HD22 | 2.47 | 0.43 |
| 1:C:1061:LYS:HD3 | 11:C:4585:HOH:O | 2.18 | 0.43 |
| 2:D:376:GLN:HA | 2:D:379:LYS:NZ | 2.33 | 0.43 |
| 1:E:735:ARG:O | 1:E:738:PHE:N | 2.51 | 0.43 |
| 1:G:509:ARG:HB2 | 1:G:509:ARG:NH1 | 2.32 | 0.43 |
| 1:A:38[B]:ARG:NH1 | 1:A:38[B]:ARG:CG | 2.80 | 0.43 |
| 1:A:682:VAL:HG11 | 1:A:689:GLN:NE2 | 2.32 | 0.43 |
| 1:A:954:LYS:HB3 | 1:A:980:VAL:HG11 | 2.01 | 0.43 |
| 2:B:249:ASP:HA | 2:B:252:ILE:HD12 | 2.00 | 0.43 |
| 2:B:269:SER:OG | 9:B:4012:GLN:HG2 | 2.18 | 0.43 |
| 1:E:579:ASP:OD1 | 1:E:605:THR:HB | 2.19 | 0.43 |
| 2:F:272:HIS:HB2 | 2:F:349:SER:HB2 | 2.01 | 0.43 |
| 1:G:339:ILE:HD11 | 1:G:531:THR:HG23 | 2.00 | 0.43 |
| 1:G:588:ALA:O | 1:G:591:GLU:HB3 | 2.19 | 0.43 |
| 1:G:695:VAL:HG11 | 1:G:701:ALA:CA | 2.48 | 0.43 |
| 1:G:1017:THR:HG22 | 1:G:1023:ILE:HG13 | 1.99 | 0.43 |
| 1:G:1021:ARG:O | 1:G:1025:ASP:OD2 | 2.36 | 0.43 |
| 1:C:167:ILE:HD12 | 1:C:167:ILE:N | 2.33 | 0.43 |
| 1:C:956:ARG:HB3 | 1:C:1044:LEU:HD23 | 1.99 | 0.43 |
| 1:E:765:ASP:O | 1:E:776:GLY:N | 2.51 | 0.43 |
| 7:E:4051:ADP:H5'2 | 11:E:4614:HOH:O | 2.18 | 0.43 |
| 1:G:246:ASP:C | 1:G:360:PRO:HG3 | 2.40 | 0.43 |
| 1:G:339:ILE:HD12 | 1:G:529:VAL:O | 2.19 | 0.43 |
| 1:G:905:PRO:HG2 | 1:G:1030:ARG:HB3 | 2.00 | 0.43 |
| 1:G:944:ARG:NH1 | 1:G:972:ASP:OD1 | 2.52 | 0.43 |
| 2:H:28:GLY:HA2 | 2:H:150:PHE:CE2 | 2.54 | 0.43 |
| 2:D:259:LEU:HD13 | 2:D:342:ARG:HH12 | 1.82 | 0.43 |
| 1:E:527:LYS:HB2 | 1:E:544:TYR:CZ | 2.54 | 0.43 |
| 2:F:102:LEU:HD23 | 2:F:102:LEU:HA | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:370:ALA:HB2 | 1:G:900:PHE:HB3 | 2.00 | 0.43 |
| 1:G:695:VAL:HG11 | 1:G:701:ALA:N | 2.34 | 0.43 |
| 1:G:733:ASP:HA | 1:G:736:ARG:HH11 | 1.83 | 0.43 |
| 2:H:66:ASN:HB3 | 2:H:93:ARG:O | 2.18 | 0.43 |
| 2:H:334:ASP:OD2 | 2:H:336:THR:HG23 | 2.19 | 0.43 |
| 1:A:267:ALA:O | 1:A:271:VAL:HG23 | 2.19 | 0.42 |
| 1:A:426:ARG:HD3 | 1:A:426:ARG:C | 2.40 | 0.42 |
| 1:A:738:PHE:O | 1:A:741:ALA:HB3 | 2.19 | 0.42 |
| 2:D:33:ASN:HA | 2:D:291:HIS:O | 2.18 | 0.42 |
| 2:D:178:THR:HG22 | 2:D:179:GLY:N | 2.32 | 0.42 |
| 1:E:456:THR:O | 1:E:457:ASN:HB2 | 2.19 | 0.42 |
| 2:H:209:LEU:HA | 2:H:209:LEU:HD23 | 1.79 | 0.42 |
| 2:D:186:LYS:H | 2:D:189:GLU:CD | 2.22 | 0.42 |
| 1:E:569:PRO:O | 1:E:571:ARG:HD2 | 2.19 | 0.42 |
| 1:E:854:SER:HA | 1:E:859:VAL:O | 2.19 | 0.42 |
| 2:F:86:PRO:HA | 11:F:2685:HOH:O | 2.19 | 0.42 |
| 2:B:208:MET:O | 2:B:211:ASP:HB2 | 2.19 | 0.42 |
| 1:C:677:ARG:O | 1:C:680:HIS:HB2 | 2.19 | 0.42 |
| 1:C:778:ILE:HD11 | 1:C:810:ARG:HG3 | 2.02 | 0.42 |
| 1:E:548:GLU:HG2 | 2:F:114:ASP:HB2 | 2.01 | 0.42 |
| 1:E:1070:ALA:HB3 | 11:E:4646:HOH:O | 2.19 | 0.42 |
| 2:H:190:LEU:HA | 2:H:191:PRO:HD3 | 1.93 | 0.42 |
| 2:H:373:LEU:HD23 | 2:H:373:LEU:HA | 1.74 | 0.42 |
| 1:A:259:LYS:HD3 | 2:B:175:TRP:CZ3 | 2.55 | 0.42 |
| 1:C:1:MET:N | 1:C:224:LYS:HE3 | 2.34 | 0.42 |
| 1:C:221:VAL:O | 1:C:228:CYS:HA | 2.19 | 0.42 |
| 1:C:493:LYS:HD2 | 1:C:493:LYS:HA | 1.86 | 0.42 |
| 1:C:905:PRO:HB2 | 1:C:1040:TYR:HH | 1.84 | 0.42 |
| 2:D:333:PHE:HD1 | 2:D:333:PHE:HA | 1.77 | 0.42 |
| 1:E:534:ALA:HB1 | 2:F:120:ARG:HG2 | 2.01 | 0.42 |
| 1:E:808:VAL:CA | 1:E:811[B]:GLN:HG3 | 2.49 | 0.42 |
| 2:F:196:ALA:HB3 | 2:F:218:ILE:HD12 | 2.01 | 0.42 |
| 1:G:267:ALA:O | 1:G:271:VAL:HG23 | 2.19 | 0.42 |
| 1:G:915:GLY:HA2 | 11:G:2979:HOH:O | 2.18 | 0.42 |
| 2:H:367:PHE:O | 2:H:370:PHE:HB3 | 2.19 | 0.42 |
| 1:A:35:LYS:HD2 | 11:A:4141:HOH:O | 2.19 | 0.42 |
| 1:A:868:VAL:HA | 1:A:872:LYS:O | 2.19 | 0.42 |
| 2:B:87:LEU:HD12 | 2:B:87:LEU:HA | 1.72 | 0.42 |
| 2:D:208:MET:O | 2:D:211:ASP:HB2 | 2.20 | 0.42 |
| 1:E:714:VAL:HG13 | 1:E:752:LEU:HD12 | 2.00 | 0.42 |
| 1:E:891:LYS:HG2 | 1:E:892:GLU:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:940:LYS:HG3 | 1:E:1011:THR:HB | 2.01 | 0.42 |
| 2:F:342:ARG:HD2 | 2:F:342:ARG:HA | 1.92 | 0.42 |
| 1:G:361:ARG:O | 1:G:380:SER:HB2 | 2.19 | 0.42 |
| 1:G:402:LEU:O | 1:G:403:GLU:HB2 | 2.19 | 0.42 |
| 1:G:482:THR:HG22 | 1:G:483:GLY:N | 2.34 | 0.42 |
| 1:G:735:ARG:O | 1:G:738:PHE:HB2 | 2.19 | 0.42 |
| 1:G:946:LEU:C | 1:G:947:LEU:HD12 | 2.39 | 0.42 |
| 1:G:1032:SER:O | 1:G:1036:TYR:HD1 | 2.02 | 0.42 |
| 1:A:775:ILE:HD13 | 1:A:775:ILE:HA | 1.86 | 0.42 |
| 1:C:730:ASP:H | 1:C:733:ASP:HB2 | 1.84 | 0.42 |
| 2:D:325:LEU:HD23 | 2:D:325:LEU:HA | 1.82 | 0.42 |
| 1:E:493:LYS:HD2 | 1:E:493:LYS:HA | 1.78 | 0.42 |
| 1:E:755:PHE:CE1 | 7:E:4051:ADP:C2 | 3.08 | 0.42 |
| 2:F:66:ASN:OD1 | 2:F:68:ALA:HB3 | 2.19 | 0.42 |
| 1:G:170:PRO:HA | 1:G:204:LEU:HD23 | 2.01 | 0.42 |
| 1:G:185:ARG:O | 1:G:188:PHE:HB3 | 2.19 | 0.42 |
| 1:G:329:GLY:CA | 11:G:2959:HOH:O | 2.68 | 0.42 |
| 1:G:828:VAL:CG1 | 1:G:839:LEU:HD11 | 2.50 | 0.42 |
| 1:G:965:LEU:HG | 1:G:971:LEU:HD11 | 2.02 | 0.42 |
| 1:A:548:GLU:OE1 | 2:B:83:ARG:HD3 | 2.19 | 0.42 |
| 1:A:981:LEU:HD12 | 1:A:988:PRO:HG3 | 2.02 | 0.42 |
| 1:E:217:GLU:HG2 | 1:E:285:GLN:HG2 | 2.01 | 0.42 |
| 2:F:91:ASN:OD1 | 2:F:93:ARG:HB2 | 2.19 | 0.42 |
| 1:A:336[B]:MET:HB3 | 1:A:342:GLY:HA2 | 2.02 | 0.42 |
| 1:C:257:THR:HG23 | 1:C:260:GLU:OE2 | 2.19 | 0.42 |
| 1:C:840:ILE:O | 1:C:841:GLU:HB3 | 2.20 | 0.42 |
| 1:C:892:GLU:OE1 | 8:C:4033:ORN:NE | 2.52 | 0.42 |
| 2:D:212:ARG:CG | 2:D:212:ARG:NH1 | 2.78 | 0.42 |
| 1:E:85:ALA:HA | 1:E:114:THR:O | 2.20 | 0.42 |
| 2:F:46:PRO:HA | 2:F:76:HIS:CB | 2.50 | 0.42 |
| 1:G:987:ASN:HA | 1:G:988:PRO:HD2 | 1.91 | 0.42 |
| 2:H:158:LEU:HA | 2:H:158:LEU:HD23 | 1.68 | 0.42 |
| 2:H:376:GLN:O | 2:H:376:GLN:HG3 | 2.20 | 0.42 |
| 1:A:1021:ARG:CG | 1:A:1021:ARG:NH1 | 2.80 | 0.42 |
| 1:E:10:ILE:HD13 | 1:E:37:LEU:HD13 | 2.02 | 0.42 |
| 1:E:248:ILE:HA | 1:E:358:LYS:O | 2.20 | 0.42 |
| 1:E:528:ARG:HG2 | 1:E:543:MET:HG2 | 2.01 | 0.42 |
| 1:G:453:PHE:CD1 | 1:G:453:PHE:C | 2.92 | 0.42 |
| 1:A:313:LYS:HE2 | 1:A:608:THR:C | 2.39 | 0.42 |
| 1:A:528:ARG:HG2 | 1:A:543:MET:HG2 | 2.02 | 0.42 |
