



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:19 PM GMT

PDB ID : 1X0R
Title : Thioredoxin Peroxidase from Aeropyrum pernix K1
Authors : Nakamura, T.; Yamamoto, T.; Inoue, T.; Matsumura, H.; Kobayashi, A.;
Hagihara, Y.; Uegaki, K.; Ataka, M.; Kai, Y.; Ishikawa, K.
Deposited on : 2005-03-28
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

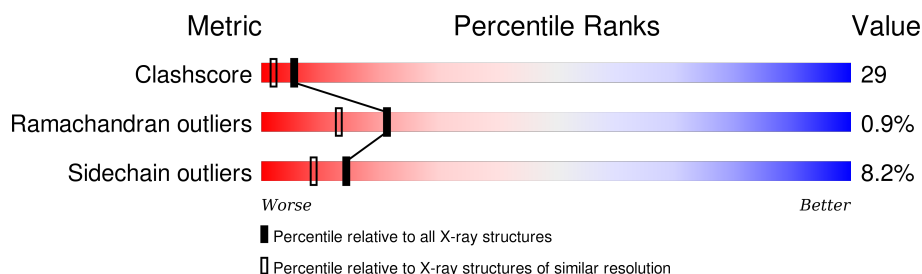
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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 | 102246 | 7340 (2.00-2.00) |
| Ramachandran outliers | 100387 | 7248 (2.00-2.00) |
| Sidechain outliers | 100360 | 7247 (2.00-2.00) |


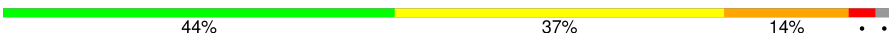

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 249 | |
| 1 | B | 249 | |
| 1 | C | 249 | |
| 1 | D | 249 | |
| 1 | E | 249 | |
| 1 | F | 249 | |
| 1 | G | 249 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | H | 249 |  |
| 1 | I | 249 |  |
| 1 | J | 249 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | EDO | A | 2001 | - | - | X | - |
| 2 | EDO | A | 2012 | - | - | X | - |
| 2 | EDO | A | 2029 | - | - | X | - |
| 2 | EDO | A | 2063 | - | - | X | - |
| 2 | EDO | A | 2065 | - | - | X | - |
| 2 | EDO | A | 2122 | - | - | X | - |
| 2 | EDO | A | 2124 | - | - | X | - |
| 2 | EDO | B | 2002 | - | - | X | - |
| 2 | EDO | B | 2021 | - | - | X | - |
| 2 | EDO | B | 2028 | - | - | X | - |
| 2 | EDO | B | 2030 | - | - | X | - |
| 2 | EDO | B | 2125 | - | X | X | - |
| 2 | EDO | C | 2004 | - | - | X | - |
| 2 | EDO | C | 2024 | - | - | X | - |
| 2 | EDO | C | 2067 | - | - | X | - |
| 2 | EDO | C | 2075 | - | - | X | - |
| 2 | EDO | C | 2081 | - | X | - | - |
| 2 | EDO | C | 2085 | - | X | X | - |
| 2 | EDO | C | 2126 | - | X | X | - |
| 2 | EDO | C | 2128 | - | - | X | - |
| 2 | EDO | D | 2003 | - | - | X | - |
| 2 | EDO | D | 2031 | - | - | X | - |
| 2 | EDO | D | 2035 | - | - | X | - |
| 2 | EDO | D | 2118 | - | - | X | - |
| 2 | EDO | E | 2005 | - | - | X | - |
| 2 | EDO | E | 2076 | - | - | X | - |
| 2 | EDO | E | 2089 | - | - | X | - |
| 2 | EDO | E | 2090 | - | - | X | - |
| 2 | EDO | E | 2091 | - | - | X | - |
| 2 | EDO | E | 2120 | - | - | X | - |
| 2 | EDO | E | 2127 | - | X | X | - |
| 2 | EDO | F | 2006 | - | X | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | EDO | F | 2034 | - | - | X | - |
| 2 | EDO | F | 2038 | - | - | X | - |
| 2 | EDO | F | 2043 | - | X | X | - |
| 2 | EDO | F | 2086 | - | X | X | - |
| 2 | EDO | F | 2094 | - | X | - | - |
| 2 | EDO | F | 2097 | - | - | X | - |
| 2 | EDO | G | 2009 | - | - | X | - |
| 2 | EDO | G | 2050 | - | - | X | - |
| 2 | EDO | G | 2056 | - | - | X | - |
| 2 | EDO | G | 2057 | - | - | X | - |
| 2 | EDO | G | 2093 | - | - | X | - |
| 2 | EDO | G | 2101 | - | X | - | - |
| 2 | EDO | H | 2010 | - | - | X | - |
| 2 | EDO | H | 2044 | - | - | X | - |
| 2 | EDO | H | 2058 | - | X | X | - |
| 2 | EDO | H | 2059 | - | X | - | - |
| 2 | EDO | H | 2060 | - | - | X | - |
| 2 | EDO | H | 2111 | - | X | - | - |
| 2 | EDO | H | 2113 | - | - | X | - |
| 2 | EDO | I | 2007 | - | X | X | - |
| 2 | EDO | I | 2046 | - | - | X | - |
| 2 | EDO | I | 2051 | - | - | X | - |
| 2 | EDO | I | 2099 | - | X | - | - |
| 2 | EDO | I | 2103 | - | X | X | - |
| 2 | EDO | I | 2107 | - | - | X | - |
| 2 | EDO | I | 2115 | - | - | X | - |
| 2 | EDO | I | 2121 | - | - | X | - |
| 2 | EDO | J | 2008 | - | - | X | - |
| 2 | EDO | J | 2049 | - | - | X | - |
| 2 | EDO | J | 2068 | - | - | X | - |
| 2 | EDO | J | 2104 | - | X | X | - |
| 2 | EDO | J | 2105 | - | - | X | - |
| 2 | EDO | J | 2109 | - | - | X | - |
| 2 | EDO | J | 2123 | - | X | X | - |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21431 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 Probable peroxiredoxin.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|---------|-------|
| 1 | A | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | B | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | C | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | D | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | E | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | F | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | G | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | H | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | I | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |
| 1 | J | 244 | Total 1973 | C 1268 | N 347 | O 352 | S 2 | Se 4 | 0 | 0 | 0 |

There are 50 discrepancies between the modelled and reference sequences:

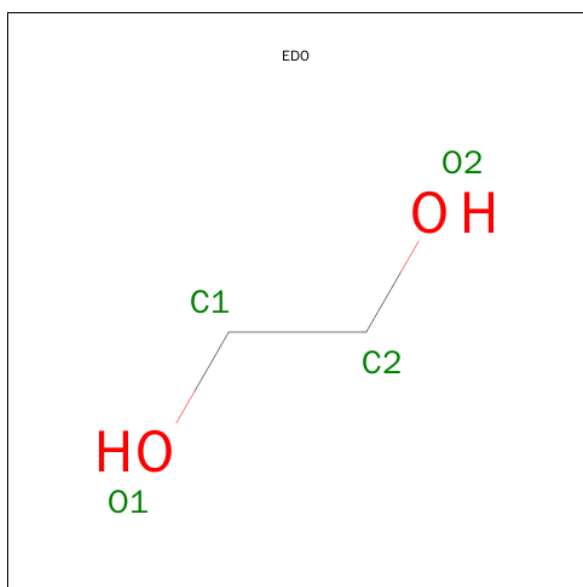
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| A | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| A | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| A | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| A | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| B | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| B | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| B | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| B | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| B | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| C | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| C | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| C | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| C | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| C | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| D | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| D | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| D | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| D | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| D | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| E | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| E | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| E | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| E | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| E | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| F | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| F | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| F | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| F | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| F | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| G | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| G | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| G | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| G | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| G | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| H | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| H | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| H | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| H | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| H | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| I | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| I | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| I | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| I | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| I | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |
| J | 15 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| J | 140 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| J | 145 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| J | 200 | MSE | MET | MODIFIED RESIDUE | UNP Q9Y9L0 |
| J | 207 | SER | CYS | ENGINEERED | UNP Q9Y9L0 |

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | D | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | E | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | F | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | I | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | J | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | G | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | H | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 2 | J | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | B | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | H | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | C | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 2 | D | 1 | Total 4 | C 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2 | E | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | I | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | A | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | J | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | A | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | B | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | C | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | E | 1 | Total C O 4 2 2 | 0 | 0 |
| 2 | C | 1 | Total C O 4 2 2 | 0 | 0 |

- Molecule 3 is water.

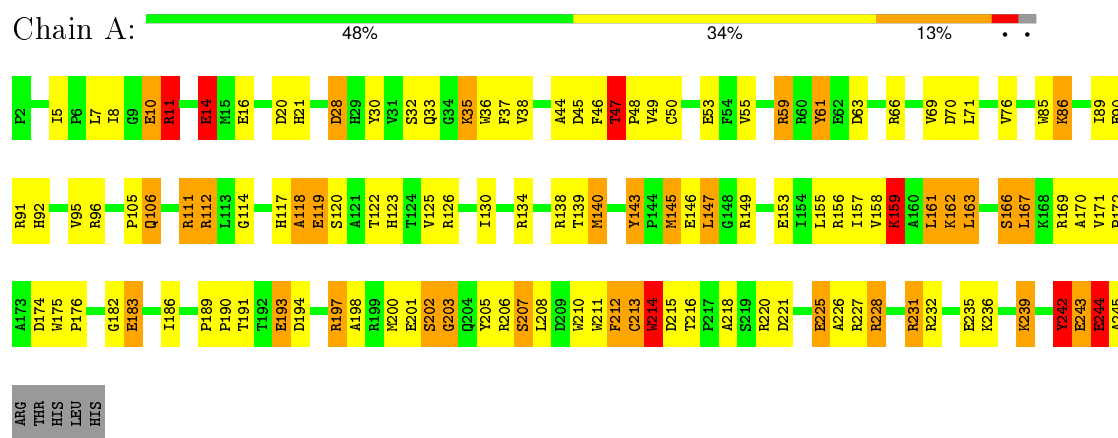
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3 | A | 140 | Total O 140 140 | 0 | 0 |
| 3 | B | 120 | Total O 120 120 | 0 | 0 |
| 3 | C | 136 | Total O 136 136 | 0 | 0 |
| 3 | D | 132 | Total O 132 132 | 0 | 0 |
| 3 | E | 133 | Total O 133 133 | 0 | 0 |
| 3 | F | 115 | Total O 115 115 | 0 | 0 |
| 3 | G | 98 | Total O 98 98 | 0 | 0 |
| 3 | H | 94 | Total O 94 94 | 0 | 0 |
| 3 | I | 106 | Total O 106 106 | 0 | 0 |
| 3 | J | 115 | Total O 115 115 | 0 | 0 |

3 Residue-property plots

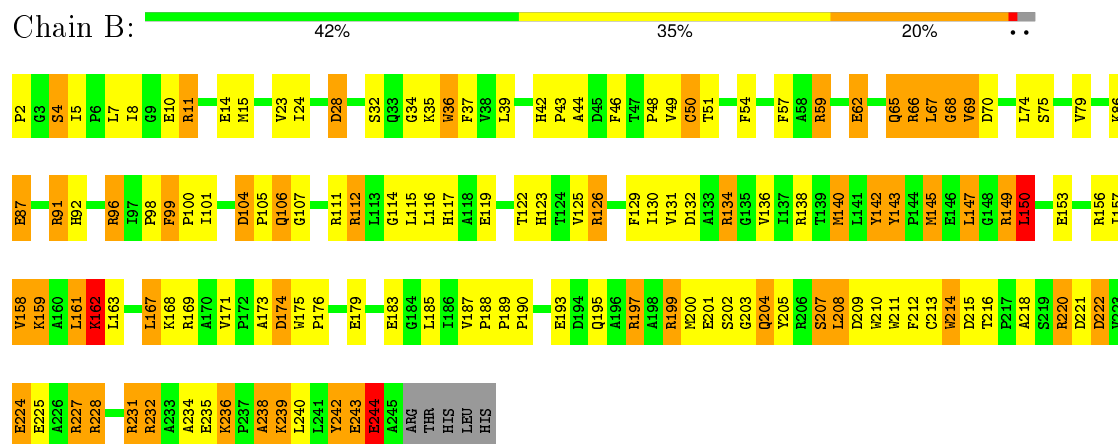
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

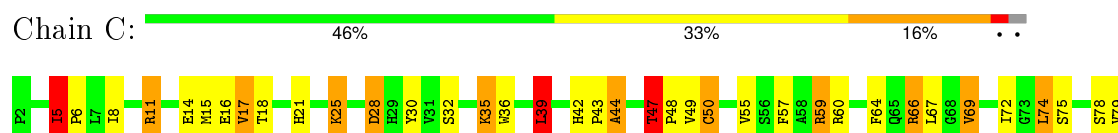
- Molecule 1: Probable peroxiredoxin

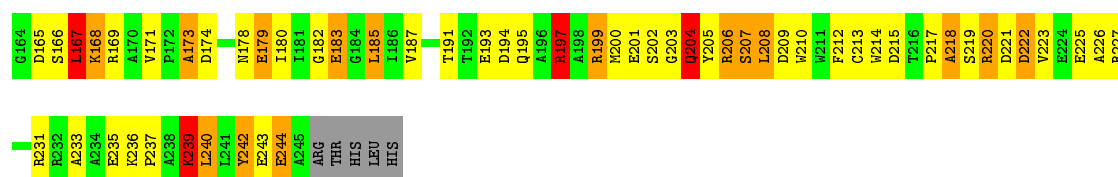


- Molecule 1: Probable peroxiredoxin



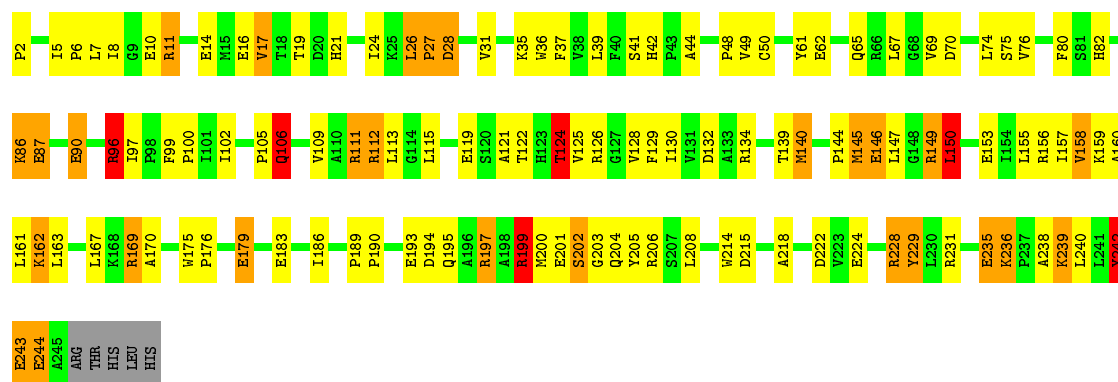
- Molecule 1: Probable peroxiredoxin





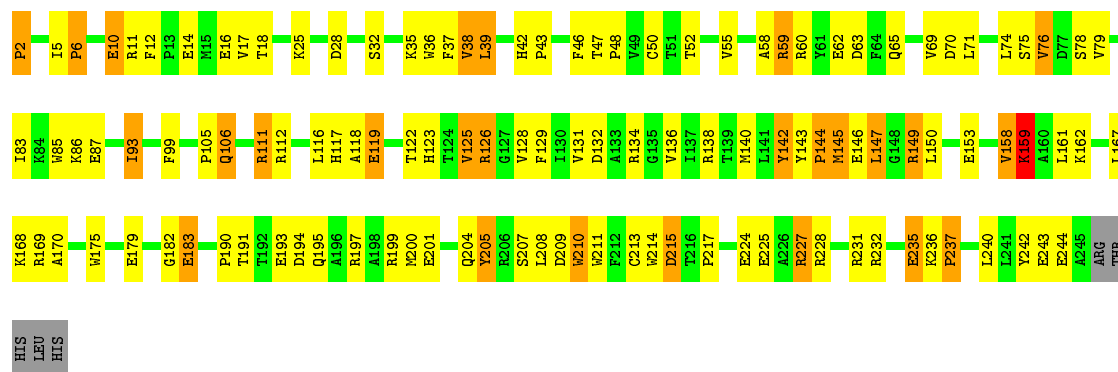
- Molecule 1: Probable peroxiredoxin

Chain G: 49% 35% 11% . .



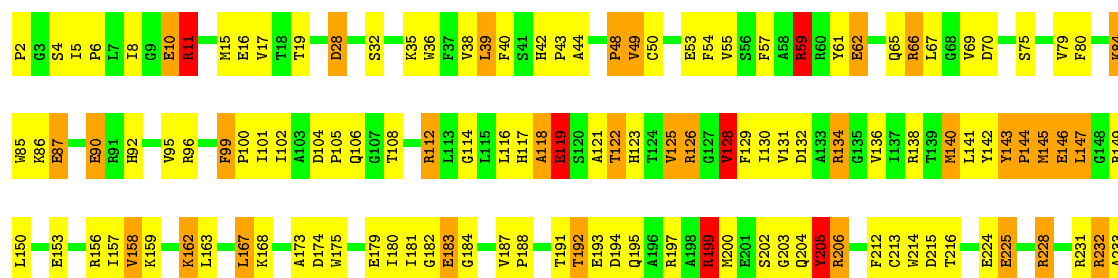
- Molecule 1: Probable peroxiredoxin

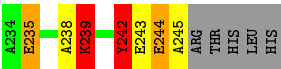
Chain H: 50% 37% 10% .



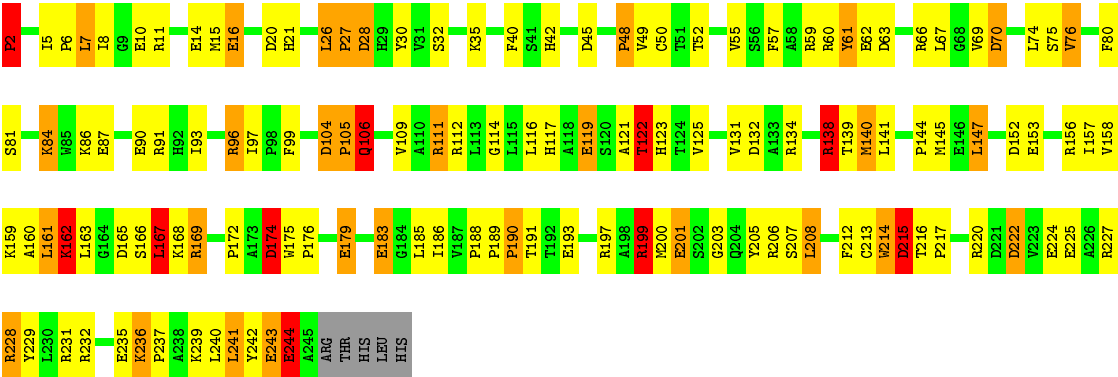
- Molecule 1: Probable peroxiredoxin

Chain I: 44% 37% 14% . .





● Molecule 1: Probable peroxiredoxin



4 Data and refinement statistics

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

| Property | Value | Source |
|--|--|-----------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 75.63Å 101.79Å 102.89Å 105.37° 105.28° 93.32° | Depositor |
| Resolution (Å) | 29.89 – 2.00 | Depositor |
| % Data completeness (in resolution range) | 89.9 (29.89-2.00) | Depositor |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.164 , 0.171 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 21431 | wwPDB-VP |
| Average B, all atoms (Å ²) | 21.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 2.20 | 78/2024 (3.9%) | 1.70 | 37/2745 (1.3%) |
| 1 | B | 2.16 | 79/2024 (3.9%) | 1.91 | 55/2745 (2.0%) |
| 1 | C | 2.16 | 79/2024 (3.9%) | 1.76 | 55/2745 (2.0%) |
| 1 | D | 2.17 | 68/2024 (3.4%) | 1.68 | 39/2745 (1.4%) |
| 1 | E | 2.25 | 96/2024 (4.7%) | 1.91 | 51/2745 (1.9%) |
| 1 | F | 2.14 | 74/2024 (3.7%) | 1.78 | 50/2745 (1.8%) |
| 1 | G | 2.12 | 65/2024 (3.2%) | 1.74 | 36/2745 (1.3%) |
| 1 | H | 2.15 | 74/2024 (3.7%) | 1.62 | 28/2745 (1.0%) |
| 1 | I | 2.12 | 74/2024 (3.7%) | 1.75 | 43/2745 (1.6%) |
| 1 | J | 2.21 | 63/2024 (3.1%) | 2.32 | 78/2745 (2.8%) |
| All | All | 2.17 | 750/20240 (3.7%) | 1.83 | 472/27450 (1.7%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 1 | B | 0 | 1 |
| 1 | D | 0 | 2 |
| 1 | E | 0 | 1 |
| 1 | G | 0 | 3 |
| 1 | H | 0 | 1 |
| 1 | I | 0 | 2 |
| 1 | J | 0 | 4 |
| All | All | 0 | 16 |

All (750) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 225 | GLU | CG-CD | 15.52 | 1.75 | 1.51 |
| 1 | H | 62 | GLU | CD-OE2 | 15.03 | 1.42 | 1.25 |
| 1 | B | 162 | LYS | CE-NZ | 14.24 | 1.84 | 1.49 |
| 1 | J | 214 | TRP | CG-CD1 | 14.23 | 1.56 | 1.36 |
| 1 | D | 68 | GLY | N-CA | 13.91 | 1.67 | 1.46 |
| 1 | G | 26 | LEU | C-N | 12.91 | 1.58 | 1.34 |
| 1 | E | 224 | GLU | CG-CD | 12.75 | 1.71 | 1.51 |
| 1 | J | 224 | GLU | CD-OE1 | 12.59 | 1.39 | 1.25 |
| 1 | D | 243 | GLU | CG-CD | 12.54 | 1.70 | 1.51 |
| 1 | F | 225 | GLU | CG-CD | 12.52 | 1.70 | 1.51 |
| 1 | I | 145 | MSE | CB-CG | 12.37 | 1.89 | 1.52 |
| 1 | E | 119 | GLU | CD-OE2 | 12.37 | 1.39 | 1.25 |
| 1 | A | 242 | TYR | CE2-CZ | 12.12 | 1.54 | 1.38 |
| 1 | B | 243 | GLU | CG-CD | 11.98 | 1.70 | 1.51 |
| 1 | A | 145 | MSE | CB-CG | 11.98 | 1.88 | 1.52 |
| 1 | A | 183 | GLU | CD-OE2 | 11.76 | 1.38 | 1.25 |
| 1 | F | 90 | GLU | CG-CD | 11.74 | 1.69 | 1.51 |
| 1 | J | 16 | GLU | CG-CD | 11.70 | 1.69 | 1.51 |
| 1 | B | 104 | ASP | CB-CG | -11.66 | 1.27 | 1.51 |
| 1 | J | 243 | GLU | CG-CD | 11.59 | 1.69 | 1.51 |
| 1 | E | 121 | ALA | CA-CB | 11.35 | 1.76 | 1.52 |
| 1 | E | 243 | GLU | CG-CD | 11.35 | 1.69 | 1.51 |
| 1 | F | 90 | GLU | CD-OE2 | 11.33 | 1.38 | 1.25 |
| 1 | I | 87 | GLU | CB-CG | -11.27 | 1.30 | 1.52 |
| 1 | D | 225 | GLU | CG-CD | 11.12 | 1.68 | 1.51 |
| 1 | J | 27 | PRO | CA-C | 10.72 | 1.74 | 1.52 |
| 1 | G | 242 | TYR | CD2-CE2 | 10.67 | 1.55 | 1.39 |
| 1 | B | 153 | GLU | CG-CD | 10.64 | 1.68 | 1.51 |
| 1 | J | 215 | ASP | CB-CG | -10.56 | 1.29 | 1.51 |
| 1 | G | 62 | GLU | CD-OE1 | 10.54 | 1.37 | 1.25 |
| 1 | D | 179 | GLU | CG-CD | 10.44 | 1.67 | 1.51 |
| 1 | A | 228 | ARG | CZ-NH1 | 10.35 | 1.46 | 1.33 |
| 1 | J | 244 | GLU | CG-CD | 10.34 | 1.67 | 1.51 |
| 1 | E | 242 | TYR | CD1-CE1 | 10.30 | 1.54 | 1.39 |
| 1 | I | 235 | GLU | CG-CD | 10.25 | 1.67 | 1.51 |
| 1 | D | 183 | GLU | CD-OE2 | 10.21 | 1.36 | 1.25 |
| 1 | E | 214 | TRP | CG-CD1 | 10.21 | 1.51 | 1.36 |
| 1 | D | 207 | SER | CB-OG | -10.13 | 1.29 | 1.42 |
| 1 | D | 136 | VAL | CB-CG2 | 10.10 | 1.74 | 1.52 |
| 1 | C | 214 | TRP | CG-CD1 | 10.08 | 1.50 | 1.36 |
| 1 | C | 224 | GLU | CG-CD | 10.06 | 1.67 | 1.51 |
| 1 | H | 145 | MSE | CB-CG | 10.05 | 1.82 | 1.52 |
| 1 | B | 79 | VAL | CB-CG2 | 10.00 | 1.73 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | H | 158 | VAL | CB-CG1 | 9.73 | 1.73 | 1.52 |
| 1 | J | 49 | VAL | CB-CG2 | 9.71 | 1.73 | 1.52 |
| 1 | E | 145 | MSE | CB-CG | 9.69 | 1.81 | 1.52 |
| 1 | F | 225 | GLU | CB-CG | 9.67 | 1.70 | 1.52 |
| 1 | C | 205 | TYR | CD2-CE2 | 9.63 | 1.53 | 1.39 |
| 1 | E | 243 | GLU | CD-OE2 | 9.59 | 1.36 | 1.25 |
| 1 | I | 225 | GLU | CG-CD | 9.57 | 1.66 | 1.51 |
| 1 | E | 224 | GLU | CD-OE1 | 9.54 | 1.36 | 1.25 |
| 1 | C | 242 | TYR | CG-CD1 | 9.53 | 1.51 | 1.39 |
| 1 | C | 224 | GLU | CD-OE1 | 9.51 | 1.36 | 1.25 |
| 1 | H | 193 | GLU | CB-CG | -9.44 | 1.34 | 1.52 |
| 1 | A | 153 | GLU | CB-CG | 9.44 | 1.70 | 1.52 |
| 1 | A | 119 | GLU | CD-OE2 | 9.39 | 1.35 | 1.25 |
| 1 | F | 193 | GLU | CB-CG | -9.39 | 1.34 | 1.52 |
| 1 | G | 235 | GLU | CG-CD | 9.38 | 1.66 | 1.51 |
| 1 | I | 183 | GLU | CD-OE2 | 9.37 | 1.35 | 1.25 |
| 1 | C | 219 | SER | CB-OG | -9.37 | 1.30 | 1.42 |
| 1 | E | 62 | GLU | CG-CD | 9.25 | 1.65 | 1.51 |
| 1 | A | 225 | GLU | CB-CG | 9.24 | 1.69 | 1.52 |
| 1 | I | 183 | GLU | CG-CD | 9.20 | 1.65 | 1.51 |
| 1 | I | 125 | VAL | CB-CG2 | -9.16 | 1.33 | 1.52 |
| 1 | A | 162 | LYS | CD-CE | 9.12 | 1.74 | 1.51 |
| 1 | F | 225 | GLU | CD-OE2 | 9.10 | 1.35 | 1.25 |
| 1 | G | 62 | GLU | CD-OE2 | 9.04 | 1.35 | 1.25 |
| 1 | I | 242 | TYR | CE1-CZ | 9.04 | 1.50 | 1.38 |
| 1 | G | 153 | GLU | CG-CD | 8.98 | 1.65 | 1.51 |
| 1 | C | 242 | TYR | CE1-CZ | 8.98 | 1.50 | 1.38 |
| 1 | J | 62 | GLU | CD-OE1 | 8.96 | 1.35 | 1.25 |
| 1 | H | 214 | TRP | CE3-CZ3 | -8.83 | 1.23 | 1.38 |
| 1 | J | 224 | GLU | CG-CD | 8.78 | 1.65 | 1.51 |
| 1 | I | 243 | GLU | CG-CD | 8.71 | 1.65 | 1.51 |
| 1 | B | 69 | VAL | CB-CG2 | 8.70 | 1.71 | 1.52 |
| 1 | E | 242 | TYR | CG-CD1 | 8.67 | 1.50 | 1.39 |
| 1 | F | 44 | ALA | CA-CB | 8.65 | 1.70 | 1.52 |
| 1 | H | 214 | TRP | CE2-CZ2 | -8.65 | 1.25 | 1.39 |
| 1 | J | 104 | ASP | CA-CB | 8.61 | 1.72 | 1.53 |
| 1 | C | 145 | MSE | CB-CG | 8.57 | 1.78 | 1.52 |
| 1 | F | 179 | GLU | CD-OE1 | 8.54 | 1.35 | 1.25 |
| 1 | B | 242 | TYR | CD1-CE1 | 8.53 | 1.52 | 1.39 |
| 1 | C | 79 | VAL | CB-CG2 | 8.53 | 1.70 | 1.52 |
| 1 | H | 175 | TRP | CB-CG | 8.53 | 1.65 | 1.50 |
| 1 | A | 214 | TRP | CG-CD1 | 8.49 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | G | 162 | LYS | CE-NZ | 8.44 | 1.70 | 1.49 |
| 1 | A | 182 | GLY | C-O | 8.43 | 1.37 | 1.23 |
| 1 | E | 76 | VAL | CB-CG1 | 8.43 | 1.70 | 1.52 |
| 1 | D | 145 | MSE | CB-CG | 8.42 | 1.77 | 1.52 |
| 1 | A | 183 | GLU | CG-CD | 8.41 | 1.64 | 1.51 |
| 1 | E | 171 | VAL | CB-CG2 | 8.40 | 1.70 | 1.52 |
| 1 | F | 87 | GLU | CG-CD | 8.38 | 1.64 | 1.51 |
| 1 | E | 225 | GLU | CD-OE1 | 8.38 | 1.34 | 1.25 |
| 1 | D | 193 | GLU | CB-CG | -8.37 | 1.36 | 1.52 |
| 1 | D | 225 | GLU | CD-OE1 | 8.36 | 1.34 | 1.25 |
| 1 | D | 243 | GLU | CD-OE2 | 8.36 | 1.34 | 1.25 |
| 1 | E | 146 | GLU | CG-CD | 8.36 | 1.64 | 1.51 |
| 1 | D | 201 | GLU | CD-OE1 | 8.35 | 1.34 | 1.25 |
| 1 | H | 168 | LYS | CD-CE | 8.33 | 1.72 | 1.51 |
| 1 | D | 16 | GLU | CD-OE1 | 8.31 | 1.34 | 1.25 |
| 1 | A | 193 | GLU | CB-CG | -8.30 | 1.36 | 1.52 |
| 1 | E | 90 | GLU | CG-CD | 8.30 | 1.64 | 1.51 |
| 1 | H | 179 | GLU | CD-OE2 | 8.30 | 1.34 | 1.25 |
| 1 | A | 76 | VAL | CB-CG1 | 8.27 | 1.70 | 1.52 |
| 1 | I | 224 | GLU | CG-CD | 8.24 | 1.64 | 1.51 |
| 1 | D | 225 | GLU | CD-OE2 | 8.21 | 1.34 | 1.25 |
| 1 | D | 37 | PHE | CE1-CZ | 8.20 | 1.52 | 1.37 |
| 1 | E | 70 | ASP | CG-OD1 | 8.18 | 1.44 | 1.25 |
| 1 | E | 236 | LYS | CD-CE | 8.18 | 1.71 | 1.51 |
| 1 | D | 243 | GLU | CD-OE1 | 8.17 | 1.34 | 1.25 |
| 1 | G | 242 | TYR | CE2-CZ | 8.17 | 1.49 | 1.38 |
| 1 | B | 4 | SER | CB-OG | 8.16 | 1.52 | 1.42 |
| 1 | G | 242 | TYR | CE1-CZ | 8.16 | 1.49 | 1.38 |
| 1 | C | 211 | TRP | CB-CG | 8.15 | 1.65 | 1.50 |
| 1 | G | 235 | GLU | CD-OE2 | 8.13 | 1.34 | 1.25 |
| 1 | F | 168 | LYS | CE-NZ | 8.12 | 1.69 | 1.49 |
| 1 | C | 90 | GLU | CB-CG | -8.11 | 1.36 | 1.52 |
| 1 | A | 85 | TRP | CZ3-CH2 | 8.05 | 1.52 | 1.40 |
| 1 | B | 225 | GLU | CD-OE1 | 8.04 | 1.34 | 1.25 |
| 1 | E | 55 | VAL | CB-CG1 | 8.04 | 1.69 | 1.52 |
| 1 | H | 214 | TRP | CB-CG | -8.03 | 1.35 | 1.50 |
| 1 | B | 162 | LYS | CD-CE | 8.02 | 1.71 | 1.51 |
| 1 | E | 35 | LYS | CD-CE | 8.01 | 1.71 | 1.51 |
| 1 | D | 96 | ARG | CZ-NH1 | 8.01 | 1.43 | 1.33 |
| 1 | C | 244 | GLU | CG-CD | 8.00 | 1.64 | 1.51 |
| 1 | I | 153 | GLU | CB-CG | 7.98 | 1.67 | 1.52 |
| 1 | G | 236 | LYS | CE-NZ | 7.95 | 1.69 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | J | 121 | ALA | CA-CB | 7.94 | 1.69 | 1.52 |
| 1 | A | 90 | GLU | CB-CG | -7.93 | 1.37 | 1.52 |
| 1 | J | 16 | GLU | CD-OE1 | 7.88 | 1.34 | 1.25 |
| 1 | C | 235 | GLU | CD-OE1 | 7.87 | 1.34 | 1.25 |
| 1 | C | 47 | THR | CB-CG2 | -7.82 | 1.26 | 1.52 |
| 1 | J | 176 | PRO | CG-CD | -7.80 | 1.25 | 1.50 |
| 1 | H | 62 | GLU | CB-CG | -7.77 | 1.37 | 1.52 |
| 1 | B | 214 | TRP | CE3-CZ3 | -7.74 | 1.25 | 1.38 |
| 1 | F | 183 | GLU | CD-OE2 | 7.74 | 1.34 | 1.25 |
| 1 | J | 138 | ARG | CD-NE | -7.74 | 1.33 | 1.46 |
| 1 | J | 215 | ASP | CA-CB | 7.73 | 1.71 | 1.53 |
| 1 | J | 140 | MSE | SE-CE | -7.72 | 1.50 | 1.95 |
| 1 | D | 222 | ASP | CG-OD2 | 7.69 | 1.43 | 1.25 |
| 1 | G | 179 | GLU | CD-OE2 | 7.69 | 1.34 | 1.25 |
| 1 | I | 87 | GLU | CG-CD | 7.67 | 1.63 | 1.51 |
| 1 | G | 229 | TYR | CD2-CE2 | 7.65 | 1.50 | 1.39 |
| 1 | G | 193 | GLU | CD-OE2 | 7.64 | 1.34 | 1.25 |
| 1 | I | 235 | GLU | CD-OE1 | 7.62 | 1.34 | 1.25 |
| 1 | G | 61 | TYR | CD2-CE2 | 7.61 | 1.50 | 1.39 |
| 1 | G | 44 | ALA | CA-CB | 7.61 | 1.68 | 1.52 |
| 1 | F | 243 | GLU | CG-CD | 7.60 | 1.63 | 1.51 |
| 1 | H | 179 | GLU | CD-OE1 | 7.60 | 1.34 | 1.25 |
| 1 | B | 199 | ARG | CB-CG | -7.59 | 1.32 | 1.52 |
| 1 | J | 220 | ARG | CG-CD | 7.58 | 1.70 | 1.51 |
| 1 | C | 16 | GLU | CD-OE1 | 7.57 | 1.33 | 1.25 |
| 1 | F | 119 | GLU | CD-OE2 | 7.56 | 1.33 | 1.25 |
| 1 | G | 76 | VAL | CB-CG1 | 7.53 | 1.68 | 1.52 |
| 1 | F | 57 | PHE | CE2-CZ | 7.51 | 1.51 | 1.37 |
| 1 | G | 197 | ARG | CG-CD | 7.51 | 1.70 | 1.51 |
| 1 | F | 207 | SER | CB-OG | -7.49 | 1.32 | 1.42 |
| 1 | A | 214 | TRP | CE3-CZ3 | -7.46 | 1.25 | 1.38 |
| 1 | A | 69 | VAL | CB-CG2 | 7.46 | 1.68 | 1.52 |
| 1 | C | 243 | GLU | CG-CD | 7.44 | 1.63 | 1.51 |
| 1 | B | 158 | VAL | CB-CG2 | -7.43 | 1.37 | 1.52 |
| 1 | J | 30 | TYR | CE2-CZ | 7.43 | 1.48 | 1.38 |
| 1 | B | 131 | VAL | CB-CG2 | 7.43 | 1.68 | 1.52 |
| 1 | B | 87 | GLU | CB-CG | -7.41 | 1.38 | 1.52 |
| 1 | F | 166 | SER | CB-OG | -7.41 | 1.32 | 1.42 |
| 1 | I | 61 | TYR | CD2-CE2 | 7.41 | 1.50 | 1.39 |
| 1 | H | 136 | VAL | CB-CG2 | 7.41 | 1.68 | 1.52 |
| 1 | F | 242 | TYR | CG-CD1 | 7.40 | 1.48 | 1.39 |
| 1 | I | 197 | ARG | CZ-NH2 | 7.40 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | E | 25 | LYS | CE-NZ | 7.39 | 1.67 | 1.49 |
| 1 | B | 134 | ARG | CG-CD | 7.39 | 1.70 | 1.51 |
| 1 | I | 244 | GLU | CB-CG | 7.37 | 1.66 | 1.52 |
| 1 | B | 68 | GLY | N-CA | 7.35 | 1.57 | 1.46 |
| 1 | H | 197 | ARG | CG-CD | 7.32 | 1.70 | 1.51 |
| 1 | C | 69 | VAL | CA-CB | 7.30 | 1.70 | 1.54 |
| 1 | A | 30 | TYR | CE1-CZ | -7.29 | 1.29 | 1.38 |
| 1 | J | 119 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 1 | F | 202 | SER | CB-OG | 7.28 | 1.51 | 1.42 |
| 1 | B | 179 | GLU | CD-OE1 | 7.26 | 1.33 | 1.25 |
| 1 | B | 207 | SER | CB-OG | -7.26 | 1.32 | 1.42 |
| 1 | G | 179 | GLU | CB-CG | 7.25 | 1.66 | 1.52 |
| 1 | J | 231 | ARG | CG-CD | 7.24 | 1.70 | 1.51 |
| 1 | A | 242 | TYR | CD1-CE1 | 7.22 | 1.50 | 1.39 |
| 1 | A | 242 | TYR | CG-CD1 | 7.21 | 1.48 | 1.39 |
| 1 | D | 138 | ARG | CB-CG | 7.20 | 1.72 | 1.52 |
| 1 | E | 104 | ASP | CB-CG | -7.19 | 1.36 | 1.51 |
| 1 | H | 62 | GLU | CD-OE1 | 7.19 | 1.33 | 1.25 |
| 1 | F | 112 | ARG | CG-CD | 7.18 | 1.70 | 1.51 |
| 1 | C | 242 | TYR | CD2-CE2 | 7.18 | 1.50 | 1.39 |
| 1 | J | 26 | LEU | C-N | 7.18 | 1.47 | 1.34 |
| 1 | I | 146 | GLU | CB-CG | 7.17 | 1.65 | 1.52 |
| 1 | C | 99 | PHE | CD2-CE2 | 7.14 | 1.53 | 1.39 |
| 1 | J | 214 | TRP | CE2-CZ2 | -7.12 | 1.27 | 1.39 |
| 1 | G | 242 | TYR | CZ-OH | 7.12 | 1.50 | 1.37 |
| 1 | D | 14 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 1 | G | 128 | VAL | CB-CG2 | -7.10 | 1.38 | 1.52 |
| 1 | C | 140 | MSE | SE-CE | -7.10 | 1.53 | 1.95 |
| 1 | F | 85 | TRP | CZ3-CH2 | 7.09 | 1.51 | 1.40 |
| 1 | E | 30 | TYR | CE2-CZ | 7.07 | 1.47 | 1.38 |
| 1 | A | 146 | GLU | CD-OE2 | 7.07 | 1.33 | 1.25 |
| 1 | A | 166 | SER | CB-OG | -7.07 | 1.33 | 1.42 |
| 1 | E | 225 | GLU | CD-OE2 | 7.07 | 1.33 | 1.25 |
| 1 | I | 16 | GLU | CD-OE2 | 7.06 | 1.33 | 1.25 |
| 1 | A | 242 | TYR | CD2-CE2 | 7.06 | 1.50 | 1.39 |
| 1 | H | 235 | GLU | CD-OE1 | 7.06 | 1.33 | 1.25 |
| 1 | B | 214 | TRP | CB-CG | -7.05 | 1.37 | 1.50 |
| 1 | D | 112 | ARG | CG-CD | 7.04 | 1.69 | 1.51 |
| 1 | A | 225 | GLU | CD-OE2 | 7.04 | 1.33 | 1.25 |
| 1 | G | 86 | LYS | CD-CE | -7.03 | 1.33 | 1.51 |
| 1 | H | 224 | GLU | CD-OE1 | 7.02 | 1.33 | 1.25 |
| 1 | G | 243 | GLU | CD-OE1 | 7.01 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 144 | PRO | CG-CD | 6.99 | 1.73 | 1.50 |
| 1 | H | 242 | TYR | CE1-CZ | 6.97 | 1.47 | 1.38 |
| 1 | F | 204 | GLN | CB-CG | -6.96 | 1.33 | 1.52 |
| 1 | F | 183 | GLU | CG-CD | 6.96 | 1.62 | 1.51 |
| 1 | D | 90 | GLU | CG-CD | 6.95 | 1.62 | 1.51 |
| 1 | E | 239 | LYS | N-CA | 6.95 | 1.60 | 1.46 |
| 1 | G | 228 | ARG | CG-CD | 6.95 | 1.69 | 1.51 |
| 1 | B | 140 | MSE | CG-SE | 6.94 | 2.19 | 1.95 |
| 1 | I | 159 | LYS | CG-CD | -6.94 | 1.28 | 1.52 |
| 1 | H | 76 | VAL | CB-CG1 | 6.91 | 1.67 | 1.52 |
| 1 | B | 119 | GLU | CB-CG | -6.91 | 1.39 | 1.52 |
| 1 | I | 140 | MSE | CG-SE | 6.89 | 2.18 | 1.95 |
| 1 | D | 212 | PHE | CB-CG | 6.88 | 1.63 | 1.51 |
| 1 | A | 95 | VAL | CB-CG1 | 6.88 | 1.67 | 1.52 |
| 1 | D | 233 | ALA | CA-CB | 6.87 | 1.66 | 1.52 |
| 1 | H | 214 | TRP | CG-CD2 | -6.84 | 1.32 | 1.43 |
| 1 | G | 31 | VAL | CB-CG1 | 6.82 | 1.67 | 1.52 |
| 1 | J | 61 | TYR | CG-CD1 | -6.82 | 1.30 | 1.39 |
| 1 | E | 37 | PHE | CD1-CE1 | 6.82 | 1.52 | 1.39 |
| 1 | E | 61 | TYR | CD1-CE1 | 6.82 | 1.49 | 1.39 |
| 1 | E | 66 | ARG | CG-CD | 6.81 | 1.69 | 1.51 |
| 1 | H | 224 | GLU | CG-CD | 6.80 | 1.62 | 1.51 |
| 1 | B | 220 | ARG | CG-CD | 6.80 | 1.69 | 1.51 |
| 1 | E | 38 | VAL | CB-CG1 | 6.79 | 1.67 | 1.52 |
| 1 | J | 201 | GLU | CG-CD | 6.79 | 1.62 | 1.51 |
| 1 | B | 143 | TYR | CD1-CE1 | 6.78 | 1.49 | 1.39 |
| 1 | F | 25 | LYS | CE-NZ | 6.78 | 1.66 | 1.49 |
| 1 | G | 244 | GLU | CG-CD | 6.77 | 1.62 | 1.51 |
| 1 | I | 202 | SER | CB-OG | 6.77 | 1.51 | 1.42 |
| 1 | E | 214 | TRP | CE3-CZ3 | -6.77 | 1.26 | 1.38 |
| 1 | I | 173 | ALA | CA-CB | 6.76 | 1.66 | 1.52 |
| 1 | B | 145 | MSE | CB-CG | 6.76 | 1.72 | 1.52 |
| 1 | A | 225 | GLU | CD-OE1 | 6.75 | 1.33 | 1.25 |
| 1 | F | 129 | PHE | CE2-CZ | 6.74 | 1.50 | 1.37 |
| 1 | C | 57 | PHE | CE2-CZ | 6.73 | 1.50 | 1.37 |
| 1 | H | 211 | TRP | CB-CG | 6.70 | 1.62 | 1.50 |
| 1 | I | 239 | LYS | CD-CE | 6.70 | 1.68 | 1.51 |
| 1 | J | 40 | PHE | CE1-CZ | 6.68 | 1.50 | 1.37 |
| 1 | B | 37 | PHE | CE2-CZ | 6.68 | 1.50 | 1.37 |
| 1 | E | 12 | PHE | CB-CG | -6.67 | 1.40 | 1.51 |
| 1 | F | 225 | GLU | CD-OE1 | 6.67 | 1.32 | 1.25 |
| 1 | G | 179 | GLU | CG-CD | 6.67 | 1.61 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | J | 61 | TYR | CD2-CE2 | 6.66 | 1.49 | 1.39 |
| 1 | G | 140 | MSE | SE-CE | -6.66 | 1.56 | 1.95 |
| 1 | H | 214 | TRP | CG-CD1 | 6.65 | 1.46 | 1.36 |
| 1 | I | 95 | VAL | CB-CG2 | 6.64 | 1.66 | 1.52 |
| 1 | D | 96 | ARG | CZ-NH2 | 6.63 | 1.41 | 1.33 |
| 1 | I | 162 | LYS | CD-CE | 6.63 | 1.67 | 1.51 |
| 1 | I | 32 | SER | CB-OG | -6.60 | 1.33 | 1.42 |
| 1 | G | 201 | GLU | CD-OE1 | 6.59 | 1.32 | 1.25 |
| 1 | F | 223 | VAL | CA-CB | 6.59 | 1.68 | 1.54 |
| 1 | A | 243 | GLU | CD-OE2 | 6.59 | 1.32 | 1.25 |
| 1 | C | 134 | ARG | NE-CZ | 6.59 | 1.41 | 1.33 |
| 1 | I | 231 | ARG | CG-CD | 6.59 | 1.68 | 1.51 |
| 1 | C | 243 | GLU | CD-OE1 | 6.57 | 1.32 | 1.25 |
| 1 | D | 239 | LYS | CE-NZ | 6.57 | 1.65 | 1.49 |
| 1 | J | 62 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 1 | I | 53 | GLU | CD-OE2 | -6.56 | 1.18 | 1.25 |
| 1 | E | 14 | GLU | CD-OE1 | 6.56 | 1.32 | 1.25 |
| 1 | D | 235 | GLU | CB-CG | -6.54 | 1.39 | 1.52 |
| 1 | J | 239 | LYS | CE-NZ | 6.53 | 1.65 | 1.49 |
| 1 | C | 157 | ILE | CA-CB | 6.53 | 1.69 | 1.54 |
| 1 | G | 90 | GLU | CG-CD | 6.52 | 1.61 | 1.51 |
| 1 | H | 228 | ARG | CG-CD | 6.52 | 1.68 | 1.51 |
| 1 | I | 119 | GLU | CG-CD | 6.52 | 1.61 | 1.51 |
| 1 | J | 14 | GLU | CD-OE2 | 6.51 | 1.32 | 1.25 |
| 1 | F | 57 | PHE | CB-CG | -6.51 | 1.40 | 1.51 |
| 1 | F | 14 | GLU | CB-CG | -6.49 | 1.39 | 1.52 |
| 1 | I | 70 | ASP | CG-OD1 | 6.49 | 1.40 | 1.25 |
| 1 | H | 16 | GLU | CG-CD | 6.48 | 1.61 | 1.51 |
| 1 | J | 80 | PHE | CE1-CZ | 6.48 | 1.49 | 1.37 |
| 1 | E | 243 | GLU | CD-OE1 | 6.46 | 1.32 | 1.25 |
| 1 | A | 211 | TRP | CE3-CZ3 | 6.46 | 1.49 | 1.38 |
| 1 | G | 37 | PHE | CE1-CZ | 6.46 | 1.49 | 1.37 |
| 1 | H | 242 | TYR | CD2-CE2 | 6.45 | 1.49 | 1.39 |
| 1 | H | 183 | GLU | CD-OE1 | 6.45 | 1.32 | 1.25 |
| 1 | C | 187 | VAL | CB-CG2 | 6.45 | 1.66 | 1.52 |
| 1 | C | 229 | TYR | CD1-CE1 | 6.42 | 1.49 | 1.39 |
| 1 | C | 99 | PHE | CE1-CZ | 6.41 | 1.49 | 1.37 |
| 1 | F | 111 | ARG | CZ-NH1 | 6.40 | 1.41 | 1.33 |
| 1 | H | 205 | TYR | CD1-CE1 | -6.40 | 1.29 | 1.39 |
| 1 | E | 111 | ARG | CZ-NH2 | 6.40 | 1.41 | 1.33 |
| 1 | F | 239 | LYS | CD-CE | 6.40 | 1.67 | 1.51 |
| 1 | A | 212 | PHE | CD1-CE1 | 6.39 | 1.52 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | D | 214 | TRP | CE3-CZ3 | 6.39 | 1.49 | 1.38 |
| 1 | A | 36 | TRP | CG-CD1 | 6.38 | 1.45 | 1.36 |
| 1 | E | 153 | GLU | CB-CG | 6.36 | 1.64 | 1.52 |
| 1 | C | 112 | ARG | CG-CD | 6.36 | 1.67 | 1.51 |
| 1 | C | 201 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | A | 243 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | E | 211 | TRP | CE3-CZ3 | 6.35 | 1.49 | 1.38 |
| 1 | F | 79 | VAL | CB-CG2 | 6.35 | 1.66 | 1.52 |
| 1 | A | 70 | ASP | CG-OD1 | 6.34 | 1.40 | 1.25 |
| 1 | D | 174 | ASP | CB-CG | 6.34 | 1.65 | 1.51 |
| 1 | F | 112 | ARG | CZ-NH2 | 6.34 | 1.41 | 1.33 |
| 1 | I | 179 | GLU | CD-OE2 | 6.33 | 1.32 | 1.25 |
| 1 | B | 36 | TRP | CE3-CZ3 | 6.32 | 1.49 | 1.38 |
| 1 | E | 179 | GLU | CG-CD | 6.32 | 1.61 | 1.51 |
| 1 | E | 140 | MSE | SE-CE | -6.31 | 1.58 | 1.95 |
| 1 | D | 227 | ARG | CG-CD | 6.31 | 1.67 | 1.51 |
| 1 | E | 60 | ARG | CG-CD | 6.31 | 1.67 | 1.51 |
| 1 | F | 179 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 1 | C | 96 | ARG | CZ-NH2 | 6.30 | 1.41 | 1.33 |
| 1 | D | 81 | SER | CB-OG | 6.30 | 1.50 | 1.42 |
| 1 | E | 232 | ARG | CB-CG | 6.30 | 1.69 | 1.52 |
| 1 | J | 242 | TYR | CD1-CE1 | 6.29 | 1.48 | 1.39 |
| 1 | C | 64 | PHE | CE2-CZ | 6.29 | 1.49 | 1.37 |
| 1 | H | 243 | GLU | CG-CD | 6.29 | 1.61 | 1.51 |
| 1 | E | 90 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | H | 58 | ALA | CA-CB | 6.28 | 1.65 | 1.52 |
| 1 | B | 158 | VAL | CB-CG1 | -6.28 | 1.39 | 1.52 |
| 1 | F | 242 | TYR | CE1-CZ | 6.28 | 1.46 | 1.38 |
| 1 | B | 14 | GLU | CB-CG | -6.28 | 1.40 | 1.52 |
| 1 | G | 119 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | C | 228 | ARG | CD-NE | 6.25 | 1.57 | 1.46 |
| 1 | C | 170 | ALA | CA-CB | 6.25 | 1.65 | 1.52 |
| 1 | J | 111 | ARG | CZ-NH2 | 6.24 | 1.41 | 1.33 |
| 1 | E | 88 | TRP | CG-CD1 | 6.24 | 1.45 | 1.36 |
| 1 | D | 78 | SER | CB-OG | 6.24 | 1.50 | 1.42 |
| 1 | C | 81 | SER | CB-OG | 6.23 | 1.50 | 1.42 |
| 1 | F | 235 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |
| 1 | A | 86 | LYS | CD-CE | 6.21 | 1.66 | 1.51 |
| 1 | H | 244 | GLU | CD-OE1 | 6.21 | 1.32 | 1.25 |
| 1 | E | 197 | ARG | CZ-NH1 | 6.19 | 1.41 | 1.33 |
| 1 | I | 131 | VAL | CB-CG1 | 6.19 | 1.65 | 1.52 |
| 1 | E | 231 | ARG | CZ-NH2 | 6.19 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | F | 193 | GLU | CD-OE1 | 6.19 | 1.32 | 1.25 |
| 1 | H | 111 | ARG | CZ-NH2 | 6.18 | 1.41 | 1.33 |
| 1 | A | 47 | THR | CB-CG2 | -6.18 | 1.31 | 1.52 |
| 1 | I | 44 | ALA | CA-CB | 6.18 | 1.65 | 1.52 |
| 1 | A | 158 | VAL | CB-CG2 | 6.17 | 1.65 | 1.52 |
| 1 | D | 10 | GLU | CB-CG | -6.17 | 1.40 | 1.52 |
| 1 | A | 220 | ARG | CZ-NH2 | 6.17 | 1.41 | 1.33 |
| 1 | B | 156 | ARG | CZ-NH1 | 6.17 | 1.41 | 1.33 |
| 1 | A | 95 | VAL | C-O | 6.15 | 1.35 | 1.23 |
| 1 | E | 61 | TYR | CE2-CZ | -6.14 | 1.30 | 1.38 |
| 1 | J | 160 | ALA | CA-CB | 6.14 | 1.65 | 1.52 |
| 1 | A | 210 | TRP | CB-CG | 6.14 | 1.61 | 1.50 |
| 1 | G | 242 | TYR | CD1-CE1 | 6.13 | 1.48 | 1.39 |
| 1 | F | 55 | VAL | CB-CG2 | 6.13 | 1.65 | 1.52 |
| 1 | E | 41 | SER | CA-CB | 6.13 | 1.62 | 1.52 |
| 1 | G | 96 | ARG | CB-CG | -6.12 | 1.36 | 1.52 |
| 1 | I | 136 | VAL | CB-CG2 | 6.12 | 1.65 | 1.52 |
| 1 | B | 224 | GLU | CD-OE2 | 6.11 | 1.32 | 1.25 |
| 1 | E | 85 | TRP | CZ3-CH2 | 6.10 | 1.49 | 1.40 |
| 1 | B | 179 | GLU | CG-CD | 6.10 | 1.61 | 1.51 |
| 1 | E | 168 | LYS | CE-NZ | 6.09 | 1.64 | 1.49 |
| 1 | A | 35 | LYS | CD-CE | 6.08 | 1.66 | 1.51 |
| 1 | C | 228 | ARG | NE-CZ | 6.08 | 1.41 | 1.33 |
| 1 | I | 54 | PHE | CD2-CE2 | 6.08 | 1.51 | 1.39 |
| 1 | J | 57 | PHE | CE2-CZ | 6.08 | 1.48 | 1.37 |
| 1 | A | 85 | TRP | CG-CD1 | 6.07 | 1.45 | 1.36 |
| 1 | I | 90 | GLU | CD-OE1 | 6.07 | 1.32 | 1.25 |
| 1 | C | 32 | SER | CA-CB | 6.06 | 1.62 | 1.52 |
| 1 | F | 242 | TYR | CE2-CZ | 6.05 | 1.46 | 1.38 |
| 1 | I | 125 | VAL | CB-CG1 | -6.05 | 1.40 | 1.52 |
| 1 | A | 69 | VAL | CB-CG1 | 6.04 | 1.65 | 1.52 |
| 1 | C | 242 | TYR | CE2-CZ | 6.04 | 1.46 | 1.38 |
| 1 | F | 193 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | B | 193 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | E | 183 | GLU | CG-CD | 6.03 | 1.60 | 1.51 |
| 1 | J | 153 | GLU | CB-CG | 6.03 | 1.63 | 1.52 |
| 1 | A | 214 | TRP | CG-CD2 | -6.03 | 1.33 | 1.43 |