| 1:C:40:GLU:CG | 1:C:325:LYS:HE2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1064:SER:OG | 1:C:1067:GLU:HG3 | 2.20 | 0.42 |
| 1:E:514:ARG:HD3 | 11:E:4483:HOH:O | 2.20 | 0.42 |
| 1:E:1001:ILE:CD1 | 1:E:1002:GLN:N | 2.79 | 0.42 |
| 1:G:48:ASN:O | 1:G:66:ILE:HA | 2.20 | 0.42 |
| 2:H:7:LEU:HD23 | 2:H:15:PHE:CD2 | 2.54 | 0.42 |
| 1:A:3:LYS:HB2 | 1:A:42:TYR:OH | 2.20 | 0.41 |
| 1:A:191:ILE:HD13 | 1:A:191:ILE:HG21 | 1.91 | 0.41 |
| 1:A:702:VAL:O | 1:A:706:LYS:HD3 | 2.20 | 0.41 |
| 1:C:24:CYS:HB2 | 1:C:604:GLU:HB3 | 2.02 | 0.41 |
| 1:C:1064:SER:O | 1:C:1068:MET:HG3 | 2.20 | 0.41 |
| 1:E:882:GLU:HB3 | 11:E:4757:HOH:O | 2.19 | 0.41 |
| 2:F:228:VAL:HG11 | 2:F:258:PHE:CE1 | 2.55 | 0.41 |
| 2:F:286:MET:CE | 2:F:312:HIS:ND1 | 2.83 | 0.41 |
| 1:G:752:LEU:HD12 | 1:G:752:LEU:HA | 1.72 | 0.41 |
| 2:H:150:PHE:CE1 | 2:H:152:GLY:HA2 | 2.55 | 0.41 |
| 1:A:659:VAL:HG12 | 1:A:660:PRO:N | 2.34 | 0.41 |
| 2:D:364:ALA:N | 2:D:365:PRO:CD | 2.83 | 0.41 |
| 1:E:765:ASP:OD2 | 1:E:827:ASN:HB2 | 2.20 | 0.41 |
| 2:F:325:LEU:HD23 | 2:F:325:LEU:HA | 1.83 | 0.41 |
| 1:G:145:ARG:HB2 | 1:G:208:GLU:CD | 2.40 | 0.41 |
| 1:G:755:PHE:CD1 | 7:G:4074:ADP:C2 | 3.08 | 0.41 |
| 1:A:734:LEU:CD1 | 1:A:738:PHE:CD2 | 3.03 | 0.41 |
| 2:B:75:VAL:HG11 | 2:B:107:ILE:HG13 | 2.02 | 0.41 |
| 1:C:662:ILE:HD13 | 1:C:662:ILE:HG21 | 1.84 | 0.41 |
| 1:C:967:GLN:HG3 | 1:C:1054:LEU:CD1 | 2.45 | 0.41 |
| 2:D:163:THR:OG1 | 2:D:164:THR:N | 2.54 | 0.41 |
| 1:E:489:LEU:HD12 | 1:E:489:LEU:HA | 1.89 | 0.41 |
| 1:G:734:LEU:O | 1:G:737:TYR:HB3 | 2.20 | 0.41 |
| 1:G:770:GLY:HA2 | 1:G:823:ARG:NH1 | 2.36 | 0.41 |
| 1:G:981:LEU:HD23 | 1:G:981:LEU:HA | 1.87 | 0.41 |
| 2:H:197:TYR:HB3 | 2:H:199:PHE:CZ | 2.55 | 0.41 |
| 1:A:225:ASN:ND2 | 1:A:331:THR:HG21 | 2.36 | 0.41 |
| 1:A:654:LEU:HD22 | 1:A:659:VAL:HG21 | 2.02 | 0.41 |
| 1:A:796:LEU:HD23 | 1:A:796:LEU:C | 2.40 | 0.41 |
| 1:A:946:LEU:C | 1:A:947:LEU:HD12 | 2.41 | 0.41 |
| 2:B:240:ASN:HB2 | 9:B:4012:GLN:OE1 | 2.21 | 0.41 |
| 1:C:994:VAL:HG23 | 1:C:1001:ILE:HD11 | 2.01 | 0.41 |
| 2:D:172:GLN:O | 2:D:207:ARG:HA | 2.21 | 0.41 |
| 2:D:190:LEU:HB2 | 2:D:215:ARG:HB3 | 2.02 | 0.41 |
| 2:D:229:LEU:HD23 | 2:D:229:LEU:HA | 1.82 | 0.41 |
| 1:E:726:GLU:HG3 | 1:E:727:ILE:H | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:726:GLU:OE1 | 1:G:1020:ARG:HD3 | 2.20 | 0.41 |
| 2:H:201:ALA:HB2 | 2:H:239:SER:CB | 2.51 | 0.41 |
| 1:A:654:LEU:O | 1:A:659:VAL:HG23 | 2.20 | 0.41 |
| 1:A:698:ILE:HG22 | 1:A:699:GLU:N | 2.36 | 0.41 |
| 1:A:957:VAL:HG13 | 1:A:958:VAL:N | 2.36 | 0.41 |
| 1:C:4:ARG:NH1 | 11:C:4132:HOH:O | 2.54 | 0.41 |
| 1:C:34:CYS:SG | 1:C:46:LEU:HD22 | 2.60 | 0.41 |
| 1:C:525:VAL:HG12 | 1:C:551:CYS:HB2 | 2.03 | 0.41 |
| 1:C:571:ARG:HD3 | 1:C:571:ARG:N | 2.35 | 0.41 |
| 1:C:682:VAL:HG13 | 1:C:687:LEU:HB2 | 2.02 | 0.41 |
| 2:D:171:THR:O | 2:D:185:LYS:N | 2.47 | 0.41 |
| 1:G:516:LEU:HA | 1:G:516:LEU:HD12 | 1.77 | 0.41 |
| 1:G:671:ARG:HG2 | 1:G:677:ARG:NH1 | 2.35 | 0.41 |
| 2:H:181:LEU:HA | 2:H:182:PRO:HD3 | 1.91 | 0.41 |
| 1:A:353:ASP:N | 1:A:353:ASP:OD2 | 2.51 | 0.41 |
| 1:C:964:LEU:O | 1:C:969:PHE:HB2 | 2.20 | 0.41 |
| 2:D:369:HIS:O | 2:D:372:GLU:HB2 | 2.20 | 0.41 |
| 1:E:58:PRO:HD2 | 1:E:59:GLU:OE2 | 2.20 | 0.41 |
| 1:E:78:ILE:HG23 | 1:E:83:PRO:HD2 | 2.02 | 0.41 |
| 1:E:532:CYS:O | 1:E:533:ALA:HB3 | 2.21 | 0.41 |
| 1:E:1021:ARG:CG | 1:E:1021:ARG:NH1 | 2.80 | 0.41 |
| 2:F:374:ILE:O | 2:F:374:ILE:HG22 | 2.19 | 0.41 |
| 1:G:479:VAL:HG23 | 1:G:480:GLY:O | 2.20 | 0.41 |
| 1:G:622:THR:OG1 | 1:G:625:ASP:OD1 | 2.27 | 0.41 |
| 2:H:95:THR:HG21 | 11:H:3459:HOH:O | 2.21 | 0.41 |
| 2:H:376:GLN:HG2 | 2:H:377:TYR:N | 2.35 | 0.41 |
| 1:C:85:ALA:HA | 1:C:114:THR:O | 2.20 | 0.41 |
| 2:D:188:ASP:OD2 | 2:D:188:ASP:N | 2.51 | 0.41 |
| 1:E:615:ARG:NE | 1:E:633:GLU:OE1 | 2.44 | 0.41 |
| 1:E:670:ASP:CB | 1:E:677:ARG:HH21 | 2.24 | 0.41 |
| 10:E:4058:NET:H42 | 10:E:4058:NET:H22 | 2.03 | 0.41 |
| 2:F:212:ARG:HG3 | 2:F:212:ARG:HH11 | 1.86 | 0.41 |
| 1:G:180:GLY:HA2 | 1:G:376:THR:OG1 | 2.20 | 0.41 |
| 1:G:469:LEU:O | 1:G:473[B]:GLU:HB2 | 2.20 | 0.41 |
| 2:H:354:PRO:HB2 | 2:H:367:PHE:CE2 | 2.56 | 0.41 |
| 1:C:57:ASP:HB2 | 1:C:60:MET:HG2 | 2.03 | 0.41 |
| 1:C:886:PRO:HD2 | 1:C:887:TYR:CD1 | 2.56 | 0.41 |
| 1:C:932:GLN:HG2 | 1:C:937:SER:HB3 | 2.02 | 0.41 |
| 2:D:43:LEU:HB3 | 2:D:75:VAL:HG13 | 2.03 | 0.41 |
| 2:D:259:LEU:HD23 | 2:D:259:LEU:HA | 1.87 | 0.41 |
| 1:E:696:THR:N | 1:E:700:MET:CE | 2.80 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:228:VAL:HG11 | 2:F:258:PHE:CZ | 2.55 | 0.41 |
| 1:G:895:LEU:HA | 1:G:896:PRO:HD3 | 1.98 | 0.41 |
| 2:H:350:PHE:HB2 | 2:H:366:LEU:HD22 | 2.03 | 0.41 |
| 1:A:4:ARG:NE | 1:A:7:ILE:HD12 | 2.36 | 0.41 |
| 1:A:164:PHE:HA | 1:A:165:PRO:C | 2.40 | 0.41 |
| 1:A:947:LEU:HA | 1:A:1014:ILE:HG23 | 2.03 | 0.41 |
| 1:A:1048:PHE:O | 1:A:1051:ALA:HB3 | 2.21 | 0.41 |
| 2:B:285:LYS:HG3 | 2:B:314:PHE:CZ | 2.54 | 0.41 |
| 1:C:43:ARG:NH2 | 1:C:81:GLU:OE2 | 2.50 | 0.41 |
| 1:C:563:MET:HE1 | 1:C:635:PRO:HG3 | 1.96 | 0.41 |
| 2:D:371:ILE:O | 2:D:374:ILE:HB | 2.20 | 0.41 |
| 1:E:411:PRO:HD2 | 11:E:4697:HOH:O | 2.20 | 0.41 |
| 1:E:832:VAL:HA | 1:E:836:GLU:O | 2.21 | 0.41 |
| 2:F:29:GLU:HB2 | 2:F:153:LEU:HD22 | 2.01 | 0.41 |
| 2:F:142:LEU:HA | 2:F:142:LEU:HD12 | 1.78 | 0.41 |
| 2:F:205:ILE:HD13 | 2:F:268:ILE:HD12 | 2.03 | 0.41 |
| 2:F:354:PRO:HB2 | 2:F:367:PHE:CE2 | 2.55 | 0.41 |
| 1:G:840:ILE:O | 1:G:841:GLU:HB3 | 2.21 | 0.41 |
| 1:G:861:LEU:HA | 1:G:861:LEU:HD23 | 1.75 | 0.41 |
| 1:A:294:ARG:HD2 | 5:A:4016:CL:CL | 2.58 | 0.41 |
| 1:A:930:LYS:HG3 | 1:A:1058:ALA:HB1 | 2.03 | 0.41 |
| 1:A:930:LYS:HG3 | 1:A:1058:ALA:CB | 2.51 | 0.41 |
| 2:F:322:PRO:CB | 2:F:324:ASN:HD21 | 2.31 | 0.41 |
| 2:F:327:VAL:HG13 | 2:F:337:LEU:CD1 | 2.51 | 0.41 |
| 1:G:734:LEU:HD12 | 1:G:738:PHE:CD2 | 2.55 | 0.41 |
| 1:G:780:GLU:OE2 | 1:G:798:ALA:HB1 | 2.20 | 0.41 |
| 2:H:38:GLY:HA3 | 2:H:358:PRO:CB | 2.51 | 0.41 |