| 1 | E | 169 | ARG | CZ-NH2 | 6.03 | 1.40 | 1.33 |
| 1 | E | 193 | GLU | CG-CD | 6.02 | 1.60 | 1.51 |
| 1 | A | 10 | GLU | CD-OE1 | 6.01 | 1.32 | 1.25 |
| 1 | F | 12 | PHE | CD2-CE2 | -6.01 | 1.27 | 1.39 |
| 1 | G | 244 | GLU | CB-CG | 6.00 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | H | 193 | GLU | CG-CD | 5.99 | 1.60 | 1.51 |
| 1 | A | 143 | TYR | CB-CG | -5.99 | 1.42 | 1.51 |
| 1 | D | 153 | GLU | CG-CD | 5.99 | 1.60 | 1.51 |
| 1 | E | 220 | ARG | CZ-NH1 | 5.99 | 1.40 | 1.33 |
| 1 | A | 212 | PHE | CD2-CE2 | 5.99 | 1.51 | 1.39 |
| 1 | F | 136 | VAL | CB-CG2 | 5.99 | 1.65 | 1.52 |
| 1 | I | 55 | VAL | CB-CG1 | 5.98 | 1.65 | 1.52 |
| 1 | C | 78 | SER | CB-OG | 5.97 | 1.50 | 1.42 |
| 1 | B | 202 | SER | CB-OG | 5.97 | 1.50 | 1.42 |
| 1 | E | 179 | GLU | CD-OE1 | 5.96 | 1.32 | 1.25 |
| 1 | F | 99 | PHE | CD2-CE2 | 5.96 | 1.51 | 1.39 |
| 1 | E | 69 | VAL | CB-CG2 | 5.96 | 1.65 | 1.52 |
| 1 | B | 232 | ARG | CB-CG | 5.96 | 1.68 | 1.52 |
| 1 | F | 129 | PHE | CD1-CE1 | 5.96 | 1.51 | 1.39 |
| 1 | G | 145 | MSE | CB-CG | 5.95 | 1.70 | 1.52 |
| 1 | B | 224 | GLU | CG-CD | 5.94 | 1.60 | 1.51 |
| 1 | H | 134 | ARG | CG-CD | 5.94 | 1.66 | 1.51 |
| 1 | H | 142 | TYR | CE1-CZ | 5.94 | 1.46 | 1.38 |
| 1 | F | 210 | TRP | CE3-CZ3 | -5.94 | 1.28 | 1.38 |
| 1 | H | 162 | LYS | CD-CE | 5.94 | 1.66 | 1.51 |
| 1 | F | 55 | VAL | CB-CG1 | 5.94 | 1.65 | 1.52 |
| 1 | H | 179 | GLU | CG-CD | 5.94 | 1.60 | 1.51 |
| 1 | C | 195 | GLN | CB-CG | -5.93 | 1.36 | 1.52 |
| 1 | C | 184 | GLY | C-O | 5.93 | 1.33 | 1.23 |
| 1 | D | 119 | GLU | CB-CG | -5.93 | 1.40 | 1.52 |
| 1 | B | 87 | GLU | CG-CD | 5.92 | 1.60 | 1.51 |
| 1 | F | 15 | MSE | CG-SE | 5.92 | 2.15 | 1.95 |
| 1 | F | 244 | GLU | CD-OE1 | 5.91 | 1.32 | 1.25 |
| 1 | E | 136 | VAL | CB-CG2 | 5.91 | 1.65 | 1.52 |
| 1 | D | 111 | ARG | CZ-NH2 | 5.90 | 1.40 | 1.33 |
| 1 | J | 69 | VAL | CB-CG2 | 5.89 | 1.65 | 1.52 |
| 1 | H | 210 | TRP | CG-CD1 | 5.89 | 1.45 | 1.36 |
| 1 | A | 66 | ARG | CZ-NH2 | 5.88 | 1.40 | 1.33 |
| 1 | A | 138 | ARG | CG-CD | 5.88 | 1.66 | 1.51 |
| 1 | A | 125 | VAL | CB-CG2 | -5.88 | 1.40 | 1.52 |
| 1 | F | 17 | VAL | CA-CB | 5.88 | 1.67 | 1.54 |
| 1 | B | 214 | TRP | CG-CD1 | 5.88 | 1.45 | 1.36 |
| 1 | D | 90 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | H | 46 | PHE | CE2-CZ | 5.87 | 1.48 | 1.37 |
| 1 | H | 38 | VAL | CB-CG1 | 5.87 | 1.65 | 1.52 |
| 1 | C | 214 | TRP | CG-CD2 | -5.87 | 1.33 | 1.43 |
| 1 | D | 146 | GLU | CG-CD | 5.86 | 1.60 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | F | 143 | TYR | CG-CD2 | 5.85 | 1.46 | 1.39 |
| 1 | H | 32 | SER | CA-CB | 5.85 | 1.61 | 1.52 |
| 1 | J | 144 | PRO | CG-CD | 5.85 | 1.70 | 1.50 |
| 1 | C | 16 | GLU | CG-CD | 5.84 | 1.60 | 1.51 |
| 1 | F | 129 | PHE | CE1-CZ | -5.84 | 1.26 | 1.37 |
| 1 | E | 214 | TRP | CB-CG | -5.83 | 1.39 | 1.50 |
| 1 | G | 170 | ALA | CA-CB | 5.82 | 1.64 | 1.52 |
| 1 | H | 126 | ARG | CZ-NH1 | 5.82 | 1.40 | 1.33 |
| 1 | G | 195 | GLN | CG-CD | 5.82 | 1.64 | 1.51 |
| 1 | J | 66 | ARG | CZ-NH2 | 5.82 | 1.40 | 1.33 |
| 1 | D | 204 | GLN | CB-CG | -5.81 | 1.36 | 1.52 |
| 1 | B | 224 | GLU | CD-OE1 | 5.81 | 1.32 | 1.25 |
| 1 | J | 179 | GLU | CD-OE1 | 5.81 | 1.32 | 1.25 |
| 1 | F | 2 | PRO | CA-C | -5.80 | 1.41 | 1.52 |
| 1 | G | 37 | PHE | CG-CD2 | 5.80 | 1.47 | 1.38 |
| 1 | B | 119 | GLU | CD-OE1 | 5.80 | 1.32 | 1.25 |
| 1 | C | 193 | GLU | CB-CG | -5.80 | 1.41 | 1.52 |
| 1 | A | 37 | PHE | CE2-CZ | 5.80 | 1.48 | 1.37 |
| 1 | C | 214 | TRP | CE2-CZ2 | -5.80 | 1.29 | 1.39 |
| 1 | D | 25 | LYS | CE-NZ | 5.79 | 1.63 | 1.49 |
| 1 | J | 243 | GLU | CB-CG | 5.79 | 1.63 | 1.52 |
| 1 | I | 239 | LYS | CE-NZ | 5.79 | 1.63 | 1.49 |
| 1 | A | 191 | THR | CB-CG2 | 5.79 | 1.71 | 1.52 |
| 1 | E | 231 | ARG | CG-CD | 5.79 | 1.66 | 1.51 |
| 1 | F | 233 | ALA | CA-CB | 5.79 | 1.64 | 1.52 |
| 1 | I | 206 | ARG | CZ-NH1 | 5.79 | 1.40 | 1.33 |
| 1 | H | 193 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | D | 44 | ALA | CA-CB | 5.78 | 1.64 | 1.52 |
| 1 | H | 236 | LYS | CE-NZ | 5.78 | 1.63 | 1.49 |
| 1 | C | 235 | GLU | CG-CD | 5.77 | 1.60 | 1.51 |
| 1 | H | 224 | GLU | CD-OE2 | 5.77 | 1.31 | 1.25 |
| 1 | C | 162 | LYS | CD-CE | 5.77 | 1.65 | 1.51 |
| 1 | B | 204 | GLN | CB-CG | -5.76 | 1.36 | 1.52 |
| 1 | H | 209 | ASP | CB-CG | 5.75 | 1.63 | 1.51 |
| 1 | G | 26 | LEU | C-O | 5.75 | 1.34 | 1.23 |
| 1 | H | 143 | TYR | CB-CG | -5.75 | 1.43 | 1.51 |
| 1 | B | 57 | PHE | CE2-CZ | 5.75 | 1.48 | 1.37 |
| 1 | B | 242 | TYR | CD2-CE2 | 5.75 | 1.48 | 1.39 |
| 1 | J | 14 | GLU | CG-CD | 5.74 | 1.60 | 1.51 |
| 1 | G | 158 | VAL | CB-CG1 | 5.74 | 1.64 | 1.52 |
| 1 | C | 143 | TYR | CE2-CZ | 5.73 | 1.46 | 1.38 |
| 1 | C | 224 | GLU | CD-OE2 | 5.73 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | I | 119 | GLU | N-CA | 5.72 | 1.57 | 1.46 |
| 1 | C | 239 | LYS | CE-NZ | 5.72 | 1.63 | 1.49 |
| 1 | J | 199 | ARG | CB-CG | -5.72 | 1.37 | 1.52 |
| 1 | D | 40 | PHE | CE1-CZ | 5.71 | 1.48 | 1.37 |
| 1 | C | 153 | GLU | CG-CD | 5.71 | 1.60 | 1.51 |
| 1 | H | 85 | TRP | CZ3-CH2 | 5.71 | 1.49 | 1.40 |
| 1 | E | 129 | PHE | CD1-CE1 | 5.71 | 1.50 | 1.39 |
| 1 | B | 96 | ARG | CZ-NH1 | 5.71 | 1.40 | 1.33 |
| 1 | A | 220 | ARG | CG-CD | 5.71 | 1.66 | 1.51 |
| 1 | C | 229 | TYR | CE2-CZ | 5.69 | 1.46 | 1.38 |
| 1 | D | 244 | GLU | CG-CD | 5.69 | 1.60 | 1.51 |
| 1 | G | 111 | ARG | CZ-NH2 | 5.69 | 1.40 | 1.33 |
| 1 | E | 66 | ARG | CZ-NH1 | 5.68 | 1.40 | 1.33 |
| 1 | A | 14 | GLU | CD-OE2 | 5.67 | 1.31 | 1.25 |
| 1 | H | 162 | LYS | CE-NZ | 5.67 | 1.63 | 1.49 |
| 1 | J | 104 | ASP | CB-CG | -5.67 | 1.39 | 1.51 |
| 1 | A | 205 | TYR | CG-CD2 | 5.66 | 1.46 | 1.39 |
| 1 | D | 231 | ARG | CG-CD | 5.65 | 1.66 | 1.51 |
| 1 | I | 187 | VAL | CB-CG2 | 5.65 | 1.64 | 1.52 |
| 1 | J | 224 | GLU | CD-OE2 | 5.65 | 1.31 | 1.25 |
| 1 | B | 34 | GLY | C-O | 5.65 | 1.32 | 1.23 |
| 1 | A | 85 | TRP | CD2-CE2 | 5.64 | 1.48 | 1.41 |
| 1 | A | 214 | TRP | CZ3-CH2 | -5.64 | 1.31 | 1.40 |
| 1 | J | 55 | VAL | CB-CG1 | 5.63 | 1.64 | 1.52 |
| 1 | E | 23 | VAL | CB-CG1 | 5.63 | 1.64 | 1.52 |
| 1 | G | 61 | TYR | CG-CD1 | -5.63 | 1.31 | 1.39 |
| 1 | E | 234 | ALA | CA-CB | 5.63 | 1.64 | 1.52 |
| 1 | C | 44 | ALA | CA-CB | 5.62 | 1.64 | 1.52 |
| 1 | D | 64 | PHE | CE1-CZ | 5.61 | 1.48 | 1.37 |
| 1 | B | 23 | VAL | CB-CG1 | 5.61 | 1.64 | 1.52 |
| 1 | F | 226 | ALA | CA-CB | 5.61 | 1.64 | 1.52 |
| 1 | B | 218 | ALA | CA-CB | 5.60 | 1.64 | 1.52 |
| 1 | F | 243 | GLU | CD-OE2 | 5.60 | 1.31 | 1.25 |
| 1 | C | 235 | GLU | CB-CG | -5.60 | 1.41 | 1.52 |
| 1 | E | 225 | GLU | CG-CD | 5.60 | 1.60 | 1.51 |
| 1 | I | 168 | LYS | CD-CE | 5.60 | 1.65 | 1.51 |
| 1 | B | 234 | ALA | CA-CB | 5.60 | 1.64 | 1.52 |
| 1 | J | 162 | LYS | CD-CE | 5.59 | 1.65 | 1.51 |
| 1 | G | 194 | ASP | CB-CG | 5.59 | 1.63 | 1.51 |
| 1 | H | 237 | PRO | CB-CG | 5.58 | 1.77 | 1.50 |
| 1 | B | 129 | PHE | CD1-CE1 | 5.58 | 1.50 | 1.39 |
| 1 | D | 242 | TYR | CD2-CE2 | 5.57 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | E | 242 | TYR | CD2-CE2 | 5.57 | 1.47 | 1.39 |
| 1 | I | 140 | MSE | SE-CE | -5.56 | 1.62 | 1.95 |
| 1 | D | 107 | GLY | C-O | 5.56 | 1.32 | 1.23 |
| 1 | A | 38 | VAL | CB-CG1 | 5.55 | 1.64 | 1.52 |
| 1 | A | 236 | LYS | CE-NZ | 5.55 | 1.62 | 1.49 |
| 1 | A | 61 | TYR | CD2-CE2 | 5.55 | 1.47 | 1.39 |
| 1 | C | 179 | GLU | CG-CD | 5.54 | 1.60 | 1.51 |
| 1 | B | 62 | GLU | CD-OE1 | 5.54 | 1.31 | 1.25 |
| 1 | I | 16 | GLU | CG-CD | 5.54 | 1.60 | 1.51 |
| 1 | F | 187 | VAL | CB-CG1 | 5.54 | 1.64 | 1.52 |
| 1 | C | 244 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | D | 111 | ARG | CZ-NH1 | 5.53 | 1.40 | 1.33 |
| 1 | H | 153 | GLU | CB-CG | 5.53 | 1.62 | 1.52 |
| 1 | C | 211 | TRP | CE3-CZ3 | 5.53 | 1.47 | 1.38 |
| 1 | D | 47 | THR | CB-CG2 | -5.53 | 1.34 | 1.52 |
| 1 | C | 59 | ARG | CZ-NH1 | 5.53 | 1.40 | 1.33 |
| 1 | D | 40 | PHE | CE2-CZ | 5.53 | 1.47 | 1.37 |
| 1 | H | 37 | PHE | CE2-CZ | 5.52 | 1.47 | 1.37 |
| 1 | G | 90 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | F | 173 | ALA | CA-CB | 5.52 | 1.64 | 1.52 |
| 1 | D | 46 | PHE | CE2-CZ | 5.52 | 1.47 | 1.37 |
| 1 | E | 53 | GLU | CD-OE1 | 5.51 | 1.31 | 1.25 |
| 1 | F | 61 | TYR | CG-CD2 | 5.51 | 1.46 | 1.39 |
| 1 | H | 146 | GLU | CG-CD | 5.51 | 1.60 | 1.51 |
| 1 | D | 109 | VAL | CB-CG2 | -5.51 | 1.41 | 1.52 |
| 1 | G | 160 | ALA | CA-CB | 5.51 | 1.64 | 1.52 |
| 1 | A | 197 | ARG | CG-CD | 5.50 | 1.65 | 1.51 |
| 1 | G | 146 | GLU | CD-OE1 | 5.50 | 1.31 | 1.25 |
| 1 | J | 244 | GLU | CD-OE2 | 5.50 | 1.31 | 1.25 |
| 1 | I | 35 | LYS | CE-NZ | 5.50 | 1.62 | 1.49 |
| 1 | G | 197 | ARG | CZ-NH1 | 5.49 | 1.40 | 1.33 |
| 1 | A | 226 | ALA | CA-CB | 5.49 | 1.64 | 1.52 |
| 1 | J | 99 | PHE | CE2-CZ | 5.49 | 1.47 | 1.37 |
| 1 | E | 214 | TRP | CE2-CZ2 | -5.49 | 1.30 | 1.39 |
| 1 | F | 222 | ASP | C-O | -5.49 | 1.12 | 1.23 |
| 1 | A | 159 | LYS | CG-CD | -5.49 | 1.33 | 1.52 |
| 1 | B | 193 | GLU | CG-CD | 5.49 | 1.60 | 1.51 |
| 1 | B | 159 | LYS | CG-CD | -5.48 | 1.33 | 1.52 |
| 1 | F | 70 | ASP | CG-OD1 | 5.48 | 1.38 | 1.25 |
| 1 | H | 131 | VAL | CB-CG1 | 5.48 | 1.64 | 1.52 |
| 1 | H | 235 | GLU | CB-CG | -5.48 | 1.41 | 1.52 |
| 1 | G | 134 | ARG | CZ-NH1 | 5.47 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | J | 172 | PRO | CG-CD | 5.47 | 1.68 | 1.50 |
| 1 | C | 109 | VAL | CB-CG1 | -5.46 | 1.41 | 1.52 |
| 1 | A | 59 | ARG | CG-CD | -5.46 | 1.38 | 1.51 |
| 1 | J | 199 | ARG | CZ-NH2 | 5.46 | 1.40 | 1.33 |
| 1 | A | 244 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | E | 54 | PHE | CB-CG | -5.45 | 1.42 | 1.51 |
| 1 | E | 227 | ARG | CB-CG | -5.45 | 1.37 | 1.52 |
| 1 | I | 243 | GLU | CB-CG | 5.45 | 1.62 | 1.52 |
| 1 | E | 227 | ARG | CG-CD | 5.44 | 1.65 | 1.51 |
| 1 | B | 66 | ARG | CZ-NH2 | 5.44 | 1.40 | 1.33 |
| 1 | B | 174 | ASP | CB-CG | 5.44 | 1.63 | 1.51 |
| 1 | G | 214 | TRP | CG-CD1 | 5.44 | 1.44 | 1.36 |
| 1 | B | 66 | ARG | NE-CZ | 5.44 | 1.40 | 1.33 |
| 1 | B | 239 | LYS | CE-NZ | 5.44 | 1.62 | 1.49 |
| 1 | B | 183 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | G | 121 | ALA | CA-CB | 5.43 | 1.63 | 1.52 |
| 1 | J | 168 | LYS | CE-NZ | 5.43 | 1.62 | 1.49 |
| 1 | B | 175 | TRP | CG-CD1 | 5.42 | 1.44 | 1.36 |
| 1 | I | 233 | ALA | CA-CB | 5.42 | 1.63 | 1.52 |
| 1 | E | 84 | LYS | CE-NZ | 5.41 | 1.62 | 1.49 |
| 1 | F | 179 | GLU | CB-CG | 5.40 | 1.62 | 1.52 |
| 1 | E | 37 | PHE | CD2-CE2 | 5.40 | 1.50 | 1.39 |
| 1 | J | 193 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | J | 30 | TYR | CE1-CZ | -5.39 | 1.31 | 1.38 |
| 1 | I | 121 | ALA | CA-CB | 5.39 | 1.63 | 1.52 |
| 1 | A | 55 | VAL | CB-CG1 | 5.38 | 1.64 | 1.52 |
| 1 | J | 55 | VAL | CB-CG2 | 5.38 | 1.64 | 1.52 |
| 1 | D | 238 | ALA | CA-CB | 5.38 | 1.63 | 1.52 |
| 1 | H | 128 | VAL | CB-CG1 | 5.38 | 1.64 | 1.52 |
| 1 | G | 124 | THR | CB-CG2 | -5.38 | 1.34 | 1.52 |
| 1 | G | 16 | GLU | CD-OE1 | 5.38 | 1.31 | 1.25 |
| 1 | B | 44 | ALA | CA-CB | 5.37 | 1.63 | 1.52 |
| 1 | B | 50 | CYS | N-CA | 5.37 | 1.57 | 1.46 |
| 1 | C | 236 | LYS | CD-CE | 5.37 | 1.64 | 1.51 |
| 1 | E | 131 | VAL | CB-CG2 | 5.36 | 1.64 | 1.52 |
| 1 | I | 197 | ARG | CZ-NH1 | 5.36 | 1.40 | 1.33 |
| 1 | F | 165 | ASP | CB-CG | 5.36 | 1.63 | 1.51 |
| 1 | B | 115 | LEU | CG-CD2 | 5.36 | 1.71 | 1.51 |
| 1 | F | 145 | MSE | CB-CG | 5.35 | 1.68 | 1.52 |
| 1 | I | 242 | TYR | CG-CD2 | 5.35 | 1.46 | 1.39 |
| 1 | C | 196 | ALA | CA-CB | 5.34 | 1.63 | 1.52 |
| 1 | B | 243 | GLU | CB-CG | 5.34 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 244 | GLU | CD-OE1 | 5.34 | 1.31 | 1.25 |
| 1 | E | 10 | GLU | CD-OE1 | 5.33 | 1.31 | 1.25 |
| 1 | I | 122 | THR | C-O | 5.33 | 1.33 | 1.23 |
| 1 | J | 188 | PRO | N-CA | 5.33 | 1.56 | 1.47 |
| 1 | C | 30 | TYR | CD1-CE1 | 5.33 | 1.47 | 1.39 |
| 1 | H | 62 | GLU | CG-CD | 5.32 | 1.59 | 1.51 |
| 1 | E | 205 | TYR | CD1-CE1 | -5.32 | 1.31 | 1.39 |
| 1 | A | 111 | ARG | CD-NE | 5.32 | 1.55 | 1.46 |
| 1 | E | 58 | ALA | CA-CB | 5.32 | 1.63 | 1.52 |
| 1 | C | 225 | GLU | CD-OE2 | 5.32 | 1.31 | 1.25 |
| 1 | E | 201 | GLU | CD-OE1 | 5.32 | 1.31 | 1.25 |
| 1 | F | 140 | MSE | CG-SE | 5.32 | 2.13 | 1.95 |
| 1 | G | 202 | SER | CB-OG | 5.32 | 1.49 | 1.42 |
| 1 | H | 205 | TYR | CB-CG | -5.30 | 1.43 | 1.51 |
| 1 | G | 149 | ARG | CZ-NH2 | 5.30 | 1.40 | 1.33 |
| 1 | I | 79 | VAL | CB-CG2 | 5.30 | 1.64 | 1.52 |
| 1 | A | 214 | TRP | CB-CG | -5.30 | 1.40 | 1.50 |
| 1 | I | 57 | PHE | CE2-CZ | 5.30 | 1.47 | 1.37 |
| 1 | H | 228 | ARG | CB-CG | -5.29 | 1.38 | 1.52 |
| 1 | A | 119 | GLU | CG-CD | 5.29 | 1.59 | 1.51 |
| 1 | C | 108 | THR | CB-CG2 | -5.29 | 1.34 | 1.52 |
| 1 | E | 134 | ARG | CB-CG | 5.29 | 1.66 | 1.52 |
| 1 | B | 145 | MSE | CG-SE | -5.28 | 1.77 | 1.95 |
| 1 | B | 162 | LYS | CG-CD | 5.28 | 1.70 | 1.52 |
| 1 | E | 62 | GLU | CD-OE1 | 5.28 | 1.31 | 1.25 |
| 1 | H | 119 | GLU | CG-CD | 5.28 | 1.59 | 1.51 |
| 1 | H | 153 | GLU | CG-CD | 5.28 | 1.59 | 1.51 |
| 1 | C | 95 | VAL | CB-CG2 | 5.28 | 1.64 | 1.52 |
| 1 | C | 96 | ARG | NE-CZ | 5.28 | 1.40 | 1.33 |
| 1 | E | 177 | ASN | N-CA | 5.28 | 1.56 | 1.46 |
| 1 | F | 23 | VAL | CA-CB | 5.27 | 1.65 | 1.54 |
| 1 | I | 85 | TRP | CZ3-CH2 | 5.27 | 1.48 | 1.40 |
| 1 | F | 201 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | G | 36 | TRP | CE3-CZ3 | 5.27 | 1.47 | 1.38 |
| 1 | I | 242 | TYR | CG-CD1 | 5.26 | 1.46 | 1.39 |
| 1 | J | 76 | VAL | CB-CG1 | 5.26 | 1.64 | 1.52 |
| 1 | H | 119 | GLU | CD-OE1 | 5.26 | 1.31 | 1.25 |
| 1 | D | 206 | ARG | CZ-NH1 | 5.26 | 1.39 | 1.33 |
| 1 | A | 139 | THR | CB-CG2 | 5.25 | 1.69 | 1.52 |
| 1 | F | 46 | PHE | CE2-CZ | 5.25 | 1.47 | 1.37 |
| 1 | C | 25 | LYS | CD-CE | 5.25 | 1.64 | 1.51 |
| 1 | B | 244 | GLU | CB-CG | 5.24 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | H | 146 | GLU | CD-OE1 | 5.24 | 1.31 | 1.25 |
| 1 | A | 170 | ALA | CA-CB | 5.24 | 1.63 | 1.52 |
| 1 | E | 85 | TRP | CE3-CZ3 | 5.24 | 1.47 | 1.38 |
| 1 | D | 143 | TYR | CE2-CZ | 5.24 | 1.45 | 1.38 |
| 1 | D | 153 | GLU | CB-CG | 5.23 | 1.62 | 1.52 |
| 1 | G | 218 | ALA | CA-CB | 5.23 | 1.63 | 1.52 |
| 1 | I | 65 | GLN | CG-CD | 5.23 | 1.63 | 1.51 |
| 1 | E | 174 | ASP | CB-CG | 5.23 | 1.62 | 1.51 |
| 1 | D | 179 | GLU | CD-OE1 | 5.23 | 1.31 | 1.25 |
| 1 | D | 201 | GLU | CG-CD | 5.22 | 1.59 | 1.51 |
| 1 | D | 55 | VAL | C-O | 5.22 | 1.33 | 1.23 |
| 1 | E | 194 | ASP | CB-CG | -5.21 | 1.40 | 1.51 |
| 1 | D | 70 | ASP | CG-OD1 | 5.21 | 1.37 | 1.25 |
| 1 | I | 99 | PHE | CE1-CZ | 5.21 | 1.47 | 1.37 |
| 1 | E | 138 | ARG | CZ-NH2 | 5.21 | 1.39 | 1.33 |
| 1 | B | 244 | GLU | CD-OE1 | 5.20 | 1.31 | 1.25 |
| 1 | C | 245 | ALA | C-O | 5.20 | 1.33 | 1.23 |
| 1 | C | 140 | MSE | CG-SE | 5.20 | 2.13 | 1.95 |
| 1 | D | 200 | MSE | CG-SE | 5.20 | 2.13 | 1.95 |
| 1 | D | 14 | GLU | CD-OE1 | 5.19 | 1.31 | 1.25 |
| 1 | A | 197 | ARG | CD-NE | 5.18 | 1.55 | 1.46 |
| 1 | E | 65 | GLN | CD-OE1 | 5.18 | 1.35 | 1.24 |
| 1 | H | 78 | SER | CB-OG | 5.18 | 1.49 | 1.42 |
| 1 | H | 168 | LYS | CB-CG | 5.18 | 1.66 | 1.52 |
| 1 | C | 18 | THR | CA-CB | 5.18 | 1.66 | 1.53 |
| 1 | F | 218 | ALA | CA-CB | 5.18 | 1.63 | 1.52 |
| 1 | B | 236 | LYS | CD-CE | 5.18 | 1.64 | 1.51 |
| 1 | G | 134 | ARG | CZ-NH2 | 5.17 | 1.39 | 1.33 |
| 1 | E | 96 | ARG | CZ-NH1 | 5.17 | 1.39 | 1.33 |
| 1 | F | 6 | PRO | CA-C | 5.17 | 1.63 | 1.52 |
| 1 | E | 64 | PHE | CE1-CZ | 5.17 | 1.47 | 1.37 |
| 1 | F | 146 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | E | 238 | ALA | CA-CB | 5.17 | 1.63 | 1.52 |
| 1 | C | 166 | SER | CB-OG | -5.16 | 1.35 | 1.42 |
| 1 | J | 61 | TYR | CZ-OH | 5.16 | 1.46 | 1.37 |
| 1 | D | 219 | SER | CA-CB | -5.16 | 1.45 | 1.52 |
| 1 | I | 244 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | E | 200 | MSE | CG-SE | 5.16 | 2.12 | 1.95 |
| 1 | A | 119 | GLU | CD-OE1 | 5.16 | 1.31 | 1.25 |
| 1 | E | 182 | GLY | C-O | 5.15 | 1.31 | 1.23 |
| 1 | B | 214 | TRP | CD2-CE2 | -5.15 | 1.35 | 1.41 |
| 1 | F | 60 | ARG | CG-CD | 5.14 | 1.64 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | H | 118 | ALA | CA-CB | 5.14 | 1.63 | 1.52 |
| 1 | I | 10 | GLU | CG-CD | 5.14 | 1.59 | 1.51 |
| 1 | I | 168 | LYS | CE-NZ | 5.14 | 1.61 | 1.49 |
| 1 | D | 8 | ILE | CB-CG1 | 5.14 | 1.68 | 1.54 |
| 1 | F | 236 | LYS | CE-NZ | 5.13 | 1.61 | 1.49 |
| 1 | H | 159 | LYS | CG-CD | -5.13 | 1.34 | 1.52 |
| 1 | J | 190 | PRO | CA-C | 5.13 | 1.63 | 1.52 |
| 1 | J | 2 | PRO | CA-C | -5.13 | 1.42 | 1.52 |
| 1 | C | 50 | CYS | N-CA | 5.13 | 1.56 | 1.46 |
| 1 | G | 65 | GLN | N-CA | 5.12 | 1.56 | 1.46 |
| 1 | J | 199 | ARG | CG-CD | 5.12 | 1.64 | 1.51 |
| 1 | B | 235 | GLU | CD-OE1 | 5.12 | 1.31 | 1.25 |
| 1 | A | 89 | ILE | CA-CB | 5.11 | 1.66 | 1.54 |
| 1 | E | 158 | VAL | CB-CG1 | -5.11 | 1.42 | 1.52 |
| 1 | G | 96 | ARG | CZ-NH1 | 5.11 | 1.39 | 1.33 |
| 1 | D | 35 | LYS | CE-NZ | 5.11 | 1.61 | 1.49 |
| 1 | I | 143 | TYR | CG-CD2 | 5.11 | 1.45 | 1.39 |
| 1 | C | 205 | TYR | CE1-CZ | 5.11 | 1.45 | 1.38 |
| 1 | J | 96 | ARG | CZ-NH1 | 5.11 | 1.39 | 1.33 |
| 1 | C | 142 | TYR | CG-CD1 | -5.11 | 1.32 | 1.39 |
| 1 | A | 220 | ARG | CZ-NH1 | 5.10 | 1.39 | 1.33 |
| 1 | C | 199 | ARG | CG-CD | -5.10 | 1.39 | 1.51 |
| 1 | C | 66 | ARG | CG-CD | 5.10 | 1.64 | 1.51 |
| 1 | G | 231 | ARG | CZ-NH2 | 5.10 | 1.39 | 1.33 |
| 1 | E | 242 | TYR | CE2-CZ | 5.09 | 1.45 | 1.38 |
| 1 | I | 11 | ARG | CZ-NH1 | 5.09 | 1.39 | 1.33 |
| 1 | D | 239 | LYS | CD-CE | 5.09 | 1.64 | 1.51 |
| 1 | H | 63 | ASP | C-O | 5.09 | 1.33 | 1.23 |
| 1 | I | 130 | ILE | CB-CG2 | 5.09 | 1.68 | 1.52 |
| 1 | I | 143 | TYR | CE1-CZ | 5.09 | 1.45 | 1.38 |
| 1 | E | 95 | VAL | CB-CG1 | 5.08 | 1.63 | 1.52 |
| 1 | H | 93 | ILE | CA-CB | 5.08 | 1.66 | 1.54 |
| 1 | E | 159 | LYS | CG-CD | -5.08 | 1.35 | 1.52 |
| 1 | H | 170 | ALA | CA-CB | 5.08 | 1.63 | 1.52 |
| 1 | G | 87 | GLU | CG-CD | 5.08 | 1.59 | 1.51 |
| 1 | D | 242 | TYR | CE1-CZ | 5.08 | 1.45 | 1.38 |
| 1 | B | 197 | ARG | CZ-NH1 | 5.07 | 1.39 | 1.33 |
| 1 | F | 99 | PHE | CE2-CZ | 5.07 | 1.47 | 1.37 |
| 1 | I | 11 | ARG | CZ-NH2 | 5.07 | 1.39 | 1.33 |
| 1 | E | 41 | SER | CB-OG | 5.07 | 1.48 | 1.42 |
| 1 | G | 179 | GLU | CD-OE1 | 5.07 | 1.31 | 1.25 |
| 1 | C | 129 | PHE | CD1-CE1 | 5.06 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | E | 15 | MSE | CG-SE | 5.06 | 2.12 | 1.95 |
| 1 | H | 6 | PRO | CA-C | 5.06 | 1.62 | 1.52 |
| 1 | I | 49 | VAL | CB-CG2 | 5.06 | 1.63 | 1.52 |
| 1 | F | 244 | GLU | CD-OE2 | 5.06 | 1.31 | 1.25 |
| 1 | G | 224 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | I | 15 | MSE | CG-SE | 5.05 | 2.12 | 1.95 |
| 1 | D | 195 | GLN | CG-CD | 5.05 | 1.62 | 1.51 |
| 1 | E | 8 | ILE | C-O | 5.05 | 1.32 | 1.23 |
| 1 | I | 242 | TYR | CE2-CZ | 5.05 | 1.45 | 1.38 |
| 1 | B | 79 | VAL | CA-CB | 5.05 | 1.65 | 1.54 |
| 1 | C | 112 | ARG | NE-CZ | 5.05 | 1.39 | 1.33 |
| 1 | H | 86 | LYS | CE-NZ | 5.05 | 1.61 | 1.49 |
| 1 | H | 99 | PHE | CG-CD2 | -5.04 | 1.31 | 1.38 |
| 1 | H | 143 | TYR | CD1-CE1 | 5.04 | 1.47 | 1.39 |
| 1 | I | 192 | THR | C-O | 5.04 | 1.32 | 1.23 |
| 1 | B | 228 | ARG | NE-CZ | 5.04 | 1.39 | 1.33 |
| 1 | B | 142 | TYR | CE1-CZ | 5.03 | 1.45 | 1.38 |
| 1 | A | 220 | ARG | NE-CZ | 5.03 | 1.39 | 1.33 |
| 1 | I | 204 | GLN | CG-CD | 5.03 | 1.62 | 1.51 |
| 1 | B | 112 | ARG | CZ-NH1 | 5.03 | 1.39 | 1.33 |
| 1 | J | 45 | ASP | CB-CG | 5.02 | 1.62 | 1.51 |
| 1 | B | 51 | THR | C-O | 5.02 | 1.32 | 1.23 |
| 1 | A | 146 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | A | 53 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | B | 153 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | E | 239 | LYS | CA-C | 5.02 | 1.66 | 1.52 |
| 1 | I | 80 | PHE | CD2-CE2 | 5.01 | 1.49 | 1.39 |
| 1 | B | 112 | ARG | CB-CG | 5.01 | 1.66 | 1.52 |
| 1 | G | 80 | PHE | CE1-CZ | 5.01 | 1.46 | 1.37 |
| 1 | B | 74 | LEU | N-CA | -5.01 | 1.36 | 1.46 |
| 1 | B | 99 | PHE | CD1-CE1 | -5.01 | 1.29 | 1.39 |
| 1 | A | 175 | TRP | CA-C | 5.01 | 1.66 | 1.52 |
| 1 | I | 205 | TYR | CD2-CE2 | -5.00 | 1.31 | 1.39 |
| 1 | F | 201 | GLU | CD-OE1 | 5.00 | 1.31 | 1.25 |
| 1 | I | 10 | GLU | CB-CG | -5.00 | 1.42 | 1.52 |

All (472) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | J | 138 | ARG | NE-CZ-NH2 | -36.48 | 102.06 | 120.30 |
| 1 | J | 138 | ARG | NE-CZ-NH1 | 34.23 | 137.42 | 120.30 |
| 1 | B | 104 | ASP | CB-CG-OD2 | -32.90 | 88.69 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | G | 26 | LEU | C-N-CD | -31.81 | 50.61 | 120.60 |
| 1 | J | 26 | LEU | C-N-CD | -28.89 | 57.03 | 120.60 |
| 1 | E | 175 | TRP | C-N-CD | -25.98 | 63.43 | 120.60 |
| 1 | E | 104 | ASP | CB-CG-OD2 | -24.00 | 96.70 | 118.30 |
| 1 | J | 104 | ASP | CB-CG-OD2 | -21.82 | 98.67 | 118.30 |
| 1 | F | 104 | ASP | CB-CG-OD2 | -21.61 | 98.85 | 118.30 |
| 1 | B | 104 | ASP | CB-CG-OD1 | 17.91 | 134.42 | 118.30 |
| 1 | J | 215 | ASP | CB-CG-OD1 | -17.77 | 102.31 | 118.30 |
| 1 | A | 228 | ARG | NE-CZ-NH2 | -17.48 | 111.56 | 120.30 |
| 1 | J | 215 | ASP | CB-CG-OD2 | 17.23 | 133.80 | 118.30 |
| 1 | J | 174 | ASP | CB-CG-OD2 | -16.32 | 103.61 | 118.30 |
| 1 | E | 104 | ASP | CB-CG-OD1 | 16.23 | 132.91 | 118.30 |
| 1 | F | 231 | ARG | NE-CZ-NH2 | -15.38 | 112.61 | 120.30 |
| 1 | D | 138 | ARG | NE-CZ-NH1 | -14.95 | 112.83 | 120.30 |
| 1 | J | 27 | PRO | CA-N-CD | -14.84 | 90.72 | 111.50 |
| 1 | I | 228 | ARG | NE-CZ-NH1 | 14.49 | 127.55 | 120.30 |
| 1 | F | 227 | ARG | NE-CZ-NH2 | -14.32 | 113.14 | 120.30 |
| 1 | J | 27 | PRO | N-CA-C | -14.23 | 75.10 | 112.10 |
| 1 | J | 104 | ASP | CB-CG-OD1 | 13.19 | 130.17 | 118.30 |
| 1 | H | 112 | ARG | NE-CZ-NH2 | -13.11 | 113.75 | 120.30 |
| 1 | D | 67 | LEU | C-N-CA | -13.01 | 94.97 | 122.30 |
| 1 | F | 66 | ARG | NE-CZ-NH1 | 12.42 | 126.51 | 120.30 |
| 1 | I | 228 | ARG | NE-CZ-NH2 | -12.32 | 114.14 | 120.30 |
| 1 | H | 227 | ARG | NE-CZ-NH1 | -12.30 | 114.15 | 120.30 |
| 1 | G | 215 | ASP | CB-CG-OD1 | 12.28 | 129.35 | 118.30 |
| 1 | C | 11 | ARG | NE-CZ-NH2 | -12.01 | 114.29 | 120.30 |
| 1 | B | 67 | LEU | C-N-CA | -11.97 | 97.17 | 122.30 |
| 1 | F | 112 | ARG | NE-CZ-NH2 | 11.89 | 126.24 | 120.30 |
| 1 | J | 138 | ARG | CD-NE-CZ | 11.69 | 139.97 | 123.60 |
| 1 | J | 28 | ASP | CB-CG-OD2 | -11.66 | 107.81 | 118.30 |
| 1 | F | 104 | ASP | CB-CG-OD1 | 11.63 | 128.77 | 118.30 |
| 1 | B | 112 | ARG | NE-CZ-NH1 | 11.40 | 126.00 | 120.30 |
| 1 | E | 70 | ASP | CB-CG-OD2 | -11.36 | 108.07 | 118.30 |
| 1 | B | 199 | ARG | CG-CD-NE | -11.34 | 87.99 | 111.80 |
| 1 | E | 228 | ARG | NE-CZ-NH2 | -11.32 | 114.64 | 120.30 |
| 1 | F | 59 | ARG | NE-CZ-NH2 | -11.12 | 114.74 | 120.30 |
| 1 | I | 231 | ARG | NE-CZ-NH2 | -10.97 | 114.81 | 120.30 |
| 1 | C | 17 | VAL | CG1-CB-CG2 | 10.94 | 128.40 | 110.90 |
| 1 | J | 59 | ARG | NE-CZ-NH1 | -10.73 | 114.93 | 120.30 |
| 1 | B | 227 | ARG | NE-CZ-NH1 | -10.73 | 114.94 | 120.30 |
| 1 | E | 176 | PRO | N-CA-C | -10.69 | 84.30 | 112.10 |
| 1 | C | 59 | ARG | NE-CZ-NH2 | -10.67 | 114.97 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | I | 28 | ASP | CB-CG-OD1 | 10.64 | 127.88 | 118.30 |
| 1 | A | 70 | ASP | CB-CG-OD2 | -10.50 | 108.85 | 118.30 |
| 1 | F | 227 | ARG | NE-CZ-NH1 | 10.37 | 125.48 | 120.30 |
| 1 | C | 60 | ARG | NE-CZ-NH1 | 10.36 | 125.48 | 120.30 |
| 1 | C | 206 | ARG | NE-CZ-NH2 | -10.34 | 115.13 | 120.30 |
| 1 | G | 27 | PRO | CA-N-CD | -10.31 | 97.07 | 111.50 |
| 1 | B | 138 | ARG | NE-CZ-NH1 | 10.27 | 125.44 | 120.30 |
| 1 | I | 138 | ARG | NE-CZ-NH2 | 10.24 | 125.42 | 120.30 |
| 1 | E | 138 | ARG | NE-CZ-NH1 | -10.11 | 115.25 | 120.30 |
| 1 | F | 149 | ARG | NE-CZ-NH1 | -10.00 | 115.30 | 120.30 |
| 1 | B | 96 | ARG | NE-CZ-NH2 | -9.76 | 115.42 | 120.30 |
| 1 | G | 199 | ARG | NE-CZ-NH1 | -9.67 | 115.47 | 120.30 |
| 1 | D | 239 | LYS | CD-CE-NZ | 9.66 | 133.93 | 111.70 |
| 1 | J | 158 | VAL | CG1-CB-CG2 | -9.62 | 95.50 | 110.90 |
| 1 | C | 60 | ARG | NE-CZ-NH2 | -9.50 | 115.55 | 120.30 |
| 1 | E | 227 | ARG | CG-CD-NE | -9.49 | 91.88 | 111.80 |
| 1 | J | 199 | ARG | CG-CD-NE | -9.33 | 92.20 | 111.80 |
| 1 | A | 231 | ARG | NE-CZ-NH1 | 9.31 | 124.95 | 120.30 |
| 1 | C | 199 | ARG | NE-CZ-NH1 | 9.21 | 124.91 | 120.30 |
| 1 | I | 126 | ARG | NE-CZ-NH2 | -9.21 | 115.70 | 120.30 |
| 1 | A | 163 | LEU | CB-CG-CD1 | -9.20 | 95.36 | 111.00 |
| 1 | J | 96 | ARG | NE-CZ-NH2 | -9.16 | 115.72 | 120.30 |
| 1 | I | 232 | ARG | NE-CZ-NH2 | -9.14 | 115.73 | 120.30 |
| 1 | J | 27 | PRO | N-CA-CB | 9.11 | 114.23 | 103.30 |
| 1 | G | 112 | ARG | CG-CD-NE | -9.07 | 92.75 | 111.80 |
| 1 | J | 11 | ARG | NE-CZ-NH2 | -9.06 | 115.77 | 120.30 |
| 1 | H | 149 | ARG | NE-CZ-NH1 | -9.05 | 115.78 | 120.30 |
| 1 | I | 28 | ASP | CB-CG-OD2 | -9.04 | 110.17 | 118.30 |
| 1 | J | 91 | ARG | NE-CZ-NH1 | -9.01 | 115.79 | 120.30 |
| 1 | D | 163 | LEU | CB-CG-CD1 | -9.00 | 95.70 | 111.00 |
| 1 | C | 32 | SER | CA-CB-OG | -8.96 | 87.00 | 111.20 |
| 1 | C | 232 | ARG | NE-CZ-NH1 | -8.94 | 115.83 | 120.30 |
| 1 | D | 67 | LEU | O-C-N | -8.87 | 108.13 | 123.20 |
| 1 | J | 175 | TRP | C-N-CD | -8.84 | 101.16 | 120.60 |
| 1 | H | 126 | ARG | NE-CZ-NH2 | -8.78 | 115.91 | 120.30 |
| 1 | B | 116 | LEU | CB-CG-CD1 | -8.77 | 96.09 | 111.00 |
| 1 | J | 96 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 1 | E | 138 | ARG | NE-CZ-NH2 | 8.70 | 124.65 | 120.30 |
| 1 | G | 231 | ARG | NE-CZ-NH1 | -8.65 | 115.97 | 120.30 |
| 1 | J | 104 | ASP | N-CA-CB | 8.60 | 126.08 | 110.60 |
| 1 | I | 183 | GLU | CG-CD-OE2 | 8.58 | 135.45 | 118.30 |
| 1 | F | 215 | ASP | CB-CG-OD2 | 8.55 | 125.99 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 227 | ARG | NE-CZ-NH1 | -8.54 | 116.03 | 120.30 |
| 1 | E | 175 | TRP | O-C-N | 8.49 | 137.23 | 121.10 |
| 1 | H | 112 | ARG | CG-CD-NE | -8.48 | 93.98 | 111.80 |
| 1 | J | 60 | ARG | NE-CZ-NH1 | 8.40 | 124.50 | 120.30 |
| 1 | A | 145 | MSE | CA-CB-CG | -8.39 | 99.03 | 113.30 |
| 1 | B | 159 | LYS | CD-CE-NZ | 8.36 | 130.92 | 111.70 |
| 1 | H | 60 | ARG | NE-CZ-NH1 | 8.34 | 124.47 | 120.30 |
| 1 | B | 67 | LEU | O-C-N | -8.32 | 109.06 | 123.20 |
| 1 | E | 175 | TRP | C-N-CA | 8.30 | 156.87 | 122.00 |
| 1 | H | 60 | ARG | NE-CZ-NH2 | -8.28 | 116.16 | 120.30 |
| 1 | C | 112 | ARG | NE-CZ-NH1 | 8.26 | 124.43 | 120.30 |
| 1 | F | 111 | ARG | NE-CZ-NH2 | -8.25 | 116.18 | 120.30 |
| 1 | I | 215 | ASP | CB-CG-OD2 | 8.23 | 125.71 | 118.30 |
| 1 | E | 119 | GLU | OE1-CD-OE2 | 8.21 | 133.15 | 123.30 |
| 1 | J | 63 | ASP | CB-CG-OD2 | 8.19 | 125.67 | 118.30 |
| 1 | A | 145 | MSE | CB-CG-SE | -8.19 | 88.12 | 112.70 |
| 1 | E | 131 | VAL | CG1-CB-CG2 | -8.14 | 97.87 | 110.90 |
| 1 | J | 145 | MSE | CG-SE-CE | -8.13 | 81.02 | 98.90 |
| 1 | A | 125 | VAL | CG1-CB-CG2 | 8.12 | 123.89 | 110.90 |
| 1 | J | 138 | ARG | CG-CD-NE | -8.12 | 94.75 | 111.80 |
| 1 | G | 159 | LYS | CD-CE-NZ | 8.10 | 130.33 | 111.70 |
| 1 | D | 126 | ARG | NE-CZ-NH2 | -8.10 | 116.25 | 120.30 |
| 1 | H | 145 | MSE | CA-CB-CG | -8.09 | 99.55 | 113.30 |
| 1 | B | 149 | ARG | NE-CZ-NH1 | -8.02 | 116.29 | 120.30 |
| 1 | I | 128 | VAL | CG1-CB-CG2 | 8.01 | 123.71 | 110.90 |
| 1 | J | 60 | ARG | NE-CZ-NH2 | -8.00 | 116.30 | 120.30 |
| 1 | B | 199 | ARG | NE-CZ-NH2 | -7.99 | 116.31 | 120.30 |
| 1 | C | 199 | ARG | NE-CZ-NH2 | -7.96 | 116.32 | 120.30 |
| 1 | G | 26 | LEU | O-C-N | 7.96 | 136.22 | 121.10 |
| 1 | H | 227 | ARG | NE-CZ-NH2 | 7.95 | 124.27 | 120.30 |
| 1 | G | 27 | PRO | N-CA-CB | 7.93 | 112.82 | 103.30 |
| 1 | I | 199 | ARG | NE-CZ-NH2 | -7.92 | 116.34 | 120.30 |
| 1 | E | 175 | TRP | N-CA-C | 7.89 | 132.31 | 111.00 |
| 1 | I | 138 | ARG | NE-CZ-NH1 | -7.86 | 116.37 | 120.30 |
| 1 | B | 175 | TRP | C-N-CD | -7.82 | 103.40 | 120.60 |
| 1 | E | 197 | ARG | NE-CZ-NH2 | -7.82 | 116.39 | 120.30 |
| 1 | G | 222 | ASP | CB-CG-OD2 | 7.82 | 125.33 | 118.30 |
| 1 | B | 112 | ARG | NE-CZ-NH2 | -7.75 | 116.42 | 120.30 |
| 1 | E | 111 | ARG | NE-CZ-NH1 | -7.74 | 116.43 | 120.30 |
| 1 | F | 112 | ARG | NE-CZ-NH1 | -7.70 | 116.45 | 120.30 |
| 1 | A | 228 | ARG | NE-CZ-NH1 | 7.69 | 124.14 | 120.30 |
| 1 | J | 243 | GLU | OE1-CD-OE2 | -7.68 | 114.09 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 222 | ASP | CB-CG-OD1 | 7.66 | 125.19 | 118.30 |
| 1 | G | 156 | ARG | NE-CZ-NH2 | -7.65 | 116.47 | 120.30 |
| 1 | I | 145 | MSE | CB-CG-SE | -7.64 | 89.77 | 112.70 |
| 1 | A | 112 | ARG | NE-CZ-NH2 | -7.63 | 116.48 | 120.30 |
| 1 | C | 199 | ARG | CA-CB-CG | 7.63 | 130.19 | 113.40 |
| 1 | B | 199 | ARG | NE-CZ-NH1 | 7.60 | 124.10 | 120.30 |
| 1 | A | 156 | ARG | NE-CZ-NH2 | -7.59 | 116.50 | 120.30 |
| 1 | E | 176 | PRO | CA-N-CD | -7.56 | 100.91 | 111.50 |
| 1 | E | 111 | ARG | NE-CZ-NH2 | 7.55 | 124.08 | 120.30 |
| 1 | I | 116 | LEU | CB-CG-CD1 | -7.55 | 98.17 | 111.00 |
| 1 | B | 140 | MSE | CA-CB-CG | -7.54 | 100.48 | 113.30 |
| 1 | H | 126 | ARG | NE-CZ-NH1 | 7.54 | 124.07 | 120.30 |
| 1 | B | 215 | ASP | CB-CG-OD1 | 7.53 | 125.07 | 118.30 |
| 1 | G | 124 | THR | N-CA-CB | -7.48 | 96.09 | 110.30 |
| 1 | F | 140 | MSE | CG-SE-CE | -7.47 | 82.47 | 98.90 |
| 1 | J | 174 | ASP | N-CA-C | 7.45 | 131.12 | 111.00 |
| 1 | E | 227 | ARG | NE-CZ-NH1 | -7.41 | 116.59 | 120.30 |
| 1 | F | 158 | VAL | CG1-CB-CG2 | -7.41 | 99.05 | 110.90 |
| 1 | B | 221 | ASP | CB-CG-OD2 | -7.39 | 111.65 | 118.30 |
| 1 | E | 25 | LYS | CD-CE-NZ | -7.36 | 94.78 | 111.70 |
| 1 | F | 231 | ARG | CG-CD-NE | -7.36 | 96.35 | 111.80 |
| 1 | B | 28 | ASP | CB-CG-OD2 | -7.36 | 111.68 | 118.30 |
| 1 | C | 74 | LEU | CD1-CG-CD2 | -7.35 | 88.46 | 110.50 |
| 1 | D | 231 | ARG | NE-CZ-NH1 | -7.33 | 116.63 | 120.30 |
| 1 | J | 28 | ASP | CB-CG-OD1 | 7.33 | 124.89 | 118.30 |
| 1 | E | 59 | ARG | NE-CZ-NH2 | -7.31 | 116.64 | 120.30 |
| 1 | J | 26 | LEU | O-C-N | 7.29 | 134.95 | 121.10 |
| 1 | B | 179 | GLU | CA-CB-CG | -7.28 | 97.38 | 113.40 |
| 1 | I | 193 | GLU | OE1-CD-OE2 | -7.28 | 114.56 | 123.30 |
| 1 | C | 59 | ARG | NH1-CZ-NH2 | 7.27 | 127.40 | 119.40 |
| 1 | C | 134 | ARG | NE-CZ-NH2 | 7.26 | 123.93 | 120.30 |
| 1 | F | 220 | ARG | NE-CZ-NH2 | -7.26 | 116.67 | 120.30 |
| 1 | G | 112 | ARG | NE-CZ-NH2 | -7.22 | 116.69 | 120.30 |
| 1 | A | 169 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 1 | B | 66 | ARG | NE-CZ-NH2 | 7.17 | 123.89 | 120.30 |
| 1 | B | 104 | ASP | OD1-CG-OD2 | 7.15 | 136.89 | 123.30 |
| 1 | I | 231 | ARG | CG-CD-NE | -7.15 | 96.79 | 111.80 |
| 1 | B | 231 | ARG | NE-CZ-NH1 | -7.08 | 116.76 | 120.30 |
| 1 | I | 70 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | F | 231 | ARG | NE-CZ-NH1 | 7.07 | 123.83 | 120.30 |
| 1 | B | 28 | ASP | CB-CG-OD1 | 7.02 | 124.62 | 118.30 |
| 1 | D | 126 | ARG | NE-CZ-NH1 | 7.01 | 123.81 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | H | 199 | ARG | NE-CZ-NH1 | -6.99 | 116.80 | 120.30 |
| 1 | F | 145 | MSE | CA-CB-CG | -6.99 | 101.41 | 113.30 |
| 1 | I | 84 | LYS | CD-CE-NZ | -6.97 | 95.68 | 111.70 |
| 1 | I | 2 | PRO | N-CA-CB | 6.96 | 111.65 | 103.30 |
| 1 | J | 26 | LEU | CB-CA-C | -6.95 | 96.99 | 110.20 |
| 1 | J | 174 | ASP | OD1-CG-OD2 | 6.95 | 136.50 | 123.30 |
| 1 | D | 183 | GLU | CG-CD-OE1 | -6.91 | 104.48 | 118.30 |
| 1 | J | 27 | PRO | N-CD-CG | 6.90 | 113.56 | 103.20 |
| 1 | J | 26 | LEU | CA-C-N | -6.90 | 97.79 | 117.10 |
| 1 | B | 145 | MSE | CA-CB-CG | -6.89 | 101.58 | 113.30 |
| 1 | D | 105 | PRO | O-C-N | -6.88 | 111.69 | 122.70 |
| 1 | D | 199 | ARG | NE-CZ-NH1 | -6.88 | 116.86 | 120.30 |
| 1 | E | 222 | ASP | CB-CG-OD1 | 6.86 | 124.47 | 118.30 |
| 1 | D | 231 | ARG | NE-CZ-NH2 | 6.80 | 123.70 | 120.30 |
| 1 | I | 59 | ARG | NE-CZ-NH2 | 6.78 | 123.69 | 120.30 |
| 1 | C | 215 | ASP | CB-CG-OD2 | 6.74 | 124.36 | 118.30 |
| 1 | J | 152 | ASP | CB-CG-OD2 | 6.72 | 124.35 | 118.30 |
| 1 | F | 66 | ARG | NE-CZ-NH2 | -6.67 | 116.97 | 120.30 |
| 1 | A | 59 | ARG | NE-CZ-NH1 | -6.66 | 116.97 | 120.30 |
| 1 | J | 231 | ARG | NE-CZ-NH1 | 6.64 | 123.62 | 120.30 |
| 1 | C | 5 | ILE | CG1-CB-CG2 | 6.64 | 126.00 | 111.40 |
| 1 | A | 183 | GLU | CG-CD-OE2 | 6.63 | 131.56 | 118.30 |
| 1 | C | 17 | VAL | N-CA-CB | -6.63 | 96.92 | 111.50 |
| 1 | H | 10 | GLU | OE1-CD-OE2 | -6.62 | 115.35 | 123.30 |
| 1 | J | 141 | LEU | CB-CG-CD2 | -6.62 | 99.75 | 111.00 |
| 1 | H | 6 | PRO | N-CA-C | -6.61 | 94.90 | 112.10 |
| 1 | J | 145 | MSE | CB-CG-SE | -6.60 | 92.91 | 112.70 |
| 1 | H | 228 | ARG | NE-CZ-NH1 | 6.59 | 123.60 | 120.30 |
| 1 | A | 59 | ARG | NE-CZ-NH2 | -6.58 | 117.01 | 120.30 |
| 1 | B | 227 | ARG | NH1-CZ-NH2 | 6.56 | 126.61 | 119.40 |
| 1 | C | 112 | ARG | CG-CD-NE | 6.55 | 125.56 | 111.80 |
| 1 | G | 17 | VAL | CG1-CB-CG2 | 6.55 | 121.38 | 110.90 |
| 1 | A | 96 | ARG | NE-CZ-NH2 | -6.54 | 117.03 | 120.30 |
| 1 | C | 111 | ARG | NE-CZ-NH1 | -6.54 | 117.03 | 120.30 |
| 1 | E | 26 | LEU | CB-CG-CD2 | -6.54 | 99.89 | 111.00 |
| 1 | G | 124 | THR | OG1-CB-CG2 | 6.53 | 125.03 | 110.00 |
| 1 | E | 191 | THR | N-CA-CB | -6.52 | 97.90 | 110.30 |
| 1 | I | 156 | ARG | NE-CZ-NH2 | -6.52 | 117.04 | 120.30 |
| 1 | H | 11 | ARG | NE-CZ-NH2 | 6.52 | 123.56 | 120.30 |
| 1 | D | 111 | ARG | NE-CZ-NH1 | -6.51 | 117.04 | 120.30 |
| 1 | A | 70 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | C | 126 | ARG | NE-CZ-NH1 | 6.47 | 123.54 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | E | 104 | ASP | N-CA-CB | 6.45 | 122.20 | 110.60 |
| 1 | E | 228 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | I | 35 | LYS | CD-CE-NZ | -6.43 | 96.91 | 111.70 |
| 1 | B | 243 | GLU | OE1-CD-OE2 | -6.40 | 115.61 | 123.30 |
| 1 | C | 149 | ARG | NE-CZ-NH2 | -6.40 | 117.10 | 120.30 |
| 1 | E | 105 | PRO | N-CA-C | -6.39 | 95.48 | 112.10 |
| 1 | G | 26 | LEU | CA-C-N | -6.36 | 99.29 | 117.10 |
| 1 | C | 199 | ARG | CG-CD-NE | -6.35 | 98.46 | 111.80 |
| 1 | A | 183 | GLU | CG-CD-OE1 | -6.34 | 105.62 | 118.30 |
| 1 | I | 206 | ARG | NE-CZ-NH2 | -6.33 | 117.14 | 120.30 |
| 1 | C | 241 | LEU | CB-CG-CD2 | -6.33 | 100.24 | 111.00 |
| 1 | J | 145 | MSE | CA-CB-CG | -6.33 | 102.54 | 113.30 |
| 1 | E | 238 | ALA | O-C-N | -6.32 | 112.59 | 122.70 |
| 1 | J | 236 | LYS | CD-CE-NZ | -6.32 | 97.18 | 111.70 |
| 1 | G | 115 | LEU | CB-CG-CD1 | -6.31 | 100.27 | 111.00 |
| 1 | G | 109 | VAL | CG1-CB-CG2 | -6.31 | 100.81 | 110.90 |
| 1 | C | 221 | ASP | CB-CG-OD2 | -6.29 | 112.64 | 118.30 |
| 1 | C | 140 | MSE | CA-CB-CG | -6.29 | 102.62 | 113.30 |
| 1 | B | 59 | ARG | NE-CZ-NH2 | -6.27 | 117.17 | 120.30 |
| 1 | D | 122 | THR | OG1-CB-CG2 | -6.25 | 95.62 | 110.00 |
| 1 | C | 199 | ARG | CB-CG-CD | 6.24 | 127.83 | 111.60 |
| 1 | A | 215 | ASP | CB-CG-OD1 | 6.23 | 123.91 | 118.30 |
| 1 | I | 104 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | F | 159 | LYS | CD-CE-NZ | 6.21 | 125.97 | 111.70 |
| 1 | E | 231 | ARG | NE-CZ-NH1 | -6.21 | 117.20 | 120.30 |
| 1 | A | 118 | ALA | O-C-N | -6.20 | 112.77 | 122.70 |
| 1 | D | 197 | ARG | NE-CZ-NH2 | -6.18 | 117.21 | 120.30 |
| 1 | J | 61 | TYR | CB-CG-CD1 | -6.18 | 117.29 | 121.00 |
| 1 | E | 191 | THR | OG1-CB-CG2 | 6.17 | 124.20 | 110.00 |
| 1 | D | 59 | ARG | CD-NE-CZ | -6.15 | 114.98 | 123.60 |
| 1 | C | 126 | ARG | CG-CD-NE | -6.15 | 98.89 | 111.80 |
| 1 | F | 74 | LEU | CA-CB-CG | 6.15 | 129.44 | 115.30 |
| 1 | E | 24 | ILE | CB-CG1-CD1 | -6.15 | 96.69 | 113.90 |
| 1 | J | 134 | ARG | NE-CZ-NH2 | -6.13 | 117.24 | 120.30 |
| 1 | J | 131 | VAL | CG1-CB-CG2 | -6.11 | 101.12 | 110.90 |
| 1 | B | 239 | LYS | CD-CE-NZ | -6.09 | 97.68 | 111.70 |
| 1 | B | 46 | PHE | CZ-CE2-CD2 | -6.09 | 112.79 | 120.10 |
| 1 | I | 6 | PRO | N-CA-C | -6.08 | 96.28 | 112.10 |
| 1 | J | 169 | ARG | NE-CZ-NH2 | -6.07 | 117.27 | 120.30 |
| 1 | E | 175 | TRP | CB-CA-C | -6.05 | 98.29 | 110.40 |
| 1 | I | 145 | MSE | CA-CB-CG | -6.05 | 103.01 | 113.30 |
| 1 | J | 231 | ARG | CG-CD-NE | -6.05 | 99.10 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 140 | MSE | CA-CB-CG | -6.04 | 103.02 | 113.30 |
| 1 | E | 145 | MSE | CB-CG-SE | -6.04 | 94.58 | 112.70 |
| 1 | J | 116 | LEU | CA-CB-CG | -6.04 | 101.42 | 115.30 |
| 1 | B | 91 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 1 | C | 74 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 1 | E | 134 | ARG | NE-CZ-NH2 | -6.03 | 117.29 | 120.30 |
| 1 | A | 59 | ARG | NH1-CZ-NH2 | 6.02 | 126.02 | 119.40 |
| 1 | F | 199 | ARG | NE-CZ-NH2 | 6.02 | 123.31 | 120.30 |
| 1 | A | 201 | GLU | C-N-CA | -6.00 | 106.71 | 121.70 |
| 1 | H | 47 | THR | N-CA-C | -6.00 | 94.81 | 111.00 |
| 1 | E | 158 | VAL | CG1-CB-CG2 | -5.97 | 101.34 | 110.90 |
| 1 | C | 105 | PRO | C-N-CA | -5.97 | 106.78 | 121.70 |
| 1 | D | 138 | ARG | NH1-CZ-NH2 | 5.96 | 125.96 | 119.40 |
| 1 | J | 122 | THR | OG1-CB-CG2 | -5.95 | 96.33 | 110.00 |
| 1 | B | 136 | VAL | CG1-CB-CG2 | -5.94 | 101.40 | 110.90 |
| 1 | C | 228 | ARG | CD-NE-CZ | 5.93 | 131.91 | 123.60 |
| 1 | G | 145 | MSE | CB-CG-SE | -5.92 | 94.93 | 112.70 |
| 1 | F | 39 | LEU | CD1-CG-CD2 | -5.92 | 92.75 | 110.50 |
| 1 | I | 183 | GLU | CG-CD-OE1 | -5.91 | 106.48 | 118.30 |
| 1 | I | 140 | MSE | CG-SE-CE | -5.91 | 85.90 | 98.90 |
| 1 | H | 112 | ARG | NE-CZ-NH1 | 5.91 | 123.25 | 120.30 |
| 1 | E | 206 | ARG | NE-CZ-NH1 | -5.89 | 117.35 | 120.30 |
| 1 | A | 11 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | J | 174 | ASP | CA-C-N | -5.87 | 104.29 | 117.20 |
| 1 | H | 215 | ASP | CB-CG-OD2 | 5.86 | 123.58 | 118.30 |
| 1 | D | 67 | LEU | CA-C-N | 5.85 | 127.91 | 116.20 |
| 1 | D | 141 | LEU | CB-CG-CD1 | -5.84 | 101.07 | 111.00 |
| 1 | D | 156 | ARG | NE-CZ-NH2 | -5.84 | 117.38 | 120.30 |
| 1 | E | 204 | GLN | CA-CB-CG | 5.84 | 126.24 | 113.40 |
| 1 | E | 175 | TRP | CA-C-O | -5.83 | 107.85 | 120.10 |
| 1 | C | 59 | ARG | NE-CZ-NH1 | -5.83 | 117.39 | 120.30 |
| 1 | F | 84 | LYS | CD-CE-NZ | -5.83 | 98.30 | 111.70 |
| 1 | F | 167 | LEU | CA-CB-CG | 5.82 | 128.70 | 115.30 |
| 1 | I | 134 | ARG | NE-CZ-NH1 | -5.82 | 117.39 | 120.30 |
| 1 | G | 28 | ASP | CB-CG-OD1 | 5.82 | 123.54 | 118.30 |
| 1 | D | 140 | MSE | CG-SE-CE | -5.82 | 86.10 | 98.90 |
| 1 | B | 209 | ASP | CB-CG-OD2 | 5.81 | 123.53 | 118.30 |
| 1 | F | 209 | ASP | CB-CG-OD2 | 5.81 | 123.53 | 118.30 |
| 1 | F | 207 | SER | N-CA-CB | -5.79 | 101.81 | 110.50 |
| 1 | D | 116 | LEU | CA-CB-CG | -5.77 | 102.02 | 115.30 |
| 1 | I | 159 | LYS | CD-CE-NZ | 5.77 | 124.97 | 111.70 |
| 1 | F | 70 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 238 | ALA | N-CA-C | -5.75 | 95.49 | 111.00 |
| 1 | J | 165 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | D | 4 | SER | N-CA-CB | -5.73 | 101.90 | 110.50 |
| 1 | B | 126 | ARG | CG-CD-NE | -5.73 | 99.77 | 111.80 |
| 1 | E | 222 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | E | 35 | LYS | CD-CE-NZ | 5.73 | 124.87 | 111.70 |
| 1 | D | 227 | ARG | NE-CZ-NH2 | -5.72 | 117.44 | 120.30 |
| 1 | C | 194 | ASP | CB-CG-OD1 | -5.72 | 113.15 | 118.30 |
| 1 | J | 81 | SER | CA-CB-OG | -5.72 | 95.76 | 111.20 |
| 1 | F | 194 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | J | 156 | ARG | NE-CZ-NH2 | -5.71 | 117.44 | 120.30 |
| 1 | G | 86 | LYS | CB-CG-CD | 5.71 | 126.43 | 111.60 |
| 1 | F | 161 | LEU | CD1-CG-CD2 | 5.69 | 127.58 | 110.50 |
| 1 | C | 119 | GLU | OE1-CD-OE2 | 5.69 | 130.12 | 123.30 |
| 1 | E | 45 | ASP | CB-CG-OD1 | 5.68 | 123.41 | 118.30 |
| 1 | I | 194 | ASP | CB-CG-OD1 | 5.68 | 123.42 | 118.30 |
| 1 | J | 231 | ARG | CD-NE-CZ | 5.68 | 131.55 | 123.60 |
| 1 | J | 229 | TYR | CB-CG-CD1 | -5.67 | 117.60 | 121.00 |
| 1 | B | 74 | LEU | CA-CB-CG | 5.67 | 128.34 | 115.30 |
| 1 | G | 197 | ARG | NE-CZ-NH1 | 5.67 | 123.14 | 120.30 |
| 1 | B | 228 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 1 | D | 91 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 1 | I | 118 | ALA | O-C-N | -5.67 | 113.63 | 122.70 |
| 1 | H | 116 | LEU | CA-CB-CG | -5.64 | 102.32 | 115.30 |
| 1 | C | 228 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | C | 39 | LEU | CD1-CG-CD2 | -5.63 | 93.61 | 110.50 |
| 1 | D | 147 | LEU | CA-CB-CG | 5.63 | 128.24 | 115.30 |
| 1 | F | 197 | ARG | NE-CZ-NH1 | 5.63 | 123.11 | 120.30 |
| 1 | G | 16 | GLU | N-CA-C | -5.61 | 95.85 | 111.00 |
| 1 | G | 169 | ARG | NE-CZ-NH2 | -5.61 | 117.50 | 120.30 |
| 1 | F | 35 | LYS | CD-CE-NZ | -5.60 | 98.82 | 111.70 |
| 1 | F | 185 | LEU | CA-CB-CG | -5.60 | 102.42 | 115.30 |
| 1 | J | 167 | LEU | CB-CG-CD2 | 5.60 | 120.52 | 111.00 |
| 1 | H | 194 | ASP | CB-CG-OD2 | -5.59 | 113.27 | 118.30 |
| 1 | D | 195 | GLN | CA-CB-CG | 5.59 | 125.69 | 113.40 |
| 1 | J | 2 | PRO | CA-CB-CG | -5.59 | 93.39 | 104.00 |
| 1 | J | 105 | PRO | N-CA-C | -5.59 | 97.57 | 112.10 |
| 1 | A | 206 | ARG | NE-CZ-NH1 | -5.58 | 117.51 | 120.30 |
| 1 | A | 32 | SER | CA-CB-OG | -5.58 | 96.13 | 111.20 |
| 1 | G | 140 | MSE | CA-CB-CG | -5.58 | 103.82 | 113.30 |
| 1 | E | 238 | ALA | C-N-CA | -5.57 | 107.77 | 121.70 |
| 1 | G | 24 | ILE | CB-CG1-CD1 | -5.57 | 98.30 | 113.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 35 | LYS | CD-CE-NZ | -5.57 | 98.90 | 111.70 |
| 1 | C | 222 | ASP | CB-CG-OD2 | 5.56 | 123.31 | 118.30 |
| 1 | H | 150 | LEU | N-CA-C | -5.55 | 96.01 | 111.00 |
| 1 | E | 134 | ARG | CG-CD-NE | -5.55 | 100.15 | 111.80 |
| 1 | J | 93 | ILE | CG1-CB-CG2 | -5.54 | 99.20 | 111.40 |
| 1 | A | 28 | ASP | CB-CG-OD2 | -5.54 | 113.32 | 118.30 |
| 1 | H | 46 | PHE | CB-CG-CD2 | -5.53 | 116.93 | 120.80 |
| 1 | C | 122 | THR | OG1-CB-CG2 | -5.52 | 97.30 | 110.00 |
| 1 | I | 149 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 1 | G | 238 | ALA | N-CA-C | -5.51 | 96.11 | 111.00 |
| 1 | F | 126 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |
| 1 | A | 213 | CYS | CA-CB-SG | -5.50 | 104.10 | 114.00 |
| 1 | J | 134 | ARG | CG-CD-NE | -5.50 | 100.26 | 111.80 |
| 1 | F | 102 | ILE | CG1-CB-CG2 | 5.49 | 123.48 | 111.40 |
| 1 | F | 6 | PRO | N-CA-C | -5.48 | 97.85 | 112.10 |
| 1 | D | 36 | TRP | CB-CA-C | -5.48 | 99.44 | 110.40 |
| 1 | I | 206 | ARG | NE-CZ-NH1 | -5.48 | 117.56 | 120.30 |
| 1 | J | 63 | ASP | CB-CG-OD1 | -5.48 | 113.37 | 118.30 |
| 1 | D | 174 | ASP | CB-CG-OD2 | 5.47 | 123.22 | 118.30 |
| 1 | J | 10 | GLU | CB-CA-C | -5.47 | 99.46 | 110.40 |
| 1 | H | 147 | LEU | CA-CB-CG | 5.47 | 127.87 | 115.30 |
| 1 | B | 15 | MSE | CA-CB-CG | -5.46 | 104.01 | 113.30 |
| 1 | F | 28 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 1 | C | 156 | ARG | NE-CZ-NH1 | -5.46 | 117.57 | 120.30 |
| 1 | B | 91 | ARG | NE-CZ-NH1 | 5.44 | 123.02 | 120.30 |
| 1 | B | 227 | ARG | CG-CD-NE | -5.43 | 100.39 | 111.80 |
| 1 | B | 207 | SER | CA-CB-OG | -5.43 | 96.53 | 111.20 |
| 1 | E | 145 | MSE | CG-SE-CE | 5.43 | 110.84 | 98.90 |
| 1 | B | 96 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | D | 150 | LEU | CB-CG-CD2 | -5.41 | 101.80 | 111.00 |
| 1 | C | 236 | LYS | CD-CE-NZ | -5.41 | 99.25 | 111.70 |
| 1 | F | 66 | ARG | CD-NE-CZ | 5.41 | 131.17 | 123.60 |
| 1 | F | 69 | VAL | CA-CB-CG2 | -5.41 | 102.79 | 110.90 |
| 1 | J | 241 | LEU | CB-CG-CD2 | -5.40 | 101.81 | 111.00 |
| 1 | E | 245 | ALA | CA-C-O | -5.40 | 108.75 | 120.10 |
| 1 | C | 206 | ARG | CG-CD-NE | -5.39 | 100.47 | 111.80 |
| 1 | A | 145 | MSE | CB-CA-C | 5.38 | 121.16 | 110.40 |
| 1 | J | 175 | TRP | C-N-CA | 5.37 | 144.56 | 122.00 |
| 1 | J | 20 | ASP | CB-CG-OD1 | 5.37 | 123.13 | 118.30 |
| 1 | J | 111 | ARG | NE-CZ-NH1 | -5.37 | 117.61 | 120.30 |
| 1 | C | 220 | ARG | CG-CD-NE | -5.37 | 100.53 | 111.80 |
| 1 | B | 11 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | D | 11 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 1 | I | 206 | ARG | NH1-CZ-NH2 | 5.36 | 125.30 | 119.40 |
| 1 | C | 11 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 1 | J | 227 | ARG | NE-CZ-NH1 | -5.36 | 117.62 | 120.30 |
| 1 | H | 149 | ARG | NE-CZ-NH2 | 5.35 | 122.98 | 120.30 |
| 1 | E | 57 | PHE | CB-CG-CD2 | -5.35 | 117.05 | 120.80 |
| 1 | E | 165 | ASP | CB-CG-OD1 | 5.35 | 123.11 | 118.30 |
| 1 | J | 106 | GLN | CA-CB-CG | 5.35 | 125.17 | 113.40 |
| 1 | B | 168 | LYS | CD-CE-NZ | -5.34 | 99.42 | 111.70 |
| 1 | C | 158 | VAL | CG1-CB-CG2 | -5.34 | 102.36 | 110.90 |
| 1 | E | 223 | VAL | CG1-CB-CG2 | 5.34 | 119.44 | 110.90 |
| 1 | A | 221 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | A | 140 | MSE | CG-SE-CE | 5.33 | 110.62 | 98.90 |
| 1 | F | 140 | MSE | CA-CB-CG | -5.32 | 104.25 | 113.30 |
| 1 | D | 134 | ARG | NE-CZ-NH1 | -5.32 | 117.64 | 120.30 |
| 1 | D | 165 | ASP | CB-CG-OD1 | 5.32 | 123.08 | 118.30 |
| 1 | G | 27 | PRO | N-CA-C | -5.32 | 98.28 | 112.10 |
| 1 | A | 231 | ARG | NH1-CZ-NH2 | -5.31 | 113.56 | 119.40 |
| 1 | F | 183 | GLU | CG-CD-OE1 | -5.30 | 107.69 | 118.30 |
| 1 | E | 2 | PRO | N-CA-C | 5.30 | 125.87 | 112.10 |
| 1 | H | 153 | GLU | OE1-CD-OE2 | -5.30 | 116.94 | 123.30 |
| 1 | J | 55 | VAL | CA-CB-CG2 | -5.28 | 102.98 | 110.90 |
| 1 | F | 10 | GLU | CG-CD-OE1 | 5.28 | 128.85 | 118.30 |
| 1 | J | 91 | ARG | NE-CZ-NH2 | 5.27 | 122.94 | 120.30 |
| 1 | C | 28 | ASP | CB-CG-OD2 | -5.27 | 113.56 | 118.30 |
| 1 | F | 206 | ARG | CG-CD-NE | -5.26 | 100.75 | 111.80 |
| 1 | G | 155 | LEU | CB-CG-CD2 | -5.26 | 102.06 | 111.00 |
| 1 | A | 220 | ARG | CG-CD-NE | 5.25 | 122.83 | 111.80 |
| 1 | B | 242 | TYR | CB-CG-CD1 | 5.25 | 124.15 | 121.00 |
| 1 | D | 16 | GLU | OE1-CD-OE2 | 5.24 | 129.59 | 123.30 |
| 1 | B | 176 | PRO | CA-N-CD | 5.23 | 119.02 | 111.70 |
| 1 | H | 126 | ARG | CG-CD-NE | -5.23 | 100.81 | 111.80 |
| 1 | C | 47 | THR | CB-CA-C | 5.22 | 125.71 | 111.60 |
| 1 | J | 84 | LYS | CD-CE-NZ | -5.22 | 99.68 | 111.70 |
| 1 | A | 47 | THR | N-CA-C | -5.22 | 96.90 | 111.00 |
| 1 | G | 27 | PRO | N-CD-CG | 5.22 | 111.03 | 103.20 |
| 1 | G | 195 | GLN | CA-CB-CG | 5.22 | 124.88 | 113.40 |
| 1 | I | 199 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | J | 7 | LEU | CB-CG-CD1 | -5.22 | 102.13 | 111.00 |
| 1 | B | 74 | LEU | CD1-CG-CD2 | -5.21 | 94.86 | 110.50 |
| 1 | A | 227 | ARG | NE-CZ-NH2 | -5.21 | 117.69 | 120.30 |
| 1 | B | 213 | CYS | CA-CB-SG | -5.20 | 104.64 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 132 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | D | 206 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | G | 150 | LEU | N-CA-C | -5.19 | 96.99 | 111.00 |
| 1 | A | 112 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 1 | J | 59 | ARG | NE-CZ-NH2 | 5.19 | 122.89 | 120.30 |
| 1 | F | 183 | GLU | CG-CD-OE2 | 5.18 | 128.67 | 118.30 |
| 1 | A | 155 | LEU | CA-CB-CG | -5.18 | 103.39 | 115.30 |
| 1 | I | 232 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | B | 150 | LEU | CB-CG-CD1 | -5.17 | 102.20 | 111.00 |
| 1 | I | 119 | GLU | N-CA-CB | 5.17 | 119.91 | 110.60 |
| 1 | I | 175 | TRP | C-N-CD | -5.17 | 109.23 | 120.60 |
| 1 | D | 6 | PRO | N-CA-C | -5.16 | 98.69 | 112.10 |
| 1 | G | 163 | LEU | CB-CG-CD1 | -5.16 | 102.24 | 111.00 |
| 1 | C | 60 | ARG | CD-NE-CZ | 5.15 | 130.81 | 123.60 |
| 1 | A | 138 | ARG | NE-CZ-NH1 | 5.15 | 122.87 | 120.30 |
| 1 | C | 112 | ARG | NH1-CZ-NH2 | -5.15 | 113.74 | 119.40 |
| 1 | F | 152 | ASP | CB-CG-OD2 | 5.15 | 122.93 | 118.30 |
| 1 | E | 60 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 1 | I | 32 | SER | CB-CA-C | -5.14 | 100.34 | 110.10 |
| 1 | C | 136 | VAL | CG1-CB-CG2 | -5.13 | 102.69 | 110.90 |
| 1 | D | 71 | LEU | CB-CG-CD2 | -5.12 | 102.30 | 111.00 |
| 1 | F | 2 | PRO | CA-N-CD | -5.12 | 104.33 | 111.50 |
| 1 | B | 174 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | C | 183 | GLU | OE1-CD-OE2 | 5.10 | 129.43 | 123.30 |
| 1 | F | 145 | MSE | CB-CG-SE | -5.10 | 97.41 | 112.70 |
| 1 | D | 145 | MSE | CB-CG-SE | -5.08 | 97.45 | 112.70 |
| 1 | F | 71 | LEU | CB-CG-CD2 | -5.08 | 102.36 | 111.00 |
| 1 | J | 61 | TYR | CB-CG-CD2 | 5.08 | 124.05 | 121.00 |
| 1 | J | 222 | ASP | CB-CG-OD2 | 5.08 | 122.87 | 118.30 |
| 1 | B | 104 | ASP | N-CA-CB | 5.08 | 119.74 | 110.60 |
| 1 | E | 61 | TYR | CB-CG-CD1 | 5.07 | 124.04 | 121.00 |
| 1 | C | 200 | MSE | CG-SE-CE | 5.06 | 110.04 | 98.90 |
| 1 | J | 26 | LEU | C-N-CA | 5.06 | 143.27 | 122.00 |
| 1 | A | 239 | LYS | CD-CE-NZ | -5.05 | 100.08 | 111.70 |
| 1 | C | 208 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 1 | G | 145 | MSE | CA-CB-CG | -5.04 | 104.72 | 113.30 |
| 1 | D | 67 | LEU | N-CA-C | -5.04 | 97.40 | 111.00 |
| 1 | F | 197 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 1 | I | 48 | PRO | N-CA-C | 5.03 | 125.19 | 112.10 |
| 1 | C | 199 | ARG | CD-NE-CZ | 5.03 | 130.64 | 123.60 |
| 1 | H | 2 | PRO | N-CA-CB | 5.03 | 109.33 | 103.30 |
| 1 | H | 193 | GLU | N-CA-CB | -5.03 | 101.55 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | F | 240 | LEU | CA-CB-CG | -5.03 | 103.74 | 115.30 |
| 1 | B | 149 | ARG | CG-CD-NE | -5.02 | 101.25 | 111.80 |
| 1 | G | 206 | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 1 | I | 38 | VAL | CG1-CB-CG2 | -5.02 | 102.87 | 110.90 |
| 1 | B | 87 | GLU | N-CA-CB | -5.01 | 101.58 | 110.60 |
| 1 | G | 235 | GLU | CA-CB-CG | 5.01 | 124.41 | 113.40 |
| 1 | J | 215 | ASP | CA-CB-CG | -5.00 | 102.39 | 113.40 |