| 1:A:713:VAL:HG23 | 1:A:755:PHE:HB2 | 2.03 | 0.40 |
| 1:C:78:ILE:O | 1:C:82:ARG:N | 2.34 | 0.40 |
| 1:C:220:VAL:C | 1:C:221:VAL:HG23 | 2.42 | 0.40 |
| 1:C:516:LEU:HD12 | 1:C:516:LEU:HA | 1.59 | 0.40 |
| 1:E:1:MET:CB | 1:E:224:LYS:HZ1 | 2.32 | 0.40 |
| 1:E:148:ILE:HG22 | 1:E:149:ALA:N | 2.36 | 0.40 |
| 1:E:1001:ILE:HD13 | 1:E:1029:ILE:HG13 | 2.03 | 0.40 |
| 2:F:62:ASN:OD1 | 2:F:86:PRO:HG3 | 2.22 | 0.40 |
| 1:G:250:VAL:HG12 | 1:G:357:THR:HG23 | 2.03 | 0.40 |
| 1:G:620:PRO:HB2 | 1:G:622:THR:HG23 | 2.02 | 0.40 |
| 1:G:761:GLU:HB3 | 1:G:781:HIS:ND1 | 2.37 | 0.40 |
| 1:A:126:ALA:HB3 | 1:A:302:PRO:HG3 | 2.02 | 0.40 |
| 1:C:475:LYS:O | 1:C:479:VAL:HG13 | 2.20 | 0.40 |
| 1:C:805:ILE:HD11 | 1:C:837:VAL:HG23 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:286:MET:CE | 2:F:312:HIS:O | 2.69 | 0.40 |
| 1:G:362:PHE:CD2 | 1:G:433:ALA:HB1 | 2.56 | 0.40 |
| 1:G:472:LEU:O | 1:G:476:VAL:HG23 | 2.21 | 0.40 |
| 1:G:788:HIS:ND1 | 1:G:790:GLY:N | 2.60 | 0.40 |
| 2:H:250:TYR:H | 2:H:250:TYR:HD2 | 1.63 | 0.40 |
| 1:A:1006:LYS:HB3 | 1:A:1006:LYS:HE3 | 2.00 | 0.40 |
| 2:B:34:THR:HA | 2:B:56:THR:OG1 | 2.22 | 0.40 |
| 1:C:6:ASP:N | 1:C:6:ASP:OD2 | 2.49 | 0.40 |
| 1:C:873:SER:O | 1:C:877:GLN:HG3 | 2.21 | 0.40 |
| 2:D:294:ASN:OD1 | 2:D:294:ASN:N | 2.54 | 0.40 |
| 1:G:1031:ARG:HE | 1:G:1031:ARG:HB3 | 1.56 | 0.40 |
| 2:H:236:ILE:HD12 | 2:H:263:ILE:CG2 | 2.51 | 0.40 |
| 2:H:296:PRO:HB2 | 2:H:332:LEU:HB2 | 2.02 | 0.40 |
| 1:A:732:ALA:O | 1:A:736:ARG:HB2 | 2.21 | 0.40 |
| 1:C:561:LYS:HE2 | 11:C:4472:HOH:O | 2.21 | 0.40 |
| 1:C:701:ALA:O | 1:C:705:ALA:N | 2.49 | 0.40 |
| 1:E:484:LEU:HD23 | 1:E:484:LEU:HA | 1.96 | 0.40 |
| 1:E:713:VAL:HG23 | 1:E:755:PHE:HB2 | 2.04 | 0.40 |
| 1:E:950:ARG:HH11 | 1:E:950:ARG:HD2 | 1.68 | 0.40 |
| 2:F:246:ALA:N | 2:F:247:PRO:HD2 | 2.36 | 0.40 |
| 2:F:274:LEU:HD23 | 2:F:274:LEU:HA | 1.92 | 0.40 |
| 1:G:939:MET:CE | 1:G:1050:THR:CG2 | 2.99 | 0.40 |
| 2:H:32:PHE:O | 2:H:291:HIS:HB2 | 2.20 | 0.40 |
| 1:A:165:PRO:HA | 1:A:182:ALA:O | 2.21 | 0.40 |
| 1:A:345:PRO:HG3 | 2:B:332:LEU:HB3 | 2.03 | 0.40 |
| 1:A:1004:ARG:HD2 | 1:A:1010:TYR:OH | 2.20 | 0.40 |
| 1:C:630:VAL:HG11 | 1:C:659:VAL:HG22 | 2.04 | 0.40 |
| 1:C:809:MET:O | 1:C:813:VAL:HG23 | 2.21 | 0.40 |
| 2:D:139:ASP:OD2 | 2:D:142:LEU:HB2 | 2.21 | 0.40 |
| 2:D:345:LYS:HB3 | 2:D:346:PRO:HD2 | 2.04 | 0.40 |
| 1:E:761:GLU:HB3 | 1:E:781:HIS:ND1 | 2.36 | 0.40 |
| 2:F:181:LEU:HA | 2:F:182:PRO:HD3 | 1.98 | 0.40 |
| 2:F:286:MET:HE1 | 2:F:312:HIS:ND1 | 2.36 | 0.40 |
| 2:F:299:ASP:OD1 | 2:F:302:LYS:HD2 | 2.22 | 0.40 |
| 1:G:526:TYR:CE1 | 1:G:545:SER:HB3 | 2.56 | 0.40 |
| 1:G:712:LEU:O | 1:G:727:ILE:HA | 2.20 | 0.40 |
| 1:G:839:LEU:HD12 | 1:G:839:LEU:HA | 1.83 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 1058/1073 (99%) | 1004 (95%) | 51 (5%) | 3 (0%) | 41 | 41 |
| 1 | C | 1059/1073 (99%) | 1005 (95%) | 50 (5%) | 4 (0%) | 34 | 32 |
| 1 | E | 1062/1073 (99%) | 1004 (94%) | 56 (5%) | 2 (0%) | 47 | 49 |
| 1 | G | 1056/1073 (98%) | 991 (94%) | 59 (6%) | 6 (1%) | 25 | 21 |
| 2 | B | 377/382 (99%) | 362 (96%) | 15 (4%) | 0 | 100 | 100 |
| 2 | D | 377/382 (99%) | 357 (95%) | 18 (5%) | 2 (0%) | 29 | 26 |
| 2 | F | 377/382 (99%) | 358 (95%) | 19 (5%) | 0 | 100 | 100 |
| 2 | H | 377/382 (99%) | 353 (94%) | 22 (6%) | 2 (0%) | 29 | 26 |
| All | All | 5743/5820 (99%) | 5434 (95%) | 290 (5%) | 19 (0%) | 41 | 41 |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 558 | ASP |
| 1 | E | 954 | LYS |
| 1 | G | 558 | ASP |
| 1 | G | 873 | SER |
| 1 | A | 975 | HIS |
| 1 | C | 739 | GLN |
| 1 | E | 975 | HIS |
| 1 | G | 739 | GLN |
| 1 | G | 975 | HIS |
| 2 | D | 229 | LEU |
| 2 | H | 269 | SER |
| 2 | D | 127 | ALA |
| 1 | C | 951 | GLU |
| 1 | G | 2 | PRO |
| 1 | G | 788 | HIS |
| 1 | A | 698 | ILE |
| 1 | C | 2 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | H | 243 | GLY |
| 1 | C | 698 | ILE |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 871/878 (99%) | 810 (93%) | 61 (7%) | 15 | 12 |
| 1 | C | 872/878 (99%) | 805 (92%) | 67 (8%) | 13 | 9 |
| 1 | E | 875/878 (100%) | 817 (93%) | 58 (7%) | 16 | 14 |
| 1 | G | 869/878 (99%) | 796 (92%) | 73 (8%) | 11 | 7 |
| 2 | B | 308/310 (99%) | 277 (90%) | 31 (10%) | 7 | 4 |
| 2 | D | 308/310 (99%) | 289 (94%) | 19 (6%) | 18 | 15 |
| 2 | F | 308/310 (99%) | 280 (91%) | 28 (9%) | 9 | 6 |
| 2 | H | 308/310 (99%) | 283 (92%) | 25 (8%) | 11 | 8 |
| All | All | 4719/4752 (99%) | 4357 (92%) | 362 (8%) | 13 | 9 |

All (362) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 1 | A | 5 | THR |
| 1 | A | 8 | LYS |
| 1 | A | 38[A] | ARG |
| 1 | A | 38[B] | ARG |
| 1 | A | 46 | LEU |
| 1 | A | 49 | SER |
| 1 | A | 103 | GLU |
| 1 | A | 138 | LYS |
| 1 | A | 174 | MET |
| 1 | A | 202 | LYS |
| 1 | A | 275 | ILE |
| 1 | A | 300 | MET |
| 1 | A | 312 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 326 | LEU |
| 1 | A | 343 | ARG |
| 1 | A | 363 | ASN |
| 1 | A | 416 | ASP |
| 1 | A | 542 | TYR |
| 1 | A | 548 | GLU |
| 1 | A | 559 | ARG |
| 1 | A | 571 | ARG |
| 1 | A | 591 | GLU |
| 1 | A | 652[A] | ARG |
| 1 | A | 652[B] | ARG |
| 1 | A | 671 | ARG |
| 1 | A | 675 | ARG |
| 1 | A | 684 | ARG |
| 1 | A | 688 | LYS |
| 1 | A | 696 | THR |
| 1 | A | 702 | VAL |
| 1 | A | 704 | LYS |
| 1 | A | 706 | LYS |
| 1 | A | 712 | LEU |
| 1 | A | 714 | VAL |
| 1 | A | 733 | ASP |
| 1 | A | 734 | LEU |
| 1 | A | 735 | ARG |
| 1 | A | 753 | ASP |
| 1 | A | 763 | ASP |
| 1 | A | 784 | GLN |
| 1 | A | 805 | ILE |
| 1 | A | 811 | GLN |
| 1 | A | 815 | LYS |
| 1 | A | 835 | ASN |
| 1 | A | 855 | LYS |
| 1 | A | 880 | THR |
| 1 | A | 891 | LYS |
| 1 | A | 906 | LEU |
| 1 | A | 912 | ARG |
| 1 | A | 930 | LYS |
| 1 | A | 940 | LYS |
| 1 | A | 950 | ARG |
| 1 | A | 951 | GLU |
| 1 | A | 967 | GLN |