There are no chirality outliers.

All (16) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 143 | TYR | Sidechain |
| 1 | A | 242 | TYR | Sidechain |
| 1 | B | 143 | TYR | Sidechain |
| 1 | D | 242 | TYR | Sidechain |
| 1 | D | 82 | HIS | Sidechain |
| 1 | E | 175 | TRP | Mainchain |
| 1 | G | 229 | TYR | Sidechain |
| 1 | G | 242 | TYR | Sidechain |
| 1 | G | 26 | LEU | Mainchain |
| 1 | H | 205 | TYR | Sidechain |
| 1 | I | 205 | TYR | Sidechain |
| 1 | I | 242 | TYR | Sidechain |
| 1 | J | 138 | ARG | Sidechain |
| 1 | J | 174 | ASP | Mainchain |
| 1 | J | 26 | LEU | Mainchain |
| 1 | J | 61 | TYR | Sidechain |

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 | 1973 | 0 | 1959 | 108 | 0 |
| 1 | B | 1973 | 0 | 1959 | 123 | 0 |
| 1 | C | 1973 | 0 | 1959 | 113 | 0 |
| 1 | D | 1973 | 0 | 1959 | 104 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | E | 1973 | 0 | 1959 | 138 | 0 |
| 1 | F | 1973 | 0 | 1959 | 128 | 0 |
| 1 | G | 1973 | 0 | 1959 | 98 | 0 |
| 1 | H | 1973 | 0 | 1959 | 99 | 0 |
| 1 | I | 1973 | 0 | 1959 | 135 | 0 |
| 1 | J | 1973 | 0 | 1959 | 119 | 0 |
| 2 | A | 56 | 0 | 84 | 55 | 0 |
| 2 | B | 56 | 0 | 84 | 46 | 0 |
| 2 | C | 64 | 0 | 96 | 68 | 0 |
| 2 | D | 40 | 0 | 60 | 33 | 0 |
| 2 | E | 68 | 0 | 101 | 57 | 0 |
| 2 | F | 48 | 0 | 72 | 43 | 0 |
| 2 | G | 36 | 0 | 54 | 36 | 0 |
| 2 | H | 36 | 0 | 54 | 37 | 1 |
| 2 | I | 44 | 0 | 66 | 56 | 0 |
| 2 | J | 64 | 0 | 96 | 79 | 0 |
| 3 | A | 140 | 0 | 0 | 9 | 0 |
| 3 | B | 120 | 0 | 0 | 9 | 0 |
| 3 | C | 136 | 0 | 0 | 3 | 1 |
| 3 | D | 132 | 0 | 0 | 9 | 0 |
| 3 | E | 133 | 0 | 0 | 7 | 0 |
| 3 | F | 115 | 0 | 0 | 9 | 0 |
| 3 | G | 98 | 0 | 0 | 4 | 0 |
| 3 | H | 94 | 0 | 0 | 3 | 0 |
| 3 | I | 106 | 0 | 0 | 9 | 0 |
| 3 | J | 115 | 0 | 0 | 6 | 0 |
| All | All | 21431 | 0 | 20357 | 1196 | 1 |

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 29.

All (1196) 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:I:102:ILE:CG1 | 1:I:102:ILE:CD1 | 1.76 | 1.60 |
| 1:E:145:MSE:CB | 1:E:145:MSE:CG | 1.81 | 1.58 |
| 1:D:145:MSE:CG | 1:D:145:MSE:CB | 1.77 | 1.56 |
| 1:H:145:MSE:CG | 1:H:145:MSE:CB | 1.82 | 1.56 |
| 1:F:168:LYS:CE | 1:F:168:LYS:NZ | 1.69 | 1.56 |
| 1:E:25:LYS:NZ | 1:E:25:LYS:CE | 1.67 | 1.56 |
| 1:C:145:MSE:CB | 1:C:145:MSE:CG | 1.78 | 1.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:121:ALA:CA | 1:E:121:ALA:CB | 1.76 | 1.56 |
| 1:A:225:GLU:CD | 1:A:225:GLU:CG | 1.75 | 1.54 |
| 1:G:162:LYS:NZ | 1:G:162:LYS:CE | 1.70 | 1.53 |
| 1:G:236:LYS:NZ | 1:G:236:LYS:CE | 1.68 | 1.51 |
| 1:I:145:MSE:CG | 1:I:145:MSE:CB | 1.89 | 1.50 |
| 1:H:237:PRO:CG | 1:H:237:PRO:CB | 1.77 | 1.49 |
| 1:A:145:MSE:CB | 1:A:145:MSE:CG | 1.88 | 1.48 |
| 2:A:2029:EDO:O2 | 2:A:2029:EDO:C2 | 1.63 | 1.46 |
| 2:J:2014:EDO:O1 | 2:J:2014:EDO:C1 | 1.64 | 1.46 |
| 2:E:2088:EDO:O1 | 2:E:2088:EDO:C1 | 1.64 | 1.46 |
| 2:D:2031:EDO:C2 | 2:D:2031:EDO:O2 | 1.64 | 1.46 |
| 2:J:2049:EDO:C2 | 2:J:2049:EDO:O2 | 1.64 | 1.45 |
| 2:A:2012:EDO:O1 | 2:A:2012:EDO:C1 | 1.63 | 1.45 |
| 2:B:2020:EDO:C1 | 2:B:2020:EDO:O1 | 1.64 | 1.45 |
| 2:J:2008:EDO:O2 | 2:J:2008:EDO:C2 | 1.63 | 1.45 |
| 2:J:2104:EDO:C1 | 2:J:2104:EDO:O1 | 1.63 | 1.44 |
| 2:A:2063:EDO:C1 | 2:A:2063:EDO:O1 | 1.64 | 1.44 |
| 1:F:15:MSE:SE | 1:F:15:MSE:CG | 2.15 | 1.44 |
| 2:J:2105:EDO:O2 | 2:J:2105:EDO:C2 | 1.63 | 1.44 |
| 2:G:2050:EDO:O2 | 2:G:2050:EDO:C2 | 1.66 | 1.44 |
| 2:J:2123:EDO:C1 | 2:J:2123:EDO:O1 | 1.64 | 1.44 |
| 2:G:2102:EDO:C2 | 2:G:2102:EDO:O2 | 1.65 | 1.44 |
| 1:E:145:MSE:SE | 1:E:145:MSE:CE | 2.15 | 1.43 |
| 2:C:2067:EDO:O2 | 2:C:2067:EDO:C2 | 1.65 | 1.43 |
| 2:C:2128:EDO:C2 | 2:C:2128:EDO:O2 | 1.65 | 1.43 |
| 2:J:2068:EDO:O2 | 2:J:2068:EDO:C2 | 1.64 | 1.43 |
| 2:B:2021:EDO:O1 | 2:B:2021:EDO:C1 | 1.65 | 1.43 |
| 2:E:2120:EDO:O1 | 2:E:2120:EDO:C1 | 1.64 | 1.43 |
| 2:C:2024:EDO:O2 | 2:C:2024:EDO:C2 | 1.65 | 1.43 |
| 2:H:2058:EDO:O2 | 2:H:2058:EDO:C2 | 1.64 | 1.43 |
| 2:E:2032:EDO:O2 | 2:E:2032:EDO:C2 | 1.66 | 1.42 |
| 2:I:2115:EDO:C2 | 2:I:2115:EDO:O2 | 1.67 | 1.42 |
| 2:D:2118:EDO:O2 | 2:D:2118:EDO:C2 | 1.66 | 1.42 |
| 2:F:2006:EDO:O1 | 2:F:2006:EDO:C1 | 1.68 | 1.41 |
| 2:B:2002:EDO:C2 | 2:B:2002:EDO:O2 | 1.69 | 1.41 |
| 2:B:2023:EDO:C2 | 2:B:2023:EDO:O2 | 1.67 | 1.41 |
| 2:J:2053:EDO:O2 | 2:J:2053:EDO:C2 | 1.63 | 1.41 |
| 2:G:2056:EDO:O2 | 2:G:2056:EDO:C2 | 1.65 | 1.41 |
| 2:F:2043:EDO:C2 | 2:F:2043:EDO:O2 | 1.65 | 1.41 |
| 2:G:2093:EDO:O2 | 2:G:2093:EDO:C2 | 1.64 | 1.41 |
| 2:C:2004:EDO:C1 | 2:C:2004:EDO:O1 | 1.67 | 1.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:MSE:CE | 1:A:145:MSE:SE | 2.19 | 1.40 |
| 2:J:2104:EDO:C2 | 2:J:2104:EDO:O2 | 1.66 | 1.40 |
| 2:A:2124:EDO:C1 | 2:A:2124:EDO:O1 | 1.69 | 1.40 |
| 1:I:140:MSE:CG | 1:I:140:MSE:SE | 2.18 | 1.40 |
| 2:C:2085:EDO:C2 | 2:C:2085:EDO:O2 | 1.66 | 1.40 |
| 1:J:237:PRO:CB | 1:J:237:PRO:CG | 1.74 | 1.40 |
| 2:E:2089:EDO:C2 | 2:E:2089:EDO:O2 | 1.68 | 1.40 |
| 2:H:2010:EDO:C2 | 2:H:2010:EDO:O2 | 1.70 | 1.40 |
| 2:C:2126:EDO:O2 | 2:C:2126:EDO:C2 | 1.65 | 1.40 |
| 2:B:2021:EDO:O2 | 2:B:2021:EDO:C2 | 1.68 | 1.40 |
| 2:G:2009:EDO:O1 | 2:G:2009:EDO:C1 | 1.67 | 1.40 |
| 2:D:2074:EDO:C1 | 2:D:2074:EDO:O1 | 1.70 | 1.40 |
| 1:B:140:MSE:SE | 1:B:140:MSE:CG | 2.19 | 1.40 |
| 1:H:145:MSE:CE | 1:H:145:MSE:SE | 2.17 | 1.39 |
| 2:C:2082:EDO:O2 | 2:C:2082:EDO:C2 | 1.68 | 1.39 |
| 2:A:2012:EDO:O2 | 2:A:2012:EDO:C2 | 1.70 | 1.39 |
| 2:A:2124:EDO:C2 | 2:A:2124:EDO:O2 | 1.69 | 1.39 |
| 2:A:2122:EDO:C2 | 2:A:2122:EDO:O2 | 1.69 | 1.38 |
| 2:F:2098:EDO:O2 | 2:F:2098:EDO:C2 | 1.72 | 1.38 |
| 1:G:145:MSE:CE | 1:G:145:MSE:SE | 2.19 | 1.38 |
| 2:I:2007:EDO:C1 | 2:I:2007:EDO:O1 | 1.68 | 1.38 |
| 1:C:145:MSE:SE | 1:C:145:MSE:CE | 2.20 | 1.38 |
| 2:B:2002:EDO:O1 | 2:B:2002:EDO:C1 | 1.71 | 1.38 |
| 2:C:2085:EDO:C1 | 2:C:2085:EDO:O1 | 1.68 | 1.38 |
| 1:B:162:LYS:CE | 1:B:162:LYS:NZ | 1.84 | 1.38 |
| 2:H:2059:EDO:C2 | 2:H:2059:EDO:O2 | 1.71 | 1.37 |
| 2:C:2004:EDO:O2 | 2:C:2004:EDO:C2 | 1.73 | 1.36 |
| 2:E:2005:EDO:O2 | 2:E:2005:EDO:C2 | 1.75 | 1.34 |
| 2:J:2008:EDO:O1 | 2:J:2008:EDO:C1 | 1.80 | 1.30 |
| 1:I:228:ARG:HD2 | 2:I:2107:EDO:C2 | 1.65 | 1.26 |
| 1:E:214:TRP:HH2 | 1:F:242:TYR:CD1 | 1.56 | 1.23 |
| 1:I:228:ARG:CD | 2:I:2107:EDO:H22 | 1.69 | 1.22 |
| 1:B:220:ARG:HG3 | 1:B:224:GLU:OE2 | 1.32 | 1.22 |
| 1:F:145:MSE:HE3 | 2:F:2086:EDO:O2 | 1.40 | 1.21 |
| 1:J:199:ARG:HH21 | 2:J:2104:EDO:H22 | 1.10 | 1.14 |
| 1:E:241:LEU:HD23 | 1:E:244:GLU:OE1 | 1.45 | 1.14 |
| 1:F:14:GLU:HG2 | 1:F:25:LYS:NZ | 1.62 | 1.12 |
| 2:C:2075:EDO:H11 | 2:E:2127:EDO:H22 | 1.17 | 1.12 |
| 1:C:129:PHE:CE2 | 1:C:140:MSE:HE3 | 1.84 | 1.12 |
| 1:J:215:ASP:HB3 | 1:J:217:PRO:HD3 | 1.17 | 1.11 |
| 1:B:205:TYR:H | 2:B:2030:EDO:H22 | 1.01 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:205:TYR:H | 2:D:2035:EDO:H22 | 1.02 | 1.10 |
| 1:E:129:PHE:CE2 | 1:E:140:MSE:HE3 | 1.86 | 1.10 |
| 1:C:48:PRO:HD2 | 2:C:2024:EDO:H11 | 1.28 | 1.09 |
| 1:C:108:THR:HG22 | 2:C:2117:EDO:H22 | 1.34 | 1.09 |
| 1:G:105:PRO:O | 1:G:106:GLN:HB2 | 1.47 | 1.09 |
| 1:A:118:ALA:O | 1:A:119:GLU:HB2 | 1.44 | 1.09 |
| 2:C:2075:EDO:C1 | 2:E:2127:EDO:H22 | 1.83 | 1.06 |
| 1:E:236:LYS:HZ1 | 2:F:2043:EDO:H22 | 1.16 | 1.06 |
| 1:G:49:VAL:H | 2:G:2056:EDO:H12 | 1.19 | 1.06 |
| 1:C:108:THR:CG2 | 2:C:2117:EDO:H22 | 1.85 | 1.05 |
| 1:C:59:ARG:HB3 | 2:C:2128:EDO:H21 | 1.06 | 1.05 |
| 1:J:97:ILE:H | 2:J:2109:EDO:H12 | 1.21 | 1.05 |
| 2:F:2095:EDO:H22 | 3:F:553:HOH:O | 1.55 | 1.05 |
| 1:D:145:MSE:HE3 | 2:D:2118:EDO:H21 | 1.09 | 1.04 |
| 1:E:199:ARG:HE | 2:E:2091:EDO:H12 | 1.21 | 1.04 |
| 1:E:214:TRP:CH2 | 1:F:242:TYR:CD1 | 2.45 | 1.03 |
| 1:I:228:ARG:NE | 2:I:2107:EDO:H11 | 1.75 | 1.01 |
| 1:J:105:PRO:O | 1:J:106:GLN:CB | 2.07 | 1.01 |
| 1:I:134:ARG:NH1 | 3:I:2137:HOH:O | 1.91 | 1.01 |
| 1:J:105:PRO:O | 1:J:106:GLN:HB2 | 1.19 | 1.01 |
| 2:I:2121:EDO:H21 | 3:I:2181:HOH:O | 1.61 | 1.00 |
| 1:D:205:TYR:N | 2:D:2035:EDO:H22 | 1.77 | 1.00 |
| 1:J:162:LYS:HE3 | 3:J:2146:HOH:O | 1.62 | 1.00 |
| 1:B:111:ARG:HH22 | 1:C:111:ARG:HH22 | 1.08 | 1.00 |
| 1:A:235:GLU:HB3 | 2:A:2001:EDO:H21 | 1.38 | 0.99 |
| 1:B:205:TYR:N | 2:B:2030:EDO:H22 | 1.76 | 0.99 |
| 1:B:49:VAL:H | 2:B:2028:EDO:C1 | 1.74 | 0.99 |
| 1:J:97:ILE:N | 2:J:2109:EDO:H12 | 1.77 | 0.98 |
| 1:A:145:MSE:CB | 1:A:145:MSE:SE | 2.61 | 0.98 |
| 1:D:235:GLU:HB3 | 2:D:2003:EDO:H11 | 1.44 | 0.98 |
| 1:I:108:THR:HG22 | 2:I:2046:EDO:H22 | 1.44 | 0.97 |
| 1:J:86:LYS:HB3 | 2:J:2109:EDO:H21 | 1.44 | 0.97 |
| 1:B:65:GLN:HG2 | 3:B:2233:HOH:O | 1.65 | 0.97 |
| 1:C:183:GLU:HG2 | 2:C:2085:EDO:H12 | 1.43 | 0.97 |
| 1:G:183:GLU:HG2 | 2:G:2057:EDO:O2 | 1.64 | 0.97 |
| 1:D:47:THR:HG23 | 3:D:2211:HOH:O | 1.65 | 0.97 |
| 1:A:48:PRO:HD2 | 2:A:2012:EDO:H22 | 1.48 | 0.96 |
| 1:J:199:ARG:HE | 2:J:2104:EDO:H12 | 1.27 | 0.96 |
| 1:I:228:ARG:HD2 | 2:I:2107:EDO:H22 | 0.98 | 0.96 |
| 1:I:150:LEU:HD12 | 1:J:174:ASP:HB3 | 1.47 | 0.96 |
| 1:B:220:ARG:CG | 1:B:224:GLU:OE2 | 2.14 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:59:ARG:HH11 | 1:H:59:ARG:HG3 | 1.28 | 0.95 |
| 1:C:117:HIS:HD2 | 1:D:8:ILE:H | 1.14 | 0.95 |
| 3:B:2191:HOH:O | 1:D:200:MSE:HG3 | 1.65 | 0.95 |
| 1:F:14:GLU:HG2 | 1:F:25:LYS:HZ1 | 1.19 | 0.95 |
| 1:B:48:PRO:HD2 | 2:B:2028:EDO:H21 | 1.48 | 0.94 |
| 1:C:183:GLU:H | 2:C:2085:EDO:H11 | 1.32 | 0.94 |
| 1:G:169:ARG:O | 2:G:2112:EDO:H11 | 1.66 | 0.94 |
| 1:G:8:ILE:H | 1:H:117:HIS:HD2 | 0.94 | 0.94 |
| 1:J:97:ILE:H | 2:J:2109:EDO:C1 | 1.81 | 0.94 |
| 1:G:8:ILE:H | 1:H:117:HIS:CD2 | 1.85 | 0.94 |
| 1:I:117:HIS:HD2 | 1:J:8:ILE:H | 1.16 | 0.94 |
| 1:E:236:LYS:NZ | 2:F:2043:EDO:H22 | 1.84 | 0.93 |
| 1:B:105:PRO:O | 1:B:106:GLN:HB2 | 1.69 | 0.93 |
| 1:D:239:LYS:HE3 | 1:D:244:GLU:OE2 | 1.69 | 0.93 |
| 1:A:145:MSE:CE | 1:A:145:MSE:HB3 | 2.00 | 0.92 |
| 1:I:118:ALA:O | 1:I:119:GLU:HB2 | 1.69 | 0.92 |
| 1:E:214:TRP:HH2 | 1:F:242:TYR:CE1 | 1.87 | 0.92 |
| 1:B:49:VAL:H | 2:B:2028:EDO:H11 | 1.33 | 0.92 |
| 1:E:8:ILE:H | 1:F:117:HIS:HD2 | 1.16 | 0.92 |
| 1:I:59:ARG:CG | 1:I:59:ARG:HH11 | 1.82 | 0.92 |
| 2:C:2075:EDO:H11 | 2:E:2127:EDO:C2 | 1.98 | 0.91 |
| 1:D:69:VAL:HG21 | 1:D:158:VAL:HG11 | 1.51 | 0.91 |
| 1:B:150:LEU:HD22 | 3:B:2151:HOH:O | 1.71 | 0.91 |
| 1:E:225:GLU:HG3 | 1:E:228:ARG:HH21 | 1.36 | 0.90 |
| 1:E:145:MSE:SE | 1:E:145:MSE:CB | 2.69 | 0.90 |
| 1:D:145:MSE:HE3 | 2:D:2118:EDO:C2 | 2.01 | 0.90 |
| 1:E:59:ARG:HB3 | 2:E:2040:EDO:H11 | 1.50 | 0.90 |
| 1:C:59:ARG:HB3 | 2:C:2128:EDO:C2 | 2.00 | 0.89 |
| 1:C:228:ARG:HD3 | 3:C:2171:HOH:O | 1.71 | 0.89 |
| 1:E:2:PRO:HB2 | 1:F:10:GLU:OE2 | 1.71 | 0.89 |
| 1:I:145:MSE:SE | 1:I:145:MSE:CB | 2.71 | 0.89 |
| 1:I:62:GLU:HB2 | 3:I:2223:HOH:O | 1.71 | 0.89 |
| 1:F:129:PHE:CE2 | 1:F:140:MSE:HE3 | 2.07 | 0.89 |
| 1:F:145:MSE:CE | 2:F:2086:EDO:O2 | 2.20 | 0.89 |
| 1:A:145:MSE:CE | 1:A:145:MSE:CB | 2.50 | 0.88 |
| 1:J:16:GLU:O | 2:J:2123:EDO:H21 | 1.73 | 0.88 |
| 1:E:117:HIS:HD2 | 1:F:8:ILE:H | 1.18 | 0.88 |
| 1:E:225:GLU:HG3 | 1:E:228:ARG:NH2 | 1.89 | 0.88 |
| 1:I:59:ARG:HG3 | 1:I:59:ARG:HH11 | 1.38 | 0.88 |
| 1:G:105:PRO:O | 1:G:106:GLN:CB | 2.20 | 0.88 |
| 1:D:145:MSE:CE | 2:D:2118:EDO:H21 | 2.00 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:97:ILE:HG12 | 2:J:2109:EDO:H11 | 1.53 | 0.87 |
| 1:I:8:ILE:HG22 | 1:J:119:GLU:HG3 | 1.55 | 0.87 |
| 2:A:2029:EDO:C2 | 2:B:2125:EDO:H11 | 2.03 | 0.87 |
| 1:C:48:PRO:CD | 2:C:2024:EDO:H11 | 2.04 | 0.86 |
| 1:E:239:LYS:HE2 | 1:E:244:GLU:HG2 | 1.56 | 0.86 |
| 1:D:190:PRO:HA | 1:D:195:GLN:HE21 | 1.37 | 0.86 |
| 1:C:8:ILE:H | 1:D:117:HIS:HD2 | 1.21 | 0.86 |
| 1:I:66:ARG:HB3 | 1:I:66:ARG:NH1 | 1.91 | 0.86 |
| 1:B:49:VAL:HB | 2:B:2028:EDO:H12 | 1.55 | 0.86 |
| 1:D:145:MSE:SE | 1:D:145:MSE:CB | 2.73 | 0.86 |
| 1:J:206:ARG:HA | 2:J:2106:EDO:H22 | 1.55 | 0.85 |
| 1:E:25:LYS:CD | 1:E:25:LYS:NZ | 2.39 | 0.85 |
| 1:A:8:ILE:H | 1:B:117:HIS:HD2 | 1.21 | 0.85 |
| 1:E:241:LEU:HA | 1:E:244:GLU:OE1 | 1.74 | 0.85 |
| 1:I:8:ILE:H | 1:J:117:HIS:HD2 | 1.25 | 0.85 |
| 1:I:129:PHE:CE2 | 1:I:140:MSE:HE3 | 2.11 | 0.85 |
| 1:J:96:ARG:HG3 | 2:J:2109:EDO:O2 | 1.75 | 0.85 |
| 1:H:14:GLU:HG2 | 1:H:25:LYS:HZ1 | 1.40 | 0.85 |
| 1:G:21:HIS:ND1 | 2:G:2093:EDO:H11 | 1.91 | 0.85 |
| 1:B:106:GLN:HE22 | 1:C:107:GLY:HA3 | 1.42 | 0.84 |
| 1:H:145:MSE:SE | 1:H:145:MSE:CB | 2.75 | 0.84 |
| 1:A:49:VAL:H | 2:A:2012:EDO:H21 | 1.42 | 0.84 |
| 1:D:191:THR:H | 1:D:195:GLN:NE2 | 1.76 | 0.84 |
| 2:A:2029:EDO:H21 | 2:B:2125:EDO:H11 | 1.58 | 0.84 |
| 1:C:197:ARG:HH22 | 1:E:96:ARG:HH21 | 1.26 | 0.84 |
| 1:J:207:SER:H | 2:J:2106:EDO:H12 | 1.43 | 0.83 |
| 1:A:193:GLU:OE1 | 3:A:2222:HOH:O | 1.95 | 0.83 |
| 1:C:129:PHE:HE2 | 1:C:140:MSE:HE3 | 1.43 | 0.83 |
| 1:I:205:TYR:H | 2:I:2051:EDO:H22 | 1.42 | 0.83 |
| 1:D:129:PHE:CE2 | 1:D:140:MSE:HE3 | 2.13 | 0.83 |
| 1:I:5:ILE:HD13 | 1:J:5:ILE:HD13 | 1.59 | 0.83 |
| 1:B:42:HIS:CE1 | 1:B:75:SER:HB3 | 2.14 | 0.83 |
| 1:C:197:ARG:HH22 | 1:E:96:ARG:NH2 | 1.77 | 0.83 |
| 1:F:105:PRO:O | 1:F:106:GLN:HB2 | 1.79 | 0.83 |
| 1:H:55:VAL:O | 1:H:59:ARG:HG2 | 1.77 | 0.83 |
| 1:H:105:PRO:O | 1:H:106:GLN:HB2 | 1.78 | 0.83 |
| 1:B:244:GLU:OE1 | 1:B:244:GLU:N | 2.12 | 0.83 |
| 1:A:122:THR:HG23 | 1:A:123:HIS:CD2 | 2.13 | 0.83 |
| 1:D:205:TYR:H | 2:D:2035:EDO:C2 | 1.89 | 0.82 |
| 1:G:69:VAL:HG21 | 1:G:158:VAL:HG11 | 1.61 | 0.82 |
| 1:G:48:PRO:HD2 | 2:G:2056:EDO:H11 | 1.60 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:112:ARG:HD3 | 2:I:2046:EDO:H11 | 1.62 | 0.82 |
| 1:J:228:ARG:NH2 | 2:J:2049:EDO:H22 | 1.94 | 0.82 |
| 1:C:193:GLU:OE1 | 2:E:2127:EDO:H21 | 1.79 | 0.82 |
| 1:C:8:ILE:HG22 | 1:D:119:GLU:HG3 | 1.62 | 0.82 |
| 1:I:228:ARG:CD | 2:I:2107:EDO:C2 | 2.43 | 0.81 |
| 1:H:145:MSE:CG | 1:H:145:MSE:CA | 2.57 | 0.81 |
| 1:G:183:GLU:N | 2:G:2057:EDO:O2 | 2.12 | 0.81 |
| 1:F:90:GLU:HG3 | 3:F:572:HOH:O | 1.80 | 0.80 |
| 1:G:8:ILE:N | 1:H:117:HIS:HD2 | 1.77 | 0.80 |
| 1:A:239:LYS:CE | 1:A:244:GLU:HG2 | 2.10 | 0.80 |
| 1:I:36:TRP:NE1 | 1:I:162:LYS:NZ | 2.29 | 0.80 |
| 1:J:199:ARG:NH2 | 2:J:2104:EDO:H22 | 1.92 | 0.80 |
| 1:A:167:LEU:O | 2:A:2124:EDO:H22 | 1.81 | 0.80 |
| 2:I:2121:EDO:C2 | 3:I:2181:HOH:O | 2.24 | 0.80 |
| 1:B:205:TYR:H | 2:B:2030:EDO:C2 | 1.88 | 0.80 |
| 1:C:117:HIS:CD2 | 1:D:8:ILE:H | 1.99 | 0.80 |
| 1:B:92:HIS:NE2 | 2:B:2125:EDO:H12 | 1.97 | 0.80 |
| 1:C:59:ARG:CB | 2:C:2128:EDO:H21 | 2.02 | 0.80 |
| 1:A:242:TYR:CD1 | 1:B:214:TRP:HH2 | 2.00 | 0.80 |
| 1:C:47:THR:HG23 | 2:C:2024:EDO:O1 | 1.82 | 0.80 |
| 1:A:117:HIS:HD2 | 1:B:8:ILE:H | 1.26 | 0.79 |
| 1:H:70:ASP:HB3 | 2:H:2113:EDO:H12 | 1.63 | 0.79 |
| 1:A:235:GLU:HB3 | 2:A:2001:EDO:C2 | 2.12 | 0.79 |
| 1:A:218:ALA:O | 2:A:2063:EDO:H12 | 1.83 | 0.79 |
| 1:C:197:ARG:HD3 | 2:C:2075:EDO:O1 | 1.82 | 0.79 |
| 1:E:122:THR:HG21 | 3:E:938:HOH:O | 1.81 | 0.79 |
| 1:H:14:GLU:HG2 | 1:H:25:LYS:NZ | 1.98 | 0.79 |
| 1:C:122:THR:HG23 | 1:C:123:HIS:CD2 | 2.17 | 0.79 |
| 1:D:235:GLU:O | 2:D:2003:EDO:C1 | 2.31 | 0.79 |
| 1:G:179:GLU:HG2 | 1:H:59:ARG:HH12 | 1.46 | 0.79 |
| 1:G:96:ARG:HH11 | 1:G:96:ARG:HG3 | 1.48 | 0.79 |
| 1:A:47:THR:HG23 | 2:A:2012:EDO:O2 | 1.83 | 0.79 |
| 1:H:183:GLU:HG2 | 2:H:2058:EDO:H12 | 1.63 | 0.78 |
| 2:E:2120:EDO:H22 | 1:F:88:TRP:HE1 | 1.49 | 0.78 |
| 1:I:225:GLU:HG3 | 1:I:228:ARG:HH11 | 1.47 | 0.78 |
| 1:F:145:MSE:HE3 | 2:F:2086:EDO:HO2 | 1.48 | 0.78 |
| 1:I:188:PRO:O | 1:I:199:ARG:NH2 | 2.16 | 0.78 |
| 1:D:235:GLU:O | 2:D:2003:EDO:H12 | 1.84 | 0.78 |
| 1:D:112:ARG:HH11 | 1:D:112:ARG:CG | 1.96 | 0.78 |
| 2:I:2099:EDO:H12 | 1:J:191:THR:CG2 | 2.14 | 0.77 |
| 1:E:8:ILE:H | 1:F:117:HIS:CD2 | 2.01 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:7:LEU:HA | 1:J:140:MSE:HE1 | 1.67 | 0.77 |
| 1:E:169:ARG:HH12 | 2:E:2089:EDO:H22 | 1.48 | 0.77 |
| 1:B:111:ARG:NH2 | 1:C:111:ARG:HH22 | 1.81 | 0.77 |
| 2:H:2058:EDO:C1 | 2:H:2058:EDO:O2 | 2.31 | 0.77 |
| 1:I:140:MSE:CG | 1:I:140:MSE:CE | 2.63 | 0.77 |
| 1:A:5:ILE:HD13 | 1:B:5:ILE:HD13 | 1.65 | 0.77 |
| 1:B:49:VAL:N | 2:B:2028:EDO:H11 | 2.00 | 0.77 |
| 1:C:193:GLU:OE2 | 3:C:2223:HOH:O | 2.02 | 0.77 |
| 1:I:203:GLY:CA | 2:I:2051:EDO:H21 | 2.15 | 0.77 |
| 1:H:70:ASP:CB | 2:H:2113:EDO:H12 | 2.13 | 0.77 |
| 1:E:203:GLY:HA2 | 2:E:2042:EDO:O2 | 1.85 | 0.77 |
| 1:F:112:ARG:HB3 | 1:F:112:ARG:HH11 | 1.48 | 0.77 |
| 1:F:112:ARG:NH1 | 1:F:112:ARG:HB3 | 2.01 | 0.76 |
| 1:C:145:MSE:CB | 1:C:145:MSE:SE | 2.83 | 0.76 |
| 1:B:49:VAL:CB | 2:B:2028:EDO:H12 | 2.15 | 0.76 |