| 1 | A | 992 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1006 | LYS |
| 1 | A | 1018 | SER |
| 1 | A | 1020 | ARG |
| 1 | A | 1021 | ARG |
| 1 | A | 1072 | ILE |
| 1 | A | 1073 | LYS |
| 2 | B | 2 | ILE |
| 2 | B | 6 | LEU |
| 2 | B | 18 | ARG |
| 2 | B | 25 | SER |
| 2 | B | 35 | SER |
| 2 | B | 50 | ARG |
| 2 | B | 87 | LEU |
| 2 | B | 154 | ASN |
| 2 | B | 174 | SER |
| 2 | B | 183 | GLU |
| 2 | B | 186 | LYS |
| 2 | B | 192 | PHE |
| 2 | B | 215 | ARG |
| 2 | B | 218 | ILE |
| 2 | B | 222 | GLN |
| 2 | B | 239 | SER |
| 2 | B | 257 | LYS |
| 2 | B | 269 | SER |
| 2 | B | 282 | LYS |
| 2 | B | 302 | LYS |
| 2 | B | 306 | MET |
| 2 | B | 321 | LEU |
| 2 | B | 324 | ASN |
| 2 | B | 326 | ARG |
| 2 | B | 332 | LEU |
| 2 | B | 333 | PHE |
| 2 | B | 357 | SER |
| 2 | B | 360 | PRO |
| 2 | B | 366 | LEU |
| 2 | B | 372 | GLU |
| 2 | B | 379 | LYS |
| 1 | C | 1 | MET |
| 1 | C | 5 | THR |
| 1 | C | 38 | ARG |
| 1 | C | 43 | ARG |
| 1 | C | 82 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 103 | GLU |
| 1 | C | 174 | MET |
| 1 | C | 185 | ARG |
| 1 | C | 202 | LYS |
| 1 | C | 299 | GLU |
| 1 | C | 313 | LYS |
| 1 | C | 321 | LYS |
| 1 | C | 343 | ARG |
| 1 | C | 358 | LYS |
| 1 | C | 363 | ASN |
| 1 | C | 365 | GLU |
| 1 | C | 412 | LYS |
| 1 | C | 414 | SER |
| 1 | C | 422 | THR |
| 1 | C | 423 | LYS |
| 1 | C | 509 | ARG |
| 1 | C | 542 | TYR |
| 1 | C | 548 | GLU |
| 1 | C | 555 | PRO |
| 1 | C | 559 | ARG |
| 1 | C | 571 | ARG |
| 1 | C | 591 | GLU |
| 1 | C | 652 | ARG |
| 1 | C | 665 | SER |
| 1 | C | 671 | ARG |
| 1 | C | 675 | ARG |
| 1 | C | 683 | GLU |
| 1 | C | 696 | THR |
| 1 | C | 706 | LYS |
| 1 | C | 733 | ASP |
| 1 | C | 735 | ARG |
| 1 | C | 751 | LEU |
| 1 | C | 753 | ASP |
| 1 | C | 757 | ASP |
| 1 | C | 763 | ASP |
| 1 | C | 784 | GLN |
| 1 | C | 792 | SER |
| 1 | C | 797 | PRO |
| 1 | C | 800 | THR |
| 1 | C | 805 | ILE |
| 1 | C | 812 | GLN |
| 1 | C | 827 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 833 | LYS |
| 1 | C | 849 | THR |
| 1 | C | 855 | LYS |
| 1 | C | 906 | LEU |
| 1 | C | 912 | ARG |
| 1 | C | 940 | LYS |
| 1 | C | 950 | ARG |
| 1 | C | 951 | GLU |
| 1 | C | 992 | ASN |
| 1 | C | 1000 | HIS |
| 1 | C | 1014 | ILE |
| 1 | C | 1018 | SER |
| 1 | C | 1020 | ARG |
| 1 | C | 1021 | ARG |
| 1 | C | 1031 | ARG |
| 1 | C | 1032 | SER |
| 1 | C | 1061 | LYS |
| 1 | C | 1063 | ILE |
| 1 | C | 1072 | ILE |
| 1 | C | 1073 | LYS |
| 2 | D | 6 | LEU |
| 2 | D | 18 | ARG |
| 2 | D | 47 | SER |
| 2 | D | 87 | LEU |
| 2 | D | 154 | ASN |
| 2 | D | 166 | GLU |
| 2 | D | 174 | SER |
| 2 | D | 183 | GLU |
| 2 | D | 222 | GLN |
| 2 | D | 257 | LYS |
| 2 | D | 261 | THR |
| 2 | D | 269 | SER |
| 2 | D | 282 | LYS |
| 2 | D | 324 | ASN |
| 2 | D | 326 | ARG |
| 2 | D | 332 | LEU |
| 2 | D | 333 | PHE |
| 2 | D | 366 | LEU |
| 2 | D | 379 | LYS |
| 1 | E | 1 | MET |
| 1 | E | 4 | ARG |
| 1 | E | 5 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | E | 46 | LEU |
| 1 | E | 55 | MET |
| 1 | E | 103 | GLU |
| 1 | E | 153[A] | GLU |
| 1 | E | 153[B] | GLU |
| 1 | E | 174 | MET |
| 1 | E | 236 | ASN |
| 1 | E | 275 | ILE |
| 1 | E | 307 | SER |
| 1 | E | 321 | LYS |
| 1 | E | 343 | ARG |
| 1 | E | 358 | LYS |
| 1 | E | 363 | ASN |
| 1 | E | 412 | LYS |
| 1 | E | 428 | LEU |
| 1 | E | 490 | ARG |
| 1 | E | 515 | LYS |
| 1 | E | 542 | TYR |
| 1 | E | 548 | GLU |
| 1 | E | 559 | ARG |
| 1 | E | 571 | ARG |
| 1 | E | 591 | GLU |
| 1 | E | 671 | ARG |
| 1 | E | 675 | ARG |
| 1 | E | 680 | HIS |
| 1 | E | 683 | GLU |
| 1 | E | 696 | THR |
| 1 | E | 698 | ILE |
| 1 | E | 700 | MET |
| 1 | E | 706 | LYS |
| 1 | E | 733 | ASP |
| 1 | E | 734 | LEU |
| 1 | E | 735 | ARG |
| 1 | E | 751 | LEU |
| 1 | E | 784 | GLN |
| 1 | E | 805 | ILE |
| 1 | E | 835 | ASN |
| 1 | E | 839 | LEU |
| 1 | E | 855 | LYS |
| 1 | E | 891 | LYS |
| 1 | E | 906 | LEU |
| 1 | E | 912[A] | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | E | 912[B] | ARG |
| 1 | E | 940 | LYS |
| 1 | E | 950 | ARG |
| 1 | E | 951 | GLU |
| 1 | E | 956[A] | ARG |
| 1 | E | 956[B] | ARG |
| 1 | E | 966 | LYS |
| 1 | E | 993 | LYS |
| 1 | E | 1000 | HIS |
| 1 | E | 1020 | ARG |
| 1 | E | 1021 | ARG |
| 1 | E | 1061 | LYS |
| 1 | E | 1073 | LYS |
| 2 | F | 18 | ARG |
| 2 | F | 25 | SER |
| 2 | F | 50 | ARG |
| 2 | F | 73 | SER |
| 2 | F | 87 | LEU |
| 2 | F | 106 | ASN |
| 2 | F | 151 | PRO |
| 2 | F | 153 | LEU |
| 2 | F | 154 | ASN |
| 2 | F | 166 | GLU |
| 2 | F | 169 | SER |
| 2 | F | 175 | TRP |
| 2 | F | 183 | GLU |
| 2 | F | 186 | LYS |
| 2 | F | 192 | PHE |
| 2 | F | 205 | ILE |
| 2 | F | 215 | ARG |
| 2 | F | 222 | GLN |
| 2 | F | 239 | SER |
| 2 | F | 261 | THR |
| 2 | F | 282 | LYS |
| 2 | F | 301 | GLU |
| 2 | F | 306 | MET |
| 2 | F | 324 | ASN |
| 2 | F | 326 | ARG |
| 2 | F | 332 | LEU |
| 2 | F | 366 | LEU |
| 2 | F | 379 | LYS |
| 1 | G | 4 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | G | 8 | LYS |
| 1 | G | 43 | ARG |
| 1 | G | 46 | LEU |
| 1 | G | 49 | SER |
| 1 | G | 59 | GLU |
| 1 | G | 76 | LYS |
| 1 | G | 145 | ARG |
| 1 | G | 174 | MET |
| 1 | G | 207 | ASP |
| 1 | G | 236 | ASN |
| 1 | G | 275 | ILE |
| 1 | G | 307 | SER |
| 1 | G | 313 | LYS |
| 1 | G | 321 | LYS |
| 1 | G | 326 | LEU |
| 1 | G | 343 | ARG |
| 1 | G | 363 | ASN |
| 1 | G | 387 | ILE |
| 1 | G | 412 | LYS |
| 1 | G | 416 | ASP |
| 1 | G | 428 | LEU |
| 1 | G | 482 | THR |
| 1 | G | 489 | LEU |
| 1 | G | 509 | ARG |
| 1 | G | 519 | GLN |
| 1 | G | 542 | TYR |
| 1 | G | 543 | MET |
| 1 | G | 548 | GLU |
| 1 | G | 558 | ASP |
| 1 | G | 559 | ARG |
| 1 | G | 571 | ARG |
| 1 | G | 591 | GLU |
| 1 | G | 652 | ARG |
| 1 | G | 665 | SER |
| 1 | G | 671 | ARG |
| 1 | G | 675 | ARG |
| 1 | G | 683 | GLU |
| 1 | G | 688 | LYS |
| 1 | G | 704 | LYS |