| 1:E:117:HIS:CD2 | 1:F:8:ILE:H | 2.02 | 0.76 |
| 1:D:203:GLY:HA2 | 2:D:2035:EDO:H11 | 1.67 | 0.76 |
| 1:E:214:TRP:CH2 | 1:F:242:TYR:CE1 | 2.71 | 0.76 |
| 1:H:106:GLN:O | 1:H:111:ARG:NH2 | 2.19 | 0.76 |
| 3:A:2228:HOH:O | 1:J:122:THR:HG21 | 1.85 | 0.76 |
| 1:I:117:HIS:CD2 | 1:J:8:ILE:H | 2.03 | 0.76 |
| 1:I:200:MSE:HE2 | 1:I:200:MSE:HA | 1.68 | 0.76 |
| 1:I:118:ALA:O | 1:I:119:GLU:CB | 2.24 | 0.76 |
| 1:D:145:MSE:CA | 1:D:145:MSE:CG | 2.64 | 0.76 |
| 1:A:216:THR:HB | 2:A:2063:EDO:H11 | 1.69 | 0.75 |
| 1:I:140:MSE:HB3 | 1:I:140:MSE:HE2 | 1.67 | 0.75 |
| 1:C:129:PHE:CE2 | 1:C:140:MSE:CE | 2.66 | 0.75 |
| 1:I:102:ILE:CD1 | 1:I:102:ILE:CB | 2.64 | 0.75 |
| 1:B:106:GLN:O | 1:B:111:ARG:NH2 | 2.19 | 0.75 |
| 1:D:15:MSE:CE | 1:D:112:ARG:HD3 | 2.17 | 0.75 |
| 1:I:108:THR:CG2 | 2:I:2046:EDO:H22 | 2.15 | 0.74 |
| 1:A:122:THR:HG23 | 1:A:123:HIS:HD2 | 1.52 | 0.74 |
| 1:I:10:GLU:OE2 | 1:J:2:PRO:HB2 | 1.87 | 0.74 |
| 1:G:236:LYS:HE3 | 3:G:1166:HOH:O | 1.86 | 0.74 |
| 2:C:2085:EDO:C1 | 2:C:2085:EDO:O2 | 2.34 | 0.74 |
| 1:G:49:VAL:H | 2:G:2056:EDO:C1 | 1.98 | 0.74 |
| 2:F:2043:EDO:O2 | 2:F:2043:EDO:C1 | 2.36 | 0.74 |
| 1:I:228:ARG:NE | 2:I:2107:EDO:C1 | 2.51 | 0.74 |
| 1:D:200:MSE:HA | 1:D:200:MSE:HE2 | 1.70 | 0.74 |
| 1:A:145:MSE:CA | 1:A:145:MSE:CG | 2.65 | 0.74 |
| 1:B:49:VAL:N | 2:B:2028:EDO:C1 | 2.50 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:145:MSE:CG | 1:E:145:MSE:CA | 2.66 | 0.73 |
| 1:I:181:ILE:O | 2:I:2103:EDO:H21 | 1.88 | 0.73 |
| 1:A:163:LEU:HD22 | 1:A:167:LEU:HD22 | 1.70 | 0.73 |
| 1:I:66:ARG:CG | 1:I:66:ARG:HH11 | 2.01 | 0.73 |
| 1:J:97:ILE:H | 2:J:2109:EDO:C2 | 2.01 | 0.73 |
| 1:B:239:LYS:HE2 | 1:B:244:GLU:CD | 2.08 | 0.73 |
| 1:I:145:MSE:CG | 1:I:145:MSE:CA | 2.67 | 0.73 |
| 1:F:222:ASP:OD2 | 2:F:2097:EDO:H22 | 1.88 | 0.73 |
| 1:I:228:ARG:HE | 2:I:2107:EDO:H11 | 1.52 | 0.73 |
| 1:C:108:THR:HG21 | 2:C:2117:EDO:H22 | 1.70 | 0.73 |
| 1:A:118:ALA:O | 1:A:119:GLU:CB | 2.18 | 0.72 |
| 1:B:122:THR:HG23 | 1:B:123:HIS:CD2 | 2.24 | 0.72 |
| 1:I:192:THR:OG1 | 2:I:2115:EDO:H11 | 1.88 | 0.72 |
| 1:A:11:ARG:NH1 | 1:A:14:GLU:OE2 | 2.22 | 0.72 |
| 1:D:111:ARG:HH22 | 1:E:111:ARG:HH22 | 1.38 | 0.72 |
| 1:E:17:VAL:HA | 2:E:2078:EDO:H21 | 1.71 | 0.72 |
| 1:I:36:TRP:CD1 | 1:I:162:LYS:NZ | 2.58 | 0.72 |
| 1:F:107:GLY:HA3 | 1:G:106:GLN:HE22 | 1.55 | 0.71 |
| 1:I:228:ARG:HD2 | 2:I:2107:EDO:H21 | 1.69 | 0.71 |
| 1:B:49:VAL:H | 2:B:2028:EDO:H12 | 1.53 | 0.71 |
| 1:F:74:LEU:HD23 | 1:F:102:ILE:HB | 1.73 | 0.71 |
| 1:C:145:MSE:CA | 1:C:145:MSE:CG | 2.66 | 0.71 |
| 1:A:145:MSE:HB3 | 1:A:145:MSE:HE3 | 1.70 | 0.71 |
| 1:G:48:PRO:CD | 2:G:2056:EDO:H11 | 2.20 | 0.71 |
| 1:J:199:ARG:HH21 | 2:J:2104:EDO:C2 | 1.97 | 0.71 |
| 1:F:14:GLU:CG | 1:F:25:LYS:NZ | 2.48 | 0.71 |
| 1:C:67:LEU:O | 1:C:162:LYS:HE2 | 1.90 | 0.71 |
| 1:J:21:HIS:ND1 | 2:J:2068:EDO:H21 | 2.06 | 0.71 |
| 1:H:18:THR:H | 2:H:2044:EDO:C2 | 2.04 | 0.71 |
| 1:J:199:ARG:HE | 2:J:2104:EDO:C1 | 2.04 | 0.71 |
| 1:J:228:ARG:HH21 | 2:J:2049:EDO:H22 | 1.53 | 0.70 |
| 1:J:199:ARG:NE | 2:J:2104:EDO:H12 | 2.04 | 0.70 |
| 1:I:140:MSE:CB | 1:I:140:MSE:SE | 2.90 | 0.70 |
| 1:J:215:ASP:HB3 | 1:J:217:PRO:CD | 2.10 | 0.70 |
| 1:B:239:LYS:HE2 | 1:B:244:GLU:OE2 | 1.90 | 0.70 |
| 1:C:91:ARG:HD2 | 2:C:2126:EDO:O1 | 1.91 | 0.70 |
| 1:G:49:VAL:N | 2:G:2056:EDO:H12 | 2.02 | 0.70 |
| 1:I:49:VAL:H | 2:I:2121:EDO:HO2 | 1.39 | 0.70 |
| 1:A:203:GLY:HA2 | 2:A:2065:EDO:O2 | 1.92 | 0.70 |
| 1:G:235:GLU:HB2 | 2:G:2009:EDO:H11 | 1.72 | 0.70 |
| 1:B:140:MSE:HE3 | 1:B:142:TYR:OH | 1.92 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:232:ARG:O | 2:I:2007:EDO:O1 | 2.10 | 0.70 |
| 1:J:215:ASP:CB | 1:J:217:PRO:HD3 | 2.10 | 0.70 |
| 1:G:96:ARG:NH1 | 1:G:96:ARG:HG3 | 2.03 | 0.70 |
| 1:I:200:MSE:HE1 | 1:I:213:CYS:SG | 2.31 | 0.70 |
| 2:C:2075:EDO:C1 | 2:E:2127:EDO:C2 | 2.65 | 0.69 |
| 1:I:8:ILE:H | 1:J:117:HIS:CD2 | 2.09 | 0.69 |
| 1:I:183:GLU:H | 2:I:2103:EDO:C2 | 2.05 | 0.69 |
| 1:E:206:ARG:HA | 2:E:2090:EDO:H22 | 1.72 | 0.69 |
| 3:C:2186:HOH:O | 1:D:231:ARG:HD3 | 1.91 | 0.69 |
| 1:J:203:GLY:HA2 | 2:J:2055:EDO:O2 | 1.92 | 0.69 |
| 1:E:199:ARG:HH21 | 2:E:2091:EDO:H22 | 1.55 | 0.69 |
| 1:C:8:ILE:H | 1:D:117:HIS:CD2 | 2.08 | 0.69 |
| 1:A:106:GLN:O | 1:A:111:ARG:NH2 | 2.25 | 0.69 |
| 1:F:111:ARG:NH2 | 1:G:106:GLN:HE21 | 1.91 | 0.69 |
| 1:F:24:ILE:HD11 | 1:F:26:LEU:HD21 | 1.75 | 0.69 |
| 1:C:59:ARG:HD3 | 2:C:2128:EDO:H22 | 1.75 | 0.69 |
| 1:H:183:GLU:H | 2:H:2058:EDO:C1 | 2.05 | 0.69 |
| 1:H:70:ASP:CG | 2:H:2113:EDO:H12 | 2.13 | 0.69 |
| 2:A:2124:EDO:O2 | 3:A:2197:HOH:O | 2.06 | 0.69 |
| 1:A:232:ARG:O | 2:A:2001:EDO:H22 | 1.92 | 0.69 |
| 1:D:112:ARG:HH11 | 1:D:112:ARG:HG2 | 1.56 | 0.69 |
| 1:D:228:ARG:HG3 | 2:D:2072:EDO:H11 | 1.75 | 0.69 |
| 1:E:5:ILE:HD13 | 1:F:5:ILE:HD13 | 1.74 | 0.69 |
| 1:C:183:GLU:HG2 | 2:C:2085:EDO:C1 | 2.20 | 0.69 |
| 2:A:2029:EDO:H21 | 2:B:2125:EDO:C1 | 2.23 | 0.68 |
| 1:H:105:PRO:O | 1:H:106:GLN:CB | 2.39 | 0.68 |
| 1:J:21:HIS:ND1 | 2:J:2068:EDO:C2 | 2.57 | 0.68 |
| 1:A:63:ASP:OD2 | 1:A:228:ARG:NH2 | 2.26 | 0.68 |
| 2:G:2057:EDO:H12 | 1:H:240:LEU:HD11 | 1.76 | 0.68 |
| 1:I:112:ARG:HD3 | 2:I:2046:EDO:C1 | 2.23 | 0.68 |
| 1:I:66:ARG:HH11 | 1:I:66:ARG:CB | 2.05 | 0.68 |
| 1:H:122:THR:HG23 | 1:H:123:HIS:CD2 | 2.29 | 0.68 |
| 1:A:21:HIS:ND1 | 2:A:2011:EDO:H22 | 2.07 | 0.67 |
| 1:B:232:ARG:HG3 | 2:B:2002:EDO:H11 | 1.76 | 0.67 |
| 2:I:2099:EDO:H12 | 1:J:191:THR:HG21 | 1.74 | 0.67 |
| 1:B:91:ARG:NH2 | 2:B:2125:EDO:O2 | 2.28 | 0.67 |
| 1:E:10:GLU:OE2 | 1:F:2:PRO:HB2 | 1.94 | 0.67 |
| 1:H:232:ARG:HG3 | 2:H:2010:EDO:H22 | 1.77 | 0.67 |
| 1:E:122:THR:HG23 | 1:E:123:HIS:CD2 | 2.29 | 0.67 |
| 1:A:231:ARG:HG2 | 2:A:2017:EDO:H22 | 1.76 | 0.67 |
| 1:E:199:ARG:HE | 2:E:2091:EDO:C1 | 2.05 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:224:GLU:OE1 | 1:C:231:ARG:NH2 | 2.28 | 0.67 |
| 2:J:2104:EDO:O1 | 2:J:2104:EDO:O2 | 2.12 | 0.67 |
| 1:D:43:PRO:HB2 | 2:D:2118:EDO:H22 | 1.75 | 0.66 |
| 1:F:168:LYS:CD | 1:F:168:LYS:NZ | 2.58 | 0.66 |
| 1:E:207:SER:H | 2:E:2090:EDO:H22 | 1.61 | 0.66 |
| 1:H:190:PRO:HG2 | 1:H:210:TRP:HE3 | 1.61 | 0.66 |
| 1:G:145:MSE:HE2 | 3:G:1000:HOH:O | 1.95 | 0.66 |
| 1:I:105:PRO:O | 1:I:106:GLN:HB2 | 1.96 | 0.66 |
| 1:B:140:MSE:SE | 1:B:140:MSE:CB | 2.92 | 0.66 |
| 1:E:199:ARG:NE | 2:E:2091:EDO:H12 | 2.04 | 0.66 |
| 1:A:239:LYS:HD3 | 1:A:244:GLU:CG | 2.26 | 0.66 |
| 1:D:47:THR:CG2 | 3:D:2211:HOH:O | 2.33 | 0.66 |
| 1:G:200:MSE:HG3 | 2:G:2050:EDO:O2 | 1.96 | 0.66 |
| 1:B:242:TYR:CE2 | 1:B:243:GLU:HG3 | 2.29 | 0.66 |
| 1:E:67:LEU:O | 1:E:162:LYS:HE3 | 1.95 | 0.66 |
| 2:J:2104:EDO:C1 | 2:J:2104:EDO:HO1 | 2.07 | 0.66 |
| 2:J:2104:EDO:C1 | 2:J:2104:EDO:O2 | 2.42 | 0.66 |
| 1:G:239:LYS:NZ | 1:G:244:GLU:HG2 | 2.11 | 0.66 |
| 1:J:16:GLU:C | 2:J:2123:EDO:H21 | 2.16 | 0.65 |
| 1:H:183:GLU:H | 2:H:2058:EDO:H11 | 1.61 | 0.65 |
| 1:I:43:PRO:HG3 | 1:I:145:MSE:HG2 | 1.77 | 0.65 |
| 2:H:2058:EDO:HO2 | 2:H:2058:EDO:C2 | 2.08 | 0.65 |
| 1:A:8:ILE:H | 1:B:117:HIS:CD2 | 2.11 | 0.65 |
| 2:J:2104:EDO:O1 | 2:J:2104:EDO:C2 | 2.44 | 0.65 |
| 1:F:183:GLU:HG2 | 2:F:2043:EDO:C1 | 2.26 | 0.65 |
| 1:E:129:PHE:HE2 | 1:E:140:MSE:HE3 | 1.52 | 0.65 |
| 1:A:239:LYS:HE2 | 1:A:244:GLU:HG2 | 1.77 | 0.65 |
| 2:B:2020:EDO:C1 | 2:B:2020:EDO:HO1 | 2.07 | 0.65 |
| 1:C:91:ARG:HH11 | 2:C:2126:EDO:H12 | 1.61 | 0.65 |
| 1:A:8:ILE:HG13 | 1:A:140:MSE:HE2 | 1.77 | 0.65 |
| 1:F:222:ASP:OD2 | 2:F:2097:EDO:C2 | 2.44 | 0.65 |
| 1:G:113:LEU:HB3 | 1:G:129:PHE:CZ | 2.30 | 0.65 |
| 2:E:2092:EDO:O1 | 1:G:87:GLU:OE1 | 2.15 | 0.65 |
| 1:J:232:ARG:O | 2:J:2008:EDO:O1 | 2.15 | 0.65 |
| 1:F:105:PRO:O | 1:F:106:GLN:CB | 2.44 | 0.65 |
| 1:A:235:GLU:CB | 2:A:2001:EDO:H21 | 2.19 | 0.65 |
| 1:B:48:PRO:HD2 | 2:B:2028:EDO:C2 | 2.27 | 0.65 |
| 1:J:205:TYR:O | 2:J:2055:EDO:H12 | 1.95 | 0.65 |
| 1:J:104:ASP:HB2 | 3:J:2130:HOH:O | 1.97 | 0.65 |
| 1:A:20:ASP:OD2 | 1:A:86:LYS:NZ | 2.28 | 0.65 |
| 1:B:35:LYS:HE3 | 3:B:2231:HOH:O | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:48:PRO:CD | 2:A:2012:EDO:H22 | 2.25 | 0.64 |
| 1:A:232:ARG:O | 2:A:2001:EDO:C2 | 2.45 | 0.64 |
| 1:J:42:HIS:CE1 | 1:J:75:SER:HB3 | 2.33 | 0.64 |
| 1:F:15:MSE:CB | 1:F:15:MSE:SE | 2.93 | 0.64 |
| 1:J:97:ILE:HG12 | 2:J:2109:EDO:C1 | 2.27 | 0.64 |
| 2:J:2008:EDO:C2 | 2:J:2008:EDO:HO2 | 2.07 | 0.64 |
| 1:E:42:HIS:CE1 | 1:E:75:SER:HB3 | 2.32 | 0.64 |
| 1:F:221:ASP:OD2 | 3:F:543:HOH:O | 2.15 | 0.64 |
| 1:C:112:ARG:HH11 | 1:C:112:ARG:CB | 2.10 | 0.64 |
| 2:A:2029:EDO:O2 | 2:B:2125:EDO:H11 | 1.97 | 0.64 |
| 2:G:2102:EDO:C2 | 2:G:2102:EDO:HO2 | 2.09 | 0.64 |
| 2:B:2021:EDO:HO1 | 2:B:2021:EDO:C1 | 2.08 | 0.64 |
| 1:I:126:ARG:HH22 | 2:I:2121:EDO:H11 | 1.62 | 0.64 |
| 1:D:77:ASP:OD2 | 3:D:2244:HOH:O | 2.14 | 0.64 |
| 1:H:87:GLU:OE2 | 2:H:2054:EDO:H22 | 1.97 | 0.64 |
| 1:B:105:PRO:O | 1:B:106:GLN:CB | 2.44 | 0.64 |
| 1:H:159:LYS:NZ | 1:H:225:GLU:OE2 | 2.30 | 0.64 |
| 2:E:2088:EDO:C1 | 2:E:2088:EDO:HO1 | 2.07 | 0.64 |
| 2:J:2068:EDO:HO2 | 2:J:2068:EDO:C2 | 2.08 | 0.64 |
| 1:B:43:PRO:HG3 | 1:B:145:MSE:HG2 | 1.80 | 0.64 |
| 1:H:182:GLY:HA3 | 2:H:2058:EDO:H11 | 1.80 | 0.64 |
| 2:G:2093:EDO:C1 | 2:G:2093:EDO:O2 | 2.42 | 0.64 |
| 1:A:145:MSE:HE2 | 1:A:145:MSE:CB | 2.27 | 0.63 |
| 2:A:2029:EDO:HO2 | 2:A:2029:EDO:C2 | 2.07 | 0.63 |
| 1:C:183:GLU:N | 2:C:2085:EDO:H11 | 2.10 | 0.63 |
| 1:A:239:LYS:HD3 | 1:A:244:GLU:HG2 | 1.80 | 0.63 |
| 1:G:35:LYS:HD2 | 1:G:70:ASP:OD2 | 1.97 | 0.63 |
| 2:J:2008:EDO:C1 | 2:J:2008:EDO:O2 | 2.46 | 0.63 |
| 1:I:17:VAL:HA | 2:I:2100:EDO:H12 | 1.80 | 0.63 |
| 1:D:105:PRO:HG2 | 1:E:122:THR:OG1 | 1.98 | 0.63 |
| 2:E:2120:EDO:H22 | 1:F:88:TRP:NE1 | 2.13 | 0.63 |
| 1:I:228:ARG:CZ | 2:I:2107:EDO:H11 | 2.27 | 0.63 |
| 1:I:66:ARG:HH11 | 1:I:66:ARG:HB3 | 1.61 | 0.63 |
| 1:I:59:ARG:HH12 | 1:J:179:GLU:CD | 2.02 | 0.63 |
| 1:I:66:ARG:CB | 1:I:66:ARG:NH1 | 2.62 | 0.63 |
| 1:E:176:PRO:HD2 | 1:E:177:ASN:N | 2.13 | 0.63 |
| 2:E:2120:EDO:C2 | 1:F:88:TRP:HE1 | 2.10 | 0.63 |
| 1:J:5:ILE:HG22 | 1:J:114:GLY:HA3 | 1.80 | 0.63 |
| 1:I:66:ARG:HH11 | 1:I:66:ARG:HG2 | 1.63 | 0.63 |
| 2:E:2120:EDO:HO1 | 2:E:2120:EDO:C1 | 2.07 | 0.63 |
| 1:A:200:MSE:CE | 2:A:2065:EDO:H11 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:16:GLU:O | 2:J:2123:EDO:C2 | 2.46 | 0.63 |
| 1:G:150:LEU:HD22 | 3:H:785:HOH:O | 1.97 | 0.63 |
| 1:C:183:GLU:H | 2:C:2085:EDO:C1 | 2.09 | 0.62 |
| 1:G:239:LYS:CE | 1:G:244:GLU:HG2 | 2.29 | 0.62 |
| 1:D:91:ARG:NH1 | 3:D:2175:HOH:O | 2.32 | 0.62 |
| 1:F:104:ASP:HB3 | 2:F:2087:EDO:H22 | 1.81 | 0.62 |
| 1:J:244:GLU:O | 1:J:244:GLU:CD | 2.37 | 0.62 |
| 1:B:207:SER:HB2 | 2:B:2030:EDO:H12 | 1.80 | 0.62 |
| 1:F:39:LEU:HD13 | 1:F:72:ILE:HG23 | 1.81 | 0.62 |
| 1:F:123:HIS:CD2 | 2:F:2086:EDO:C2 | 2.82 | 0.62 |
| 1:A:200:MSE:HE2 | 1:A:200:MSE:HA | 1.80 | 0.62 |
| 1:F:200:MSE:HE1 | 1:F:213:CYS:SG | 2.39 | 0.62 |
| 1:H:38:VAL:HB | 1:H:71:LEU:HD23 | 1.82 | 0.62 |
| 1:I:48:PRO:HD2 | 2:I:2121:EDO:O2 | 2.00 | 0.62 |
| 1:B:239:LYS:HG2 | 1:B:243:GLU:OE1 | 1.99 | 0.62 |
| 1:A:239:LYS:CD | 1:A:244:GLU:HG2 | 2.30 | 0.62 |
| 2:C:2024:EDO:C2 | 2:C:2024:EDO:HO2 | 2.09 | 0.62 |
| 1:D:204:GLN:N | 2:D:2035:EDO:C2 | 2.63 | 0.62 |
| 1:B:243:GLU:HB2 | 1:B:244:GLU:OE1 | 2.00 | 0.62 |
| 2:G:2093:EDO:HO2 | 2:G:2093:EDO:C2 | 2.08 | 0.62 |
| 1:I:49:VAL:N | 2:I:2121:EDO:O2 | 2.26 | 0.62 |
| 1:E:176:PRO:HD2 | 1:E:177:ASN:H | 1.65 | 0.62 |
| 1:I:191:THR:H | 1:I:195:GLN:NE2 | 1.97 | 0.62 |
| 2:J:2053:EDO:HO2 | 2:J:2053:EDO:C2 | 2.07 | 0.62 |
| 1:D:204:GLN:N | 2:D:2035:EDO:H21 | 2.15 | 0.61 |
| 2:D:2031:EDO:C2 | 2:D:2031:EDO:HO2 | 2.08 | 0.61 |
| 1:I:228:ARG:NE | 2:I:2107:EDO:C2 | 2.62 | 0.61 |
| 2:A:2022:EDO:C2 | 1:B:236:LYS:HZ1 | 2.12 | 0.61 |
| 1:D:42:HIS:CE1 | 1:D:75:SER:HB3 | 2.35 | 0.61 |
| 1:F:200:MSE:HE2 | 1:F:200:MSE:HA | 1.81 | 0.61 |
| 1:I:140:MSE:CB | 1:I:140:MSE:HE2 | 2.30 | 0.61 |
| 1:G:6:PRO:HG2 | 1:G:129:PHE:HE2 | 1.65 | 0.61 |
| 1:G:7:LEU:HA | 1:G:140:MSE:HE1 | 1.83 | 0.61 |
| 2:A:2012:EDO:HO1 | 2:A:2012:EDO:C1 | 2.07 | 0.61 |
| 1:F:111:ARG:HH21 | 1:G:106:GLN:HE21 | 1.47 | 0.61 |
| 1:H:18:THR:H | 2:H:2044:EDO:H21 | 1.64 | 0.61 |
| 1:I:99:PHE:HB2 | 1:I:100:PRO:HD2 | 1.82 | 0.61 |
| 1:G:183:GLU:H | 2:G:2057:EDO:HO2 | 1.46 | 0.61 |
| 1:J:32:SER:HA | 2:J:2108:EDO:H21 | 1.82 | 0.61 |
| 3:I:2182:HOH:O | 1:J:138:ARG:HD2 | 2.00 | 0.61 |
| 1:B:140:MSE:CE | 1:B:142:TYR:OH | 2.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:59:ARG:CG | 1:H:59:ARG:HH11 | 2.08 | 0.61 |
| 1:I:59:ARG:HG3 | 1:I:59:ARG:NH1 | 2.13 | 0.61 |
| 1:E:121:ALA:CB | 1:E:121:ALA:C | 2.66 | 0.61 |
| 1:J:200:MSE:HE1 | 1:J:213:CYS:SG | 2.40 | 0.61 |
| 1:E:104:ASP:OD2 | 1:E:104:ASP:N | 2.31 | 0.61 |
| 1:G:67:LEU:O | 1:G:162:LYS:HE3 | 2.01 | 0.60 |
| 1:B:203:GLY:CA | 2:B:2030:EDO:H21 | 2.31 | 0.60 |
| 1:F:200:MSE:CE | 2:F:2034:EDO:H21 | 2.30 | 0.60 |
| 1:D:62:GLU:HG2 | 1:D:66:ARG:NH1 | 2.16 | 0.60 |
| 1:A:216:THR:O | 2:A:2063:EDO:H11 | 2.01 | 0.60 |
| 2:G:2056:EDO:C2 | 2:G:2056:EDO:HO2 | 2.09 | 0.60 |
| 1:I:225:GLU:CG | 1:I:228:ARG:HH11 | 2.13 | 0.60 |
| 1:D:111:ARG:NH2 | 1:E:111:ARG:HH22 | 1.98 | 0.60 |
| 1:I:50:CYS:SG | 2:I:2121:EDO:O1 | 2.57 | 0.60 |
| 1:C:191:THR:H | 1:C:195:GLN:NE2 | 2.00 | 0.60 |
| 1:E:39:LEU:HD13 | 1:E:72:ILE:HG23 | 1.84 | 0.60 |
| 1:A:200:MSE:HE1 | 2:A:2065:EDO:H11 | 1.84 | 0.60 |
| 2:I:2115:EDO:C2 | 2:I:2115:EDO:HO2 | 2.10 | 0.60 |
| 1:H:145:MSE:CE | 1:H:145:MSE:CB | 2.79 | 0.60 |
| 2:C:2004:EDO:C1 | 2:C:2004:EDO:HO1 | 2.10 | 0.60 |
| 1:D:235:GLU:HA | 2:D:2119:EDO:H12 | 1.82 | 0.60 |
| 1:I:182:GLY:HA3 | 2:I:2103:EDO:H21 | 1.84 | 0.60 |
| 1:A:47:THR:CG2 | 2:A:2012:EDO:O2 | 2.50 | 0.59 |
| 1:H:69:VAL:HG21 | 1:H:158:VAL:HG11 | 1.83 | 0.59 |
| 1:B:197:ARG:O | 1:B:201:GLU:HG2 | 2.02 | 0.59 |
| 1:C:43:PRO:HG3 | 1:C:145:MSE:HG2 | 1.84 | 0.59 |
| 1:E:236:LYS:HE2 | 3:E:536:HOH:O | 2.00 | 0.59 |
| 1:H:106:GLN:O | 1:H:111:ARG:CZ | 2.49 | 0.59 |
| 1:H:17:VAL:HA | 2:H:2044:EDO:H21 | 1.85 | 0.59 |
| 1:G:74:LEU:HD23 | 1:G:102:ILE:HB | 1.83 | 0.59 |
| 1:F:14:GLU:HG2 | 1:F:25:LYS:HZ3 | 1.60 | 0.59 |
| 1:I:48:PRO:CD | 2:I:2121:EDO:O2 | 2.50 | 0.59 |
| 1:D:107:GLY:HA3 | 1:E:106:GLN:HE22 | 1.68 | 0.59 |
| 1:B:190:PRO:HB3 | 1:B:195:GLN:HB3 | 1.84 | 0.59 |
| 1:F:183:GLU:H | 2:F:2043:EDO:H11 | 1.68 | 0.59 |
| 2:A:2063:EDO:C1 | 2:A:2063:EDO:HO1 | 2.07 | 0.59 |
| 1:C:59:ARG:HD3 | 2:C:2128:EDO:C2 | 2.33 | 0.59 |
| 2:I:2099:EDO:H12 | 1:J:191:THR:HG22 | 1.84 | 0.59 |
| 1:C:200:MSE:HA | 1:C:200:MSE:HE2 | 1.84 | 0.59 |