| 1 | G | 706 | LYS |
| 1 | G | 714 | VAL |
| 1 | G | 733 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | G | 734 | LEU |
| 1 | G | 735 | ARG |
| 1 | G | 751 | LEU |
| 1 | G | 752 | LEU |
| 1 | G | 753 | ASP |
| 1 | G | 763 | ASP |
| 1 | G | 784 | GLN |
| 1 | G | 800 | THR |
| 1 | G | 805 | ILE |
| 1 | G | 815 | LYS |
| 1 | G | 849 | THR |
| 1 | G | 855 | LYS |
| 1 | G | 880 | THR |
| 1 | G | 881 | LYS |
| 1 | G | 891 | LYS |
| 1 | G | 906 | LEU |
| 1 | G | 912 | ARG |
| 1 | G | 940 | LYS |
| 1 | G | 950 | ARG |
| 1 | G | 963 | LYS |
| 1 | G | 966 | LYS |
| 1 | G | 1001 | ILE |
| 1 | G | 1006 | LYS |
| 1 | G | 1020 | ARG |
| 1 | G | 1021 | ARG |
| 1 | G | 1026 | SER |
| 1 | G | 1031 | ARG |
| 1 | G | 1061 | LYS |
| 1 | G | 1063 | ILE |
| 1 | G | 1073 | LYS |
| 2 | H | 2 | ILE |
| 2 | H | 6 | LEU |
| 2 | H | 7 | LEU |
| 2 | H | 25 | SER |
| 2 | H | 47 | SER |
| 2 | H | 78 | GLN |
| 2 | H | 104 | ARG |
| 2 | H | 125 | LYS |
| 2 | H | 153 | LEU |
| 2 | H | 154 | ASN |
| 2 | H | 156 | MET |
| 2 | H | 166 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | H | 192 | PHE |
| 2 | H | 216 | LEU |
| 2 | H | 218 | ILE |
| 2 | H | 222 | GLN |
| 2 | H | 257 | LYS |
| 2 | H | 306 | MET |
| 2 | H | 321 | LEU |
| 2 | H | 324 | ASN |
| 2 | H | 332 | LEU |
| 2 | H | 340 | ILE |
| 2 | H | 357 | SER |
| 2 | H | 366 | LEU |
| 2 | H | 379 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 105 | GLN |
| 1 | A | 266 | ASN |
| 1 | A | 457 | ASN |
| 1 | A | 689 | GLN |
| 1 | A | 784 | GLN |
| 1 | A | 803 | GLN |
| 1 | A | 814 | GLN |
| 1 | A | 834 | ASN |
| 1 | A | 835 | ASN |
| 1 | A | 936 | ASN |
| 1 | A | 942 | HIS |
| 1 | A | 967 | GLN |
| 1 | A | 987 | ASN |
| 1 | A | 992 | ASN |
| 1 | A | 1000 | HIS |
| 1 | A | 1007 | ASN |
| 1 | A | 1035 | GLN |
| 1 | A | 1071 | GLN |
| 2 | B | 51 | GLN |
| 2 | B | 154 | ASN |
| 2 | B | 222 | GLN |
| 2 | B | 324 | ASN |
| 2 | B | 351 | GLN |
| 1 | C | 105 | GLN |
| 1 | C | 266 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 457 | ASN |
| 1 | C | 645 | GLN |
| 1 | C | 689 | GLN |
| 1 | C | 784 | GLN |
| 1 | C | 942 | HIS |
| 1 | C | 987 | ASN |
| 1 | C | 992 | ASN |
| 1 | C | 1000 | HIS |
| 1 | C | 1035 | GLN |
| 1 | C | 1055 | ASN |
| 1 | C | 1071 | GLN |
| 2 | D | 51 | GLN |
| 2 | D | 154 | ASN |
| 2 | D | 222 | GLN |
| 2 | D | 324 | ASN |
| 2 | D | 351 | GLN |
| 1 | E | 105 | GLN |
| 1 | E | 266 | ASN |
| 1 | E | 457 | ASN |
| 1 | E | 679 | GLN |
| 1 | E | 689 | GLN |
| 1 | E | 784 | GLN |
| 1 | E | 803 | GLN |
| 1 | E | 814 | GLN |
| 1 | E | 835 | ASN |
| 1 | E | 942 | HIS |
| 1 | E | 987 | ASN |
| 1 | E | 992 | ASN |
| 1 | E | 1000 | HIS |
| 1 | E | 1002 | GLN |
| 1 | E | 1035 | GLN |
| 1 | E | 1055 | ASN |
| 1 | E | 1071 | GLN |
| 2 | F | 51 | GLN |
| 2 | F | 106 | ASN |
| 2 | F | 154 | ASN |
| 2 | F | 222 | GLN |
| 2 | F | 324 | ASN |
| 1 | G | 105 | GLN |
| 1 | G | 457 | ASN |
| 1 | G | 523 | HIS |
| 1 | G | 689 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | G | 784 | GLN |
| 1 | G | 803 | GLN |
| 1 | G | 834 | ASN |
| 1 | G | 936 | ASN |
| 1 | G | 942 | HIS |
| 1 | G | 987 | ASN |
| 1 | G | 992 | ASN |
| 1 | G | 1000 | HIS |
| 1 | G | 1035 | GLN |
| 1 | G | 1055 | ASN |
| 1 | G | 1071 | GLN |
| 2 | H | 51 | GLN |
| 2 | H | 78 | GLN |
| 2 | H | 154 | ASN |
| 2 | H | 324 | 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 89 ligands modelled in this entry, 60 are monoatomic - leaving 29 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 |
| 7 | ADP | G | 4068 | 3 | 24,29,29 | 1.12 | 2 (8%) | 29,45,45 | 1.43 | 6 (20%) |
| 8 | ORN | G | 4078 | - | 7,8,8 | 0.73 | 0 | 8,9,9 | 1.16 | 1 (12%) |
| 9 | GLN | C | 4035 | - | 8,9,9 | 1.25 | 1 (12%) | 10,11,11 | 1.18 | 2 (20%) |
| 9 | GLN | F | 4056 | - | 8,9,9 | 1.46 | 2 (25%) | 10,11,11 | 1.48 | 2 (20%) |
| 9 | GLN | D | 4034 | - | 8,9,9 | 1.22 | 1 (12%) | 10,11,11 | 2.09 | 4 (40%) |
| 9 | GLN | B | 4012 | - | 8,9,9 | 1.14 | 1 (12%) | 10,11,11 | 1.63 | 3 (30%) |
| 10 | NET | G | 4081 | - | 8,8,8 | 0.66 | 0 | 10,10,10 | 0.46 | 0 |
| 10 | NET | C | 4036 | - | 8,8,8 | 0.54 | 0 | 10,10,10 | 0.47 | 0 |
| 9 | GLN | H | 4079 | - | 8,9,9 | 1.25 | 1 (12%) | 10,11,11 | 1.21 | 0 |
| 8 | ORN | C | 4033 | - | 7,8,8 | 1.13 | 1 (14%) | 8,9,9 | 1.00 | 0 |
| 7 | ADP | E | 4045 | 3 | 24,29,29 | 1.11 | 2 (8%) | 29,45,45 | 1.20 | 2 (6%) |
| 10 | NET | E | 4058 | - | 8,8,8 | 0.55 | 0 | 10,10,10 | 0.74 | 0 |
| 6 | PO4 | A | 4006 | 3,4 | 4,4,4 | 2.38 | 2 (50%) | 6,6,6 | 0.99 | 0 |
| 7 | ADP | A | 4000 | 3 | 24,29,29 | 1.20 | 3 (12%) | 29,45,45 | 1.18 | 2 (6%) |
| 7 | ADP | C | 4023 | 3 | 24,29,29 | 1.13 | 1 (4%) | 29,45,45 | 0.96 | 1 (3%) |
| 9 | GLN | G | 4080 | - | 8,9,9 | 1.34 | 1 (12%) | 10,11,11 | 0.77 | 0 |
| 7 | ADP | C | 4029 | 3,4 | 24,29,29 | 1.22 | 3 (12%) | 29,45,45 | 1.19 | 5 (17%) |
| 6 | PO4 | G | 4073 | 3,4 | 4,4,4 | 1.97 | 2 (50%) | 6,6,6 | 1.02 | 0 |
| 7 | ADP | E | 4051 | 3,4 | 24,29,29 | 1.05 | 3 (12%) | 29,45,45 | 0.96 | 1 (3%) |
| 9 | GLN | E | 4057 | - | 8,9,9 | 1.39 | 2 (25%) | 10,11,11 | 1.47 | 2 (20%) |
| 7 | ADP | A | 4007 | 3,4 | 24,29,29 | 0.91 | 0 | 29,45,45 | 1.29 | 2 (6%) |
| 6 | PO4 | C | 4028 | 3,4 | 4,4,4 | 2.89 | 3 (75%) | 6,6,6 | 1.13 | 0 |
| 6 | PO4 | E | 4067 | - | 4,4,4 | 1.42 | 0 | 6,6,6 | 0.68 | 0 |
| 10 | NET | A | 4014 | - | 8,8,8 | 0.69 | 0 | 10,10,10 | 0.56 | 0 |
| 8 | ORN | A | 4011 | - | 7,8,8 | 1.08 | 0 | 8,9,9 | 1.52 | 2 (25%) |
| 7 | ADP | G | 4074 | 3,4 | 24,29,29 | 1.27 | 3 (12%) | 29,45,45 | 1.37 | 3 (10%) |
| 6 | PO4 | E | 4050 | 3,4 | 4,4,4 | 2.40 | 3 (75%) | 6,6,6 | 1.14 | 0 |
| 8 | ORN | E | 4055 | - | 7,8,8 | 1.00 | 0 | 8,9,9 | 0.74 | 0 |
| 9 | GLN | A | 4013 | - | 8,9,9 | 1.40 | 1 (12%) | 10,11,11 | 1.19 | 0 |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 7 | ADP | G | 4068 | 3 | - | 1/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 8 | ORN | G | 4078 | - | - | 6/8/8/8 | - |
| 9 | GLN | C | 4035 | - | - | 2/9/9/9 | - |
| 9 | GLN | F | 4056 | - | - | 2/9/9/9 | - |
| 9 | GLN | D | 4034 | - | - | 3/9/9/9 | - |
| 9 | GLN | B | 4012 | - | - | 6/9/9/9 | - |
| 10 | NET | G | 4081 | - | - | 0/12/12/12 | - |
| 10 | NET | C | 4036 | - | - | 3/12/12/12 | - |
| 9 | GLN | H | 4079 | - | - | 5/9/9/9 | - |
| 8 | ORN | C | 4033 | - | - | 6/8/8/8 | - |
| 7 | ADP | E | 4045 | 3 | - | 1/12/32/32 | 0/3/3/3 |
| 10 | NET | E | 4058 | - | - | 3/12/12/12 | - |
| 7 | ADP | A | 4000 | 3 | - | 1/12/32/32 | 0/3/3/3 |
| 7 | ADP | C | 4023 | 3 | - | 2/12/32/32 | 0/3/3/3 |
| 9 | GLN | G | 4080 | - | - | 0/9/9/9 | - |
| 7 | ADP | C | 4029 | 3,4 | - | 3/12/32/32 | 0/3/3/3 |
| 7 | ADP | E | 4051 | 3,4 | - | 4/12/32/32 | 0/3/3/3 |
| 9 | GLN | E | 4057 | - | - | 1/9/9/9 | - |
| 7 | ADP | A | 4007 | 3,4 | - | 4/12/32/32 | 0/3/3/3 |
| 10 | NET | A | 4014 | - | - | 0/12/12/12 | - |
| 8 | ORN | A | 4011 | - | - | 5/8/8/8 | - |
| 7 | ADP | G | 4074 | 3,4 | - | 2/12/32/32 | 0/3/3/3 |
| 8 | ORN | E | 4055 | - | - | 5/8/8/8 | - |
| 9 | GLN | A | 4013 | - | - | 3/9/9/9 | - |

All (38) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6 | C | 4028 | PO4 | P-O4 | -3.77 | 1.43 | 1.54 |
| 7 | G | 4074 | ADP | O3'-C3' | 3.72 | 1.51 | 1.43 |
| 7 | C | 4029 | ADP | O3'-C3' | 3.60 | 1.51 | 1.43 |
| 6 | C | 4028 | PO4 | P-O2 | -3.44 | 1.44 | 1.54 |
| 6 | A | 4006 | PO4 | P-O2 | -3.12 | 1.45 | 1.54 |
| 6 | G | 4073 | PO4 | P-O2 | -3.01 | 1.45 | 1.54 |
| 9 | C | 4035 | GLN | CA-N | -2.99 | 1.33 | 1.48 |
| 7 | G | 4068 | ADP | O3'-C3' | 2.92 | 1.49 | 1.43 |
| 9 | E | 4057 | GLN | CA-N | -2.90 | 1.33 | 1.48 |
| 9 | H | 4079 | GLN | CA-N | -2.89 | 1.33 | 1.48 |
| 7 | E | 4045 | ADP | O3'-C3' | 2.86 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | G | 4080 | GLN | CA-N | -2.86 | 1.34 | 1.48 |
| 9 | F | 4056 | GLN | CA-N | -2.80 | 1.34 | 1.48 |
| 7 | C | 4023 | ADP | O2'-C2' | 2.80 | 1.49 | 1.43 |
| 6 | E | 4050 | PO4 | P-O3 | -2.80 | 1.46 | 1.54 |
| 6 | A | 4006 | PO4 | P-O4 | -2.78 | 1.46 | 1.54 |
| 9 | A | 4013 | GLN | CA-N | -2.72 | 1.34 | 1.48 |
| 6 | E | 4050 | PO4 | P-O2 | -2.72 | 1.46 | 1.54 |
| 7 | C | 4029 | ADP | O2'-C2' | 2.60 | 1.49 | 1.43 |
| 7 | G | 4074 | ADP | O2'-C2' | 2.60 | 1.49 | 1.43 |
| 9 | B | 4012 | GLN | CA-N | -2.58 | 1.35 | 1.48 |
| 6 | E | 4050 | PO4 | P-O4 | -2.56 | 1.46 | 1.54 |
| 8 | C | 4033 | ORN | O-C | 2.55 | 1.29 | 1.22 |
| 7 | G | 4074 | ADP | O4'-C1' | -2.47 | 1.37 | 1.41 |
| 7 | A | 4000 | ADP | O3'-C3' | 2.45 | 1.48 | 1.43 |
| 9 | D | 4034 | GLN | CA-N | -2.44 | 1.36 | 1.48 |
| 9 | F | 4056 | GLN | O-C | 2.43 | 1.29 | 1.22 |
| 7 | A | 4000 | ADP | O4'-C1' | -2.35 | 1.37 | 1.41 |
| 7 | G | 4068 | ADP | O2'-C2' | 2.30 | 1.48 | 1.43 |
| 9 | E | 4057 | GLN | O-C | 2.28 | 1.29 | 1.22 |
| 7 | E | 4051 | ADP | C2-N1 | 2.27 | 1.38 | 1.33 |
| 7 | C | 4029 | ADP | C2-N1 | 2.27 | 1.38 | 1.33 |
| 7 | E | 4045 | ADP | O4'-C1' | -2.26 | 1.37 | 1.41 |
| 7 | E | 4051 | ADP | O2'-C2' | 2.22 | 1.48 | 1.43 |
| 6 | C | 4028 | PO4 | P-O3 | -2.20 | 1.48 | 1.54 |
| 7 | E | 4051 | ADP | O4'-C1' | -2.19 | 1.38 | 1.41 |
| 6 | G | 4073 | PO4 | P-O4 | -2.12 | 1.48 | 1.54 |
| 7 | A | 4000 | ADP | C2-N1 | 2.10 | 1.37 | 1.33 |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7 | A | 4007 | ADP | C5-C6-N6 | 4.26 | 126.83 | 120.35 |
| 9 | D | 4034 | GLN | CG-CB-CA | -3.88 | 104.78 | 113.84 |
| 7 | G | 4068 | ADP | O3B-PB-O3A | -3.66 | 92.38 | 104.64 |
| 7 | G | 4074 | ADP | C5-C6-N6 | 3.49 | 125.66 | 120.35 |
| 9 | D | 4034 | GLN | CB-CA-C | -3.26 | 102.53 | 110.30 |
| 7 | E | 4045 | ADP | C3'-C2'-C1' | 3.00 | 105.49 | 100.98 |
| 9 | B | 4012 | GLN | CB-CA-C | -2.89 | 103.42 | 110.30 |
| 7 | G | 4074 | ADP | O3B-PB-O3A | 2.88 | 114.30 | 104.64 |
| 7 | E | 4045 | ADP | C5-C6-N6 | 2.82 | 124.63 | 120.35 |
| 9 | F | 4056 | GLN | CG-CB-CA | -2.76 | 107.39 | 113.84 |
| 7 | G | 4068 | ADP | O3'-C3'-C2' | 2.70 | 120.57 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7 | G | 4074 | ADP | O3'-C3'-C2' | 2.69 | 120.51 | 111.82 |
| 9 | E | 4057 | GLN | OXT-C-O | -2.69 | 117.99 | 124.09 |
| 7 | A | 4000 | ADP | C5-C6-N1 | -2.64 | 114.37 | 120.35 |
| 9 | E | 4057 | GLN | OXT-C-CA | 2.60 | 122.26 | 113.38 |
| 7 | C | 4029 | ADP | C3'-C2'-C1' | 2.60 | 104.89 | 100.98 |
| 9 | D | 4034 | GLN | OE1-CD-CG | -2.59 | 113.45 | 121.07 |
| 7 | G | 4068 | ADP | N6-C6-N1 | 2.56 | 123.88 | 118.57 |
| 9 | B | 4012 | GLN | OXT-C-CA | 2.50 | 121.90 | 113.38 |
| 7 | A | 4007 | ADP | C2'-C3'-C4' | -2.50 | 97.79 | 102.64 |
| 8 | G | 4078 | ORN | OXT-C-CA | 2.47 | 121.79 | 113.38 |
| 7 | C | 4023 | ADP | C3'-C2'-C1' | 2.47 | 104.69 | 100.98 |
| 7 | G | 4068 | ADP | O2'-C2'-C3' | 2.46 | 119.78 | 111.82 |
| 7 | G | 4068 | ADP | C5-C6-N1 | -2.38 | 114.96 | 120.35 |
| 7 | C | 4029 | ADP | C5-C6-N6 | 2.38 | 123.96 | 120.35 |
| 8 | A | 4011 | ORN | OXT-C-CA | 2.34 | 121.35 | 113.38 |
| 7 | C | 4029 | ADP | C5-C6-N1 | -2.30 | 115.13 | 120.35 |
| 9 | B | 4012 | GLN | OXT-C-O | -2.21 | 119.07 | 124.09 |
| 9 | C | 4035 | GLN | OXT-C-O | -2.20 | 119.09 | 124.09 |
| 9 | C | 4035 | GLN | OXT-C-CA | 2.17 | 120.78 | 113.38 |
| 8 | A | 4011 | ORN | CB-CA-C | -2.16 | 105.16 | 110.30 |
| 7 | A | 4000 | ADP | O3B-PB-O3A | -2.13 | 97.49 | 104.64 |
| 7 | C | 4029 | ADP | O3'-C3'-C2' | 2.11 | 118.66 | 111.82 |
| 9 | F | 4056 | GLN | CB-CA-C | -2.10 | 105.29 | 110.30 |
| 7 | C | 4029 | ADP | O2'-C2'-C3' | 2.09 | 118.59 | 111.82 |
| 7 | G | 4068 | ADP | O3B-PB-O2B | 2.04 | 115.45 | 107.64 |
| 9 | D | 4034 | GLN | CG-CD-NE2 | 2.02 | 122.80 | 116.51 |
| 7 | E | 4051 | ADP | C4-C5-N7 | 2.00 | 111.48 | 109.40 |

There are no chirality outliers.

All (68) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 7 | C | 4029 | ADP | PA-O3A-PB-O3B |
| 7 | E | 4051 | ADP | PA-O3A-PB-O3B |
| 8 | A | 4011 | ORN | N-CA-CB-CG |
| 8 | A | 4011 | ORN | C-CA-CB-CG |
| 8 | C | 4033 | ORN | N-CA-CB-CG |
| 8 | C | 4033 | ORN | C-CA-CB-CG |
| 8 | E | 4055 | ORN | N-CA-CB-CG |
| 8 | E | 4055 | ORN | C-CA-CB-CG |
| 8 | G | 4078 | ORN | N-CA-CB-CG |
| 9 | A | 4013 | GLN | C-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 9 | B | 4012 | GLN | C-CA-CB-CG |
| 9 | C | 4035 | GLN | N-CA-CB-CG |
| 9 | C | 4035 | GLN | C-CA-CB-CG |
| 9 | E | 4057 | GLN | C-CA-CB-CG |
| 9 | H | 4079 | GLN | N-CA-CB-CG |
| 9 | H | 4079 | GLN | C-CA-CB-CG |
| 9 | B | 4012 | GLN | CA-CB-CG-CD |
| 8 | E | 4055 | ORN | OXT-C-CA-N |
| 8 | E | 4055 | ORN | CA-CB-CG-CD |
| 10 | C | 4036 | NET | C8-C7-N1-C3 |
| 8 | G | 4078 | ORN | OXT-C-CA-N |
| 10 | C | 4036 | NET | C8-C7-N1-C5 |
| 10 | C | 4036 | NET | C8-C7-N1-C1 |
| 8 | C | 4033 | ORN | OXT-C-CA-N |
| 7 | A | 4007 | ADP | PA-O3A-PB-O1B |
| 7 | E | 4051 | ADP | PA-O3A-PB-O1B |
| 9 | H | 4079 | GLN | NE2-CD-CG-CB |
| 8 | C | 4033 | ORN | CA-CB-CG-CD |
| 8 | C | 4033 | ORN | O-C-CA-N |
| 8 | E | 4055 | ORN | O-C-CA-N |
| 8 | G | 4078 | ORN | O-C-CA-N |
| 9 | B | 4012 | GLN | OE1-CD-CG-CB |
| 10 | E | 4058 | NET | C4-C3-N1-C5 |
| 9 | H | 4079 | GLN | OE1-CD-CG-CB |
| 8 | A | 4011 | ORN | CA-CB-CG-CD |
| 8 | G | 4078 | ORN | CA-CB-CG-CD |
| 7 | A | 4007 | ADP | PA-O3A-PB-O3B |
| 8 | G | 4078 | ORN | C-CA-CB-CG |
| 7 | A | 4000 | ADP | PB-O3A-PA-O1A |
| 7 | E | 4045 | ADP | PB-O3A-PA-O1A |
| 10 | E | 4058 | NET | C4-C3-N1-C1 |
| 9 | B | 4012 | GLN | NE2-CD-CG-CB |
| 9 | A | 4013 | GLN | N-CA-CB-CG |
| 10 | E | 4058 | NET | C4-C3-N1-C7 |
| 9 | F | 4056 | GLN | OE1-CD-CG-CB |
| 7 | G | 4074 | ADP | PA-O3A-PB-O1B |
| 9 | F | 4056 | GLN | NE2-CD-CG-CB |
| 8 | G | 4078 | ORN | NE-CD-CG-CB |
| 8 | A | 4011 | ORN | OXT-C-CA-N |
| 7 | A | 4007 | ADP | PB-O3A-PA-O2A |
| 7 | C | 4029 | ADP | PB-O3A-PA-O2A |
| 7 | E | 4051 | ADP | PB-O3A-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 9 | H | 4079 | GLN | CA-CB-CG-CD |
| 8 | A | 4011 | ORN | O-C-CA-N |
| 7 | G | 4068 | ADP | PB-O3A-PA-O1A |
| 7 | C | 4029 | ADP | PA-O3A-PB-O1B |
| 9 | D | 4034 | GLN | OXT-C-CA-N |
| 7 | G | 4074 | ADP | C5'-O5'-PA-O3A |
| 8 | C | 4033 | ORN | NE-CD-CG-CB |
| 9 | D | 4034 | GLN | NE2-CD-CG-CB |
| 9 | B | 4012 | GLN | OXT-C-CA-N |
| 7 | A | 4007 | ADP | PB-O3A-PA-O1A |
| 7 | C | 4023 | ADP | PB-O3A-PA-O1A |
| 7 | E | 4051 | ADP | PB-O3A-PA-O1A |
| 7 | C | 4023 | ADP | C5'-O5'-PA-O1A |
| 9 | D | 4034 | GLN | OE1-CD-CG-CB |
| 9 | B | 4012 | GLN | N-CA-CB-CG |
| 9 | A | 4013 | GLN | OXT-C-CA-N |

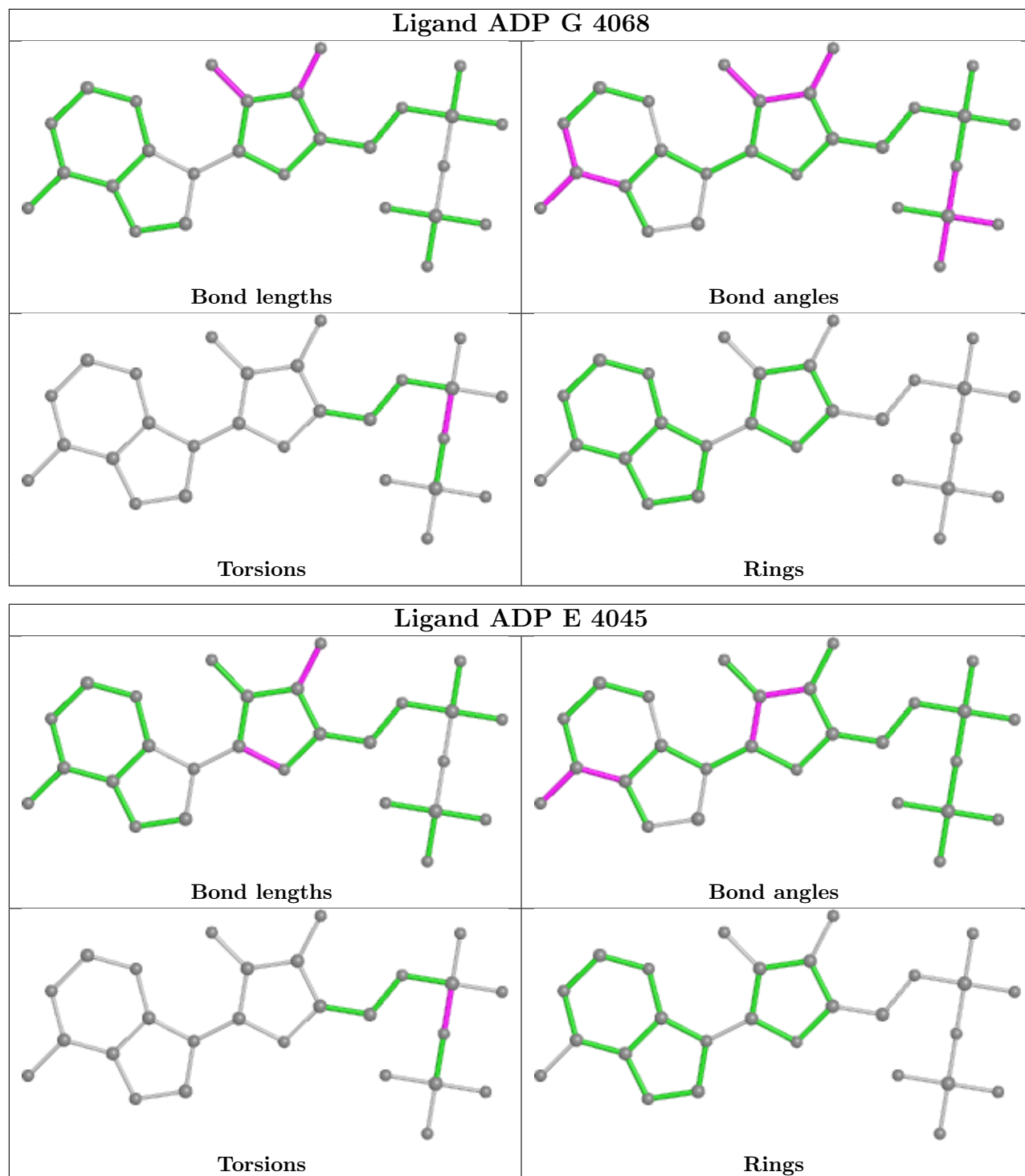
There are no ring outliers.

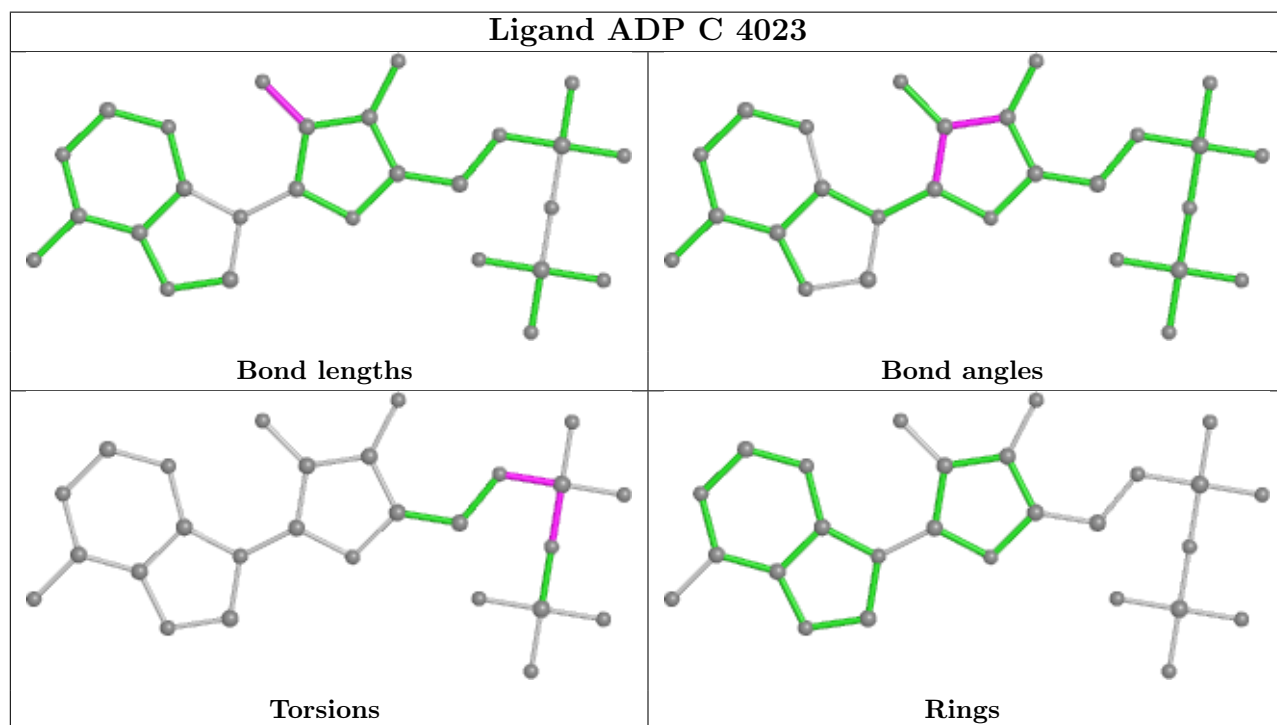
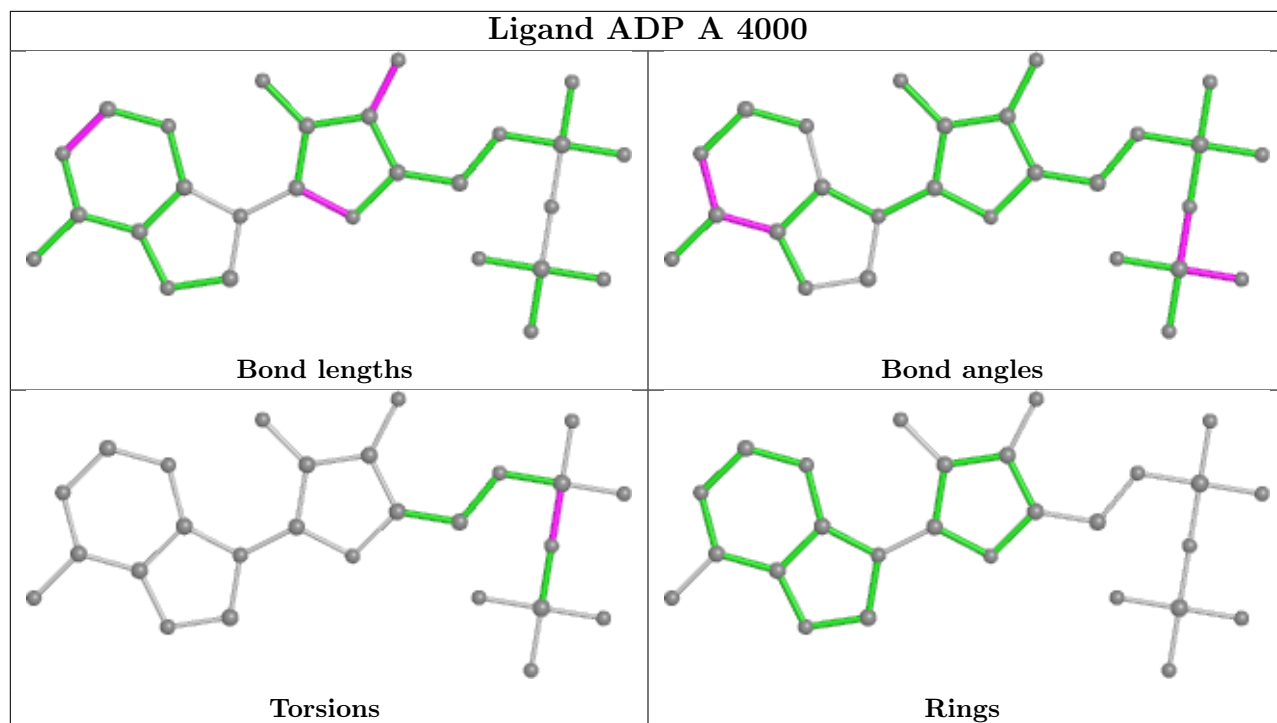
13 monomers are involved in 22 short contacts:

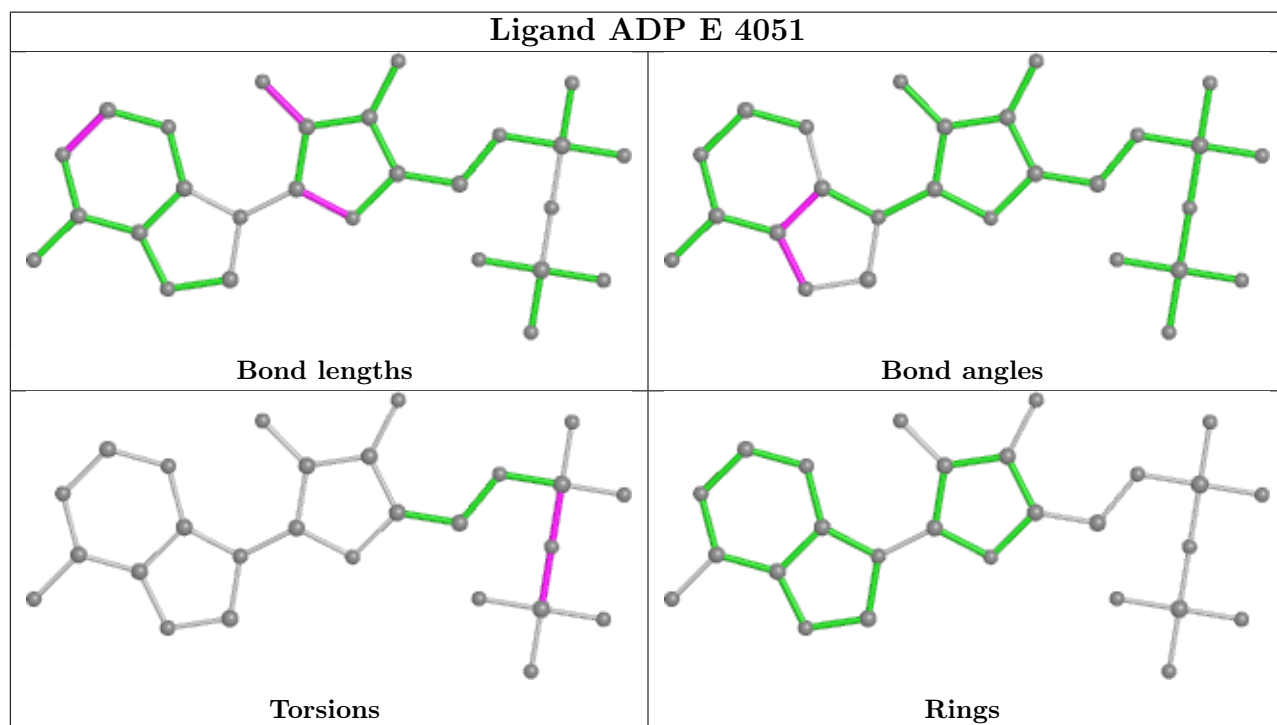
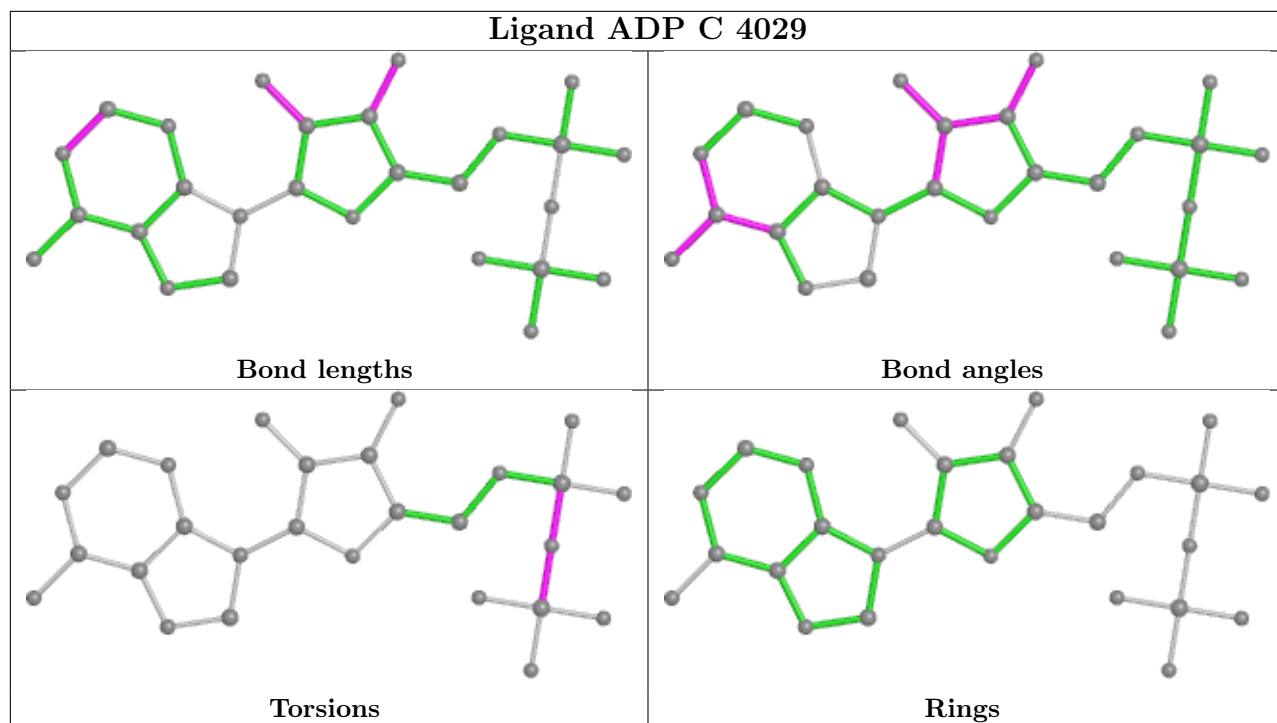
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 7 | G | 4068 | ADP | 1 | 0 |
| 9 | F | 4056 | GLN | 3 | 0 |
| 9 | D | 4034 | GLN | 2 | 0 |
| 9 | B | 4012 | GLN | 3 | 0 |
| 10 | C | 4036 | NET | 1 | 0 |
| 9 | H | 4079 | GLN | 2 | 0 |
| 8 | C | 4033 | ORN | 1 | 0 |
| 7 | E | 4045 | ADP | 2 | 0 |
| 10 | E | 4058 | NET | 2 | 0 |
| 7 | C | 4029 | ADP | 1 | 0 |
| 7 | E | 4051 | ADP | 2 | 0 |
| 8 | A | 4011 | ORN | 1 | 0 |
| 7 | G | 4074 | ADP | 1 | 0 |

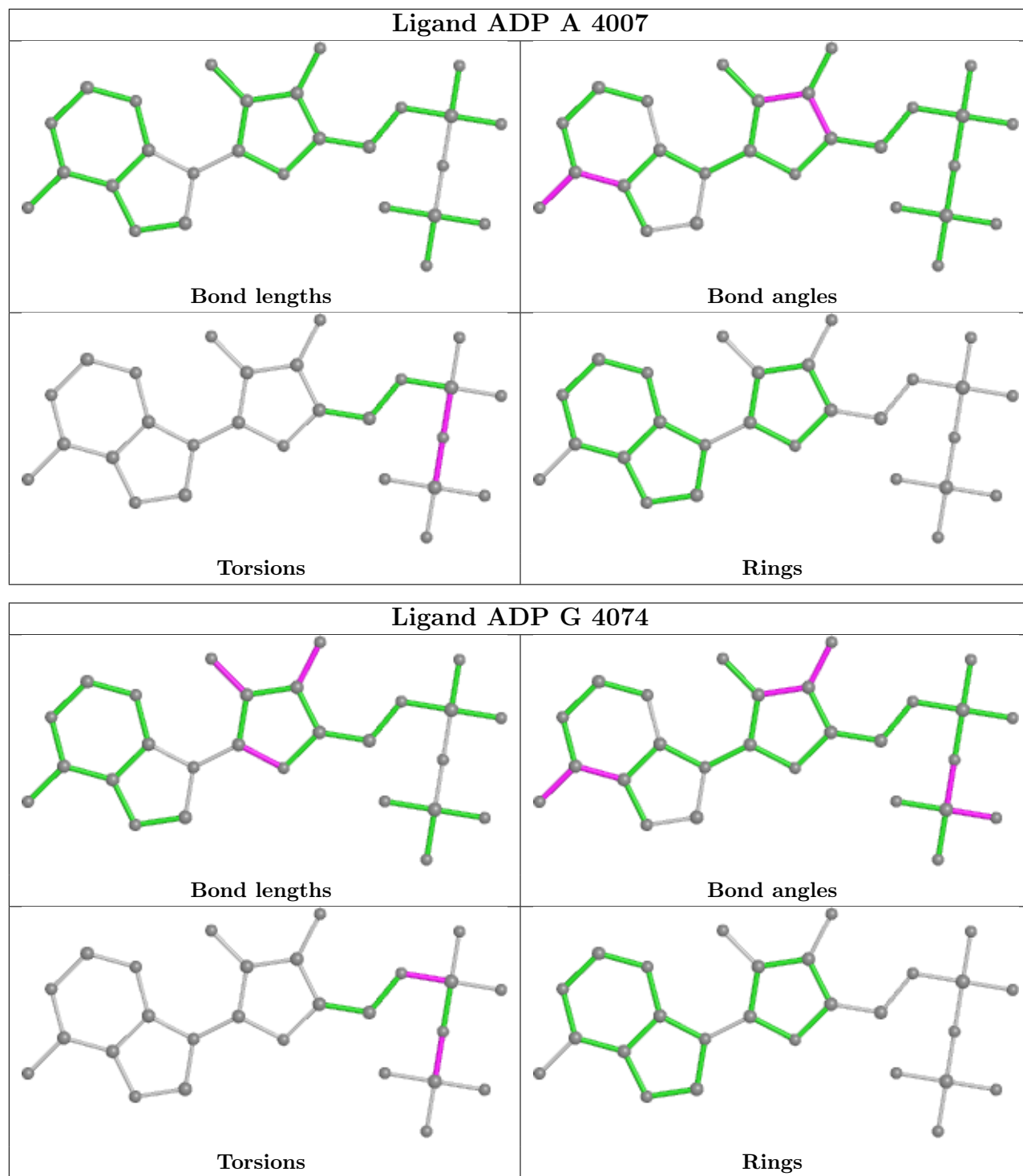
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.