| 2:C:2128:EDO:C2 | 2:C:2128:EDO:HO2 | 2.08 | 0.59 |
| 1:B:205:TYR:O | 2:B:2030:EDO:H11 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:222:ASP:OD2 | 2:J:2110:EDO:O1 | 2.18 | 0.59 |
| 2:C:2067:EDO:HO2 | 2:C:2067:EDO:C2 | 2.09 | 0.59 |
| 2:F:2006:EDO:HO1 | 2:F:2006:EDO:C1 | 2.11 | 0.59 |
| 1:C:112:ARG:HB3 | 1:C:112:ARG:HH11 | 1.67 | 0.59 |
| 1:A:228:ARG:HH22 | 1:A:232:ARG:HH12 | 1.49 | 0.59 |
| 1:I:203:GLY:HA2 | 2:I:2051:EDO:H21 | 1.85 | 0.59 |
| 2:E:2032:EDO:HO2 | 2:E:2032:EDO:C2 | 2.10 | 0.59 |
| 1:H:18:THR:HB | 2:H:2044:EDO:O2 | 2.03 | 0.59 |
| 1:C:5:ILE:HG23 | 1:C:6:PRO:O | 2.03 | 0.59 |
| 1:B:49:VAL:N | 2:B:2028:EDO:H12 | 2.16 | 0.58 |
| 1:A:145:MSE:HE2 | 1:A:145:MSE:HB2 | 1.85 | 0.58 |
| 1:A:44:ALA:O | 1:A:47:THR:HB | 2.03 | 0.58 |
| 1:J:106:GLN:O | 1:J:111:ARG:NH2 | 2.37 | 0.58 |
| 1:C:179:GLU:CD | 1:D:59:ARG:NH1 | 2.57 | 0.58 |
| 1:A:228:ARG:HH22 | 1:A:232:ARG:NH1 | 2.02 | 0.58 |
| 1:B:35:LYS:CE | 3:B:2231:HOH:O | 2.51 | 0.58 |
| 1:J:35:LYS:HD3 | 1:J:70:ASP:OD2 | 2.03 | 0.58 |
| 1:D:106:GLN:O | 1:D:111:ARG:NH2 | 2.36 | 0.58 |
| 1:E:176:PRO:CD | 1:E:177:ASN:N | 2.63 | 0.58 |
| 1:D:68:GLY:H | 1:D:162:LYS:HE3 | 1.67 | 0.58 |
| 2:H:2059:EDO:H22 | 3:H:1074:HOH:O | 2.04 | 0.58 |
| 1:B:35:LYS:HD3 | 1:B:70:ASP:OD2 | 2.03 | 0.58 |
| 1:I:48:PRO:HG2 | 1:J:186:ILE:HG21 | 1.86 | 0.57 |
| 1:H:190:PRO:HG2 | 1:H:210:TRP:CE3 | 2.39 | 0.57 |
| 1:E:92:HIS:NE2 | 2:E:2076:EDO:H21 | 2.18 | 0.57 |
| 2:J:2049:EDO:O2 | 2:J:2049:EDO:C1 | 2.47 | 0.57 |
| 3:B:2225:HOH:O | 1:C:122:THR:HG21 | 2.03 | 0.57 |
| 1:F:105:PRO:HG2 | 1:G:122:THR:HB | 1.87 | 0.57 |
| 1:B:106:GLN:NE2 | 1:C:107:GLY:HA3 | 2.17 | 0.57 |
| 1:B:163:LEU:O | 1:B:167:LEU:HB2 | 2.04 | 0.57 |
| 1:C:193:GLU:OE1 | 2:E:2127:EDO:C2 | 2.52 | 0.57 |
| 1:G:162:LYS:CD | 1:G:162:LYS:NZ | 2.65 | 0.57 |
| 1:E:232:ARG:O | 2:E:2005:EDO:O2 | 2.23 | 0.57 |
| 1:E:176:PRO:CD | 1:E:177:ASN:H | 2.15 | 0.57 |
| 1:G:124:THR:HG23 | 1:G:125:VAL:O | 2.03 | 0.57 |
| 1:B:205:TYR:O | 2:B:2030:EDO:C1 | 2.52 | 0.57 |
| 2:C:2085:EDO:C2 | 2:C:2085:EDO:HO2 | 2.10 | 0.57 |
| 1:D:106:GLN:O | 1:D:111:ARG:CZ | 2.53 | 0.57 |
| 1:C:49:VAL:H | 2:C:2024:EDO:H12 | 1.70 | 0.57 |
| 1:E:238:ALA:O | 1:E:239:LYS:CB | 2.50 | 0.57 |
| 1:I:126:ARG:NH2 | 2:I:2121:EDO:H11 | 2.19 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:198:ALA:O | 1:A:202:SER:HB3 | 2.05 | 0.57 |
| 1:E:5:ILE:HG22 | 1:E:114:GLY:HA3 | 1.87 | 0.57 |
| 1:H:191:THR:H | 1:H:195:GLN:NE2 | 2.02 | 0.57 |
| 1:H:200:MSE:CE | 2:H:2060:EDO:H22 | 2.34 | 0.57 |
| 1:B:203:GLY:C | 2:B:2030:EDO:H21 | 2.25 | 0.56 |
| 1:J:97:ILE:CG1 | 2:J:2109:EDO:H11 | 2.32 | 0.56 |
| 1:C:5:ILE:HG12 | 1:C:142:TYR:OH | 2.05 | 0.56 |
| 1:E:132:ASP:CG | 2:E:2039:EDO:H12 | 2.25 | 0.56 |
| 2:J:2049:EDO:C2 | 2:J:2049:EDO:HO2 | 2.08 | 0.56 |
| 1:A:243:GLU:CD | 3:A:2163:HOH:O | 2.42 | 0.56 |
| 1:I:50:CYS:HG | 2:I:2121:EDO:HO1 | 1.49 | 0.56 |
| 1:E:105:PRO:O | 1:E:106:GLN:HB2 | 2.05 | 0.56 |
| 1:E:105:PRO:O | 1:E:106:GLN:CB | 2.52 | 0.56 |
| 1:F:104:ASP:HB2 | 3:F:467:HOH:O | 2.03 | 0.56 |
| 1:C:104:ASP:N | 1:C:105:PRO:HD3 | 2.20 | 0.56 |
| 1:H:126:ARG:HB3 | 1:H:149:ARG:CZ | 2.35 | 0.56 |
| 1:A:171:VAL:HB | 1:B:147:LEU:HD23 | 1.88 | 0.56 |
| 2:J:2104:EDO:HO2 | 2:J:2104:EDO:C2 | 2.10 | 0.56 |
| 1:C:235:GLU:OE1 | 2:C:2080:EDO:H21 | 2.04 | 0.56 |
| 1:E:169:ARG:HH12 | 2:E:2089:EDO:C2 | 2.17 | 0.56 |
| 1:E:235:GLU:O | 2:E:2005:EDO:O2 | 2.17 | 0.56 |
| 2:J:2014:EDO:HO1 | 2:J:2014:EDO:C1 | 2.07 | 0.56 |
| 1:A:218:ALA:O | 2:A:2063:EDO:C1 | 2.51 | 0.56 |
| 2:B:2002:EDO:C2 | 2:B:2002:EDO:HO2 | 2.12 | 0.56 |
| 1:D:47:THR:HG22 | 1:D:50:CYS:SG | 2.45 | 0.56 |
| 1:J:87:GLU:HB3 | 2:J:2014:EDO:H11 | 1.88 | 0.56 |
| 2:C:2085:EDO:HO1 | 2:C:2085:EDO:C1 | 2.11 | 0.56 |
| 1:I:200:MSE:CE | 1:I:200:MSE:HA | 2.36 | 0.56 |
| 1:G:39:LEU:HD23 | 1:G:39:LEU:C | 2.26 | 0.56 |
| 2:J:2105:EDO:HO2 | 2:J:2105:EDO:C2 | 2.07 | 0.55 |
| 2:E:2005:EDO:H21 | 1:F:179:GLU:OE2 | 2.05 | 0.55 |
| 1:J:90:GLU:OE2 | 1:J:96:ARG:HG3 | 2.06 | 0.55 |
| 1:I:132:ASP:CG | 2:I:2045:EDO:H21 | 2.26 | 0.55 |
| 1:F:84:LYS:HD2 | 1:F:87:GLU:OE1 | 2.06 | 0.55 |
| 1:C:44:ALA:O | 1:C:47:THR:HB | 2.06 | 0.55 |
| 1:I:39:LEU:HD12 | 1:I:40:PHE:N | 2.21 | 0.55 |
| 2:E:2079:EDO:H22 | 3:E:337:HOH:O | 2.07 | 0.55 |
| 2:A:2122:EDO:C2 | 2:A:2122:EDO:HO2 | 2.13 | 0.55 |
| 1:D:232:ARG:N | 2:D:2072:EDO:H22 | 2.20 | 0.55 |
| 1:B:134:ARG:HG3 | 2:B:2025:EDO:H22 | 1.87 | 0.55 |
| 1:F:104:ASP:OD2 | 1:F:104:ASP:N | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:70:ASP:OD1 | 2:H:2113:EDO:H12 | 2.07 | 0.55 |
| 1:J:228:ARG:CZ | 2:J:2049:EDO:H22 | 2.36 | 0.55 |
| 2:A:2122:EDO:O1 | 2:A:2122:EDO:O2 | 2.21 | 0.55 |
| 1:C:49:VAL:H | 2:C:2024:EDO:C1 | 2.20 | 0.54 |
| 1:E:200:MSE:HE3 | 1:E:210:TRP:HA | 1.89 | 0.54 |
| 2:A:2022:EDO:C2 | 1:B:236:LYS:NZ | 2.71 | 0.54 |
| 1:F:204:GLN:NE2 | 3:F:1120:HOH:O | 2.40 | 0.54 |
| 1:G:203:GLY:HA2 | 2:G:2047:EDO:O2 | 2.07 | 0.54 |
| 1:J:197:ARG:O | 1:J:201:GLU:HG3 | 2.07 | 0.54 |
| 1:F:42:HIS:CE1 | 1:F:75:SER:HB3 | 2.43 | 0.54 |
| 1:E:119:GLU:HG3 | 1:F:8:ILE:HG22 | 1.89 | 0.54 |
| 1:I:59:ARG:NH1 | 1:J:179:GLU:CD | 2.60 | 0.54 |
| 1:D:112:ARG:NH1 | 1:D:112:ARG:CG | 2.69 | 0.54 |
| 1:E:207:SER:N | 2:E:2090:EDO:H22 | 2.23 | 0.54 |
| 1:F:126:ARG:HB3 | 1:F:149:ARG:CZ | 2.37 | 0.54 |
| 2:B:2002:EDO:O2 | 2:B:2002:EDO:C1 | 2.51 | 0.54 |
| 1:D:112:ARG:NH1 | 1:D:112:ARG:HG2 | 2.22 | 0.54 |
| 1:C:49:VAL:HG23 | 2:C:2024:EDO:H12 | 1.90 | 0.54 |
| 1:G:183:GLU:N | 2:G:2057:EDO:HO2 | 2.04 | 0.54 |
| 1:G:96:ARG:HD2 | 3:G:780:HOH:O | 2.08 | 0.54 |
| 1:E:47:THR:HB | 1:E:48:PRO:HD2 | 1.90 | 0.54 |
| 1:C:235:GLU:OE1 | 2:C:2004:EDO:C2 | 2.56 | 0.54 |
| 2:C:2126:EDO:HO2 | 2:C:2126:EDO:C2 | 2.08 | 0.54 |
| 1:F:123:HIS:CD2 | 2:F:2086:EDO:H22 | 2.43 | 0.54 |
| 2:C:2075:EDO:H12 | 2:E:2127:EDO:H22 | 1.82 | 0.54 |
| 1:I:105:PRO:O | 1:I:106:GLN:CB | 2.55 | 0.54 |
| 1:G:86:LYS:HD2 | 1:G:97:ILE:HB | 1.88 | 0.54 |
| 1:E:5:ILE:CD1 | 1:F:5:ILE:HG21 | 2.38 | 0.54 |
| 1:I:49:VAL:N | 2:I:2121:EDO:HO2 | 2.03 | 0.54 |
| 1:C:39:LEU:HD13 | 1:C:72:ILE:HG23 | 1.89 | 0.54 |
| 1:D:43:PRO:HB2 | 2:D:2118:EDO:C2 | 2.38 | 0.53 |
| 1:D:44:ALA:O | 1:D:47:THR:HB | 2.08 | 0.53 |
| 1:F:169:ARG:HB3 | 1:F:185:LEU:HB3 | 1.90 | 0.53 |
| 1:A:147:LEU:HD23 | 1:B:171:VAL:HB | 1.90 | 0.53 |
| 1:H:43:PRO:HG3 | 1:H:145:MSE:HG2 | 1.90 | 0.53 |
| 1:I:192:THR:HG1 | 2:I:2115:EDO:H11 | 1.73 | 0.53 |
| 1:I:67:LEU:O | 1:I:162:LYS:HE2 | 2.08 | 0.53 |
| 1:G:90:GLU:OE2 | 1:G:96:ARG:HG2 | 2.09 | 0.53 |
| 1:D:111:ARG:HH21 | 1:E:106:GLN:HE21 | 1.56 | 0.53 |
| 1:A:216:THR:C | 2:A:2063:EDO:H11 | 2.28 | 0.53 |
| 1:G:145:MSE:CE | 1:G:145:MSE:CB | 2.86 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:59:ARG:HH11 | 1:I:59:ARG:CB | 2.20 | 0.53 |
| 1:A:105:PRO:O | 1:A:106:GLN:CB | 2.56 | 0.53 |
| 1:I:206:ARG:HD2 | 1:I:214:TRP:CZ2 | 2.44 | 0.53 |
| 1:E:146:GLU:HG3 | 3:F:516:HOH:O | 2.08 | 0.53 |
| 1:D:114:GLY:O | 1:D:117:HIS:HE1 | 1.92 | 0.53 |
| 1:C:48:PRO:HG2 | 1:D:186:ILE:HG21 | 1.89 | 0.53 |
| 1:G:158:VAL:HG12 | 1:G:162:LYS:HD2 | 1.90 | 0.53 |
| 1:D:112:ARG:HH11 | 1:D:112:ARG:CB | 2.21 | 0.53 |
| 1:F:200:MSE:HE1 | 2:F:2034:EDO:H21 | 1.91 | 0.53 |
| 1:A:47:THR:HG22 | 1:A:50:CYS:SG | 2.49 | 0.53 |
| 1:D:204:GLN:N | 2:D:2035:EDO:H22 | 2.24 | 0.53 |
| 1:F:205:TYR:HB2 | 2:F:2034:EDO:H12 | 1.89 | 0.53 |
| 1:J:222:ASP:OD2 | 2:J:2110:EDO:C1 | 2.56 | 0.53 |
| 1:A:130:ILE:HD12 | 1:A:157:ILE:HG21 | 1.91 | 0.53 |
| 1:B:62:GLU:O | 1:B:66:ARG:HG3 | 2.08 | 0.53 |
| 1:C:169:ARG:HB3 | 1:C:185:LEU:HB3 | 1.91 | 0.53 |
| 1:C:145:MSE:HE3 | 2:C:2067:EDO:H22 | 1.91 | 0.53 |
| 1:B:126:ARG:HB3 | 1:B:149:ARG:CZ | 2.39 | 0.53 |
| 1:F:96:ARG:O | 2:F:2095:EDO:H11 | 2.09 | 0.53 |
| 1:B:111:ARG:HH22 | 1:C:111:ARG:NH2 | 1.91 | 0.53 |
| 1:B:243:GLU:CB | 1:B:244:GLU:OE1 | 2.56 | 0.53 |
| 1:A:200:MSE:C | 1:A:202:SER:H | 2.11 | 0.53 |
| 1:A:10:GLU:OE2 | 1:B:2:PRO:N | 2.42 | 0.53 |
| 1:G:228:ARG:NH2 | 3:G:767:HOH:O | 2.41 | 0.53 |
| 2:G:2009:EDO:HO1 | 2:G:2009:EDO:C1 | 2.10 | 0.52 |
| 1:F:163:LEU:HD22 | 1:F:167:LEU:HD22 | 1.91 | 0.52 |
| 1:F:200:MSE:CE | 1:F:200:MSE:HA | 2.40 | 0.52 |
| 1:F:205:TYR:H | 2:F:2034:EDO:H12 | 1.73 | 0.52 |
| 2:B:2021:EDO:C2 | 2:B:2021:EDO:HO2 | 2.12 | 0.52 |
| 1:F:183:GLU:HG2 | 2:F:2043:EDO:H11 | 1.90 | 0.52 |
| 1:A:231:ARG:NH1 | 2:A:2017:EDO:H11 | 2.24 | 0.52 |
| 1:H:145:MSE:HE2 | 1:H:145:MSE:CB | 2.40 | 0.52 |
| 1:H:59:ARG:NH1 | 1:H:59:ARG:HG3 | 2.07 | 0.52 |
| 1:I:5:ILE:HG22 | 1:I:114:GLY:HA3 | 1.91 | 0.52 |
| 1:H:129:PHE:CE2 | 1:H:140:MSE:HE3 | 2.45 | 0.52 |
| 1:C:174:ASP:HB3 | 3:D:2163:HOH:O | 2.09 | 0.52 |
| 1:C:21:HIS:CB | 2:C:2064:EDO:H22 | 2.40 | 0.52 |
| 1:J:84:LYS:HD2 | 1:J:87:GLU:OE2 | 2.09 | 0.52 |
| 1:J:200:MSE:HE2 | 1:J:200:MSE:HA | 1.91 | 0.52 |
| 2:A:2124:EDO:O2 | 2:A:2124:EDO:C1 | 2.50 | 0.52 |
| 2:F:2043:EDO:C2 | 2:F:2043:EDO:HO2 | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:14:GLU:CG | 1:F:25:LYS:CE | 2.88 | 0.52 |
| 1:F:24:ILE:HD11 | 1:F:26:LEU:CD2 | 2.39 | 0.52 |
| 1:E:91:ARG:HD3 | 2:E:2076:EDO:H11 | 1.91 | 0.52 |
| 1:F:69:VAL:HG21 | 1:F:158:VAL:HG21 | 1.92 | 0.52 |
| 1:J:240:LEU:N | 1:J:243:GLU:OE1 | 2.38 | 0.52 |
| 1:C:126:ARG:HB3 | 1:C:149:ARG:CZ | 2.39 | 0.52 |
| 1:B:99:PHE:HB2 | 1:B:100:PRO:HD2 | 1.92 | 0.52 |
| 1:J:185:LEU:O | 1:J:214:TRP:HB2 | 2.10 | 0.52 |
| 1:D:15:MSE:SE | 1:D:109:VAL:HG13 | 2.60 | 0.51 |
| 2:G:2102:EDO:C1 | 2:G:2102:EDO:O2 | 2.51 | 0.51 |
| 1:A:134:ARG:HA | 2:A:2116:EDO:H21 | 1.92 | 0.51 |
| 1:C:47:THR:HG22 | 1:C:50:CYS:SG | 2.50 | 0.51 |
| 1:I:228:ARG:NE | 2:I:2107:EDO:H22 | 2.22 | 0.51 |
| 2:F:2038:EDO:H11 | 1:H:191:THR:CG2 | 2.40 | 0.51 |
| 1:H:42:HIS:CE1 | 1:H:75:SER:HB3 | 2.46 | 0.51 |
| 2:J:2105:EDO:C1 | 2:J:2105:EDO:O2 | 2.50 | 0.51 |
| 2:E:2032:EDO:O2 | 2:E:2032:EDO:C1 | 2.53 | 0.51 |
| 1:I:140:MSE:CB | 1:I:140:MSE:CE | 2.88 | 0.51 |
| 1:E:207:SER:HB3 | 1:E:213:CYS:SG | 2.51 | 0.51 |
| 1:J:222:ASP:OD2 | 2:J:2110:EDO:H11 | 2.09 | 0.51 |
| 2:B:2023:EDO:C2 | 2:B:2023:EDO:HO2 | 2.11 | 0.51 |
| 1:E:238:ALA:O | 1:E:239:LYS:HB3 | 2.10 | 0.51 |
| 2:D:2074:EDO:HO1 | 2:D:2074:EDO:C1 | 2.13 | 0.51 |
| 1:D:203:GLY:N | 2:D:2035:EDO:H21 | 2.26 | 0.51 |
| 1:J:97:ILE:H | 2:J:2109:EDO:H22 | 1.75 | 0.51 |
| 1:E:62:GLU:HG2 | 1:E:66:ARG:HE | 1.76 | 0.51 |
| 2:C:2128:EDO:C1 | 2:C:2128:EDO:O2 | 2.55 | 0.51 |
| 1:E:206:ARG:CA | 2:E:2090:EDO:H22 | 2.40 | 0.51 |
| 1:F:191:THR:H | 1:F:195:GLN:NE2 | 2.09 | 0.51 |
| 1:H:183:GLU:N | 2:H:2058:EDO:H11 | 2.24 | 0.50 |
| 1:J:112:ARG:NH1 | 2:J:2053:EDO:O2 | 2.44 | 0.50 |
| 1:I:225:GLU:CB | 1:I:228:ARG:HH11 | 2.24 | 0.50 |
| 1:D:205:TYR:O | 2:D:2035:EDO:H12 | 2.12 | 0.50 |
| 1:B:50:CYS:HG | 2:B:2028:EDO:HO1 | 1.56 | 0.50 |
| 1:D:200:MSE:HA | 1:D:200:MSE:CE | 2.33 | 0.50 |
| 1:G:130:ILE:HD12 | 1:G:157:ILE:HG21 | 1.93 | 0.50 |
| 1:A:118:ALA:O | 1:A:120:SER:N | 2.43 | 0.50 |
| 1:A:239:LYS:HD3 | 1:A:244:GLU:OE2 | 2.11 | 0.50 |
| 1:G:75:SER:OG | 1:G:82:HIS:HE1 | 1.93 | 0.50 |
| 1:C:153:GLU:OE1 | 1:D:150:LEU:HD22 | 2.11 | 0.50 |
| 1:I:48:PRO:CG | 1:J:186:ILE:HG21 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:7:LEU:HD21 | 1:F:3:GLY:HA3 | 1.93 | 0.50 |
| 1:G:126:ARG:HB3 | 1:G:149:ARG:CZ | 2.41 | 0.50 |
| 1:E:126:ARG:HB3 | 1:E:149:ARG:CZ | 2.41 | 0.50 |
| 1:B:238:ALA:O | 1:B:239:LYS:CB | 2.58 | 0.50 |
| 1:B:239:LYS:CG | 1:B:243:GLU:OE1 | 2.59 | 0.50 |
| 1:B:132:ASP:CG | 2:B:2025:EDO:H21 | 2.32 | 0.50 |
| 1:I:90:GLU:OE1 | 1:I:96:ARG:HG3 | 2.11 | 0.50 |
| 1:J:228:ARG:HE | 2:J:2049:EDO:H11 | 1.76 | 0.50 |
| 1:G:99:PHE:HB2 | 1:G:100:PRO:HD2 | 1.94 | 0.50 |
| 1:G:145:MSE:HB3 | 1:G:145:MSE:CE | 2.41 | 0.50 |
| 2:C:2082:EDO:HO2 | 2:C:2082:EDO:C2 | 2.12 | 0.50 |
| 1:D:203:GLY:CA | 2:D:2035:EDO:H21 | 2.42 | 0.50 |
| 1:E:215:ASP:OD2 | 1:E:217:PRO:HD3 | 2.12 | 0.50 |
| 1:H:140:MSE:CE | 1:H:142:TYR:OH | 2.60 | 0.50 |
| 2:D:2118:EDO:HO2 | 2:D:2118:EDO:C2 | 2.10 | 0.50 |
| 1:G:2:PRO:N | 1:H:10:GLU:OE2 | 2.44 | 0.50 |
| 1:B:92:HIS:NE2 | 2:B:2125:EDO:C1 | 2.72 | 0.49 |
| 1:H:169:ARG:O | 2:H:2111:EDO:H11 | 2.12 | 0.49 |
| 1:B:200:MSE:HA | 1:B:200:MSE:HE2 | 1.92 | 0.49 |
| 1:C:48:PRO:HD2 | 2:C:2024:EDO:C1 | 2.20 | 0.49 |
| 1:G:42:HIS:HB2 | 1:G:50:CYS:SG | 2.52 | 0.49 |
| 1:F:239:LYS:HG3 | 1:F:244:GLU:OE2 | 2.13 | 0.49 |
| 1:E:209:ASP:OD2 | 2:E:2120:EDO:H21 | 2.12 | 0.49 |
| 2:A:2122:EDO:O2 | 2:A:2122:EDO:C1 | 2.53 | 0.49 |
| 1:E:90:GLU:OE2 | 2:E:2127:EDO:O1 | 2.25 | 0.49 |
| 1:I:134:ARG:HG3 | 2:I:2045:EDO:H22 | 1.94 | 0.49 |
| 2:G:2057:EDO:H12 | 1:H:240:LEU:CD1 | 2.41 | 0.49 |
| 1:D:122:THR:OG1 | 1:E:105:PRO:HG2 | 2.12 | 0.49 |
| 1:E:240:LEU:O | 1:E:244:GLU:HG3 | 2.12 | 0.49 |
| 1:I:59:ARG:NH1 | 1:J:179:GLU:OE1 | 2.45 | 0.49 |
| 1:A:207:SER:HB3 | 2:A:2065:EDO:H22 | 1.95 | 0.49 |
| 1:A:147:LEU:HG | 1:B:161:LEU:HD13 | 1.94 | 0.49 |
| 1:C:235:GLU:HB3 | 2:C:2004:EDO:C2 | 2.43 | 0.49 |
| 1:H:200:MSE:HE2 | 2:H:2060:EDO:H22 | 1.95 | 0.49 |
| 1:G:11:ARG:NH1 | 1:G:14:GLU:OE2 | 2.43 | 0.49 |
| 1:E:242:TYR:OH | 1:F:206:ARG:HG2 | 2.13 | 0.49 |
| 1:G:74:LEU:HD13 | 1:G:74:LEU:C | 2.32 | 0.49 |
| 1:F:107:GLY:HA3 | 1:G:106:GLN:NE2 | 2.26 | 0.49 |
| 1:F:222:ASP:OD2 | 2:F:2097:EDO:O2 | 2.30 | 0.49 |
| 1:I:128:VAL:HG13 | 1:I:141:LEU:HB2 | 1.93 | 0.49 |
| 1:G:197:ARG:HA | 2:G:2050:EDO:C2 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:183:GLU:HG2 | 2:F:2043:EDO:H12 | 1.95 | 0.49 |
| 1:B:5:ILE:HG22 | 1:B:114:GLY:HA3 | 1.95 | 0.49 |
| 1:B:203:GLY:HA2 | 2:B:2030:EDO:H21 | 1.95 | 0.49 |
| 1:C:42:HIS:CE1 | 1:C:75:SER:HB3 | 2.47 | 0.49 |
| 1:E:241:LEU:CD2 | 1:E:244:GLU:OE1 | 2.38 | 0.49 |
| 1:J:122:THR:HG23 | 1:J:123:HIS:CD2 | 2.48 | 0.49 |
| 1:D:199:ARG:NH1 | 3:D:2192:HOH:O | 2.33 | 0.49 |
| 1:F:25:LYS:NZ | 3:F:556:HOH:O | 2.41 | 0.48 |
| 1:F:199:ARG:HG2 | 1:F:200:MSE:CE | 2.43 | 0.48 |
| 1:C:186:ILE:HG21 | 1:D:48:PRO:HG2 | 1.95 | 0.48 |
| 1:H:235:GLU:OE1 | 2:H:2010:EDO:H21 | 2.13 | 0.48 |
| 1:G:169:ARG:O | 2:G:2112:EDO:C1 | 2.51 | 0.48 |
| 1:D:32:SER:O | 3:D:2214:HOH:O | 2.20 | 0.48 |
| 1:F:67:LEU:O | 1:F:162:LYS:HE3 | 2.13 | 0.48 |
| 1:A:105:PRO:O | 1:A:106:GLN:HB2 | 2.13 | 0.48 |
| 1:A:200:MSE:C | 1:A:202:SER:N | 2.66 | 0.48 |
| 1:A:119:GLU:HG3 | 1:B:8:ILE:HG22 | 1.94 | 0.48 |
| 1:E:199:ARG:HH21 | 2:E:2091:EDO:C2 | 2.22 | 0.48 |
| 1:A:183:GLU:HG2 | 2:A:2022:EDO:O2 | 2.14 | 0.48 |
| 1:E:90:GLU:OE2 | 2:E:2127:EDO:C1 | 2.62 | 0.48 |
| 1:H:59:ARG:NH1 | 1:H:59:ARG:CG | 2.73 | 0.48 |
| 1:E:67:LEU:HD13 | 1:E:158:VAL:HG23 | 1.95 | 0.48 |
| 1:C:167:LEU:HD11 | 2:C:2036:EDO:H21 | 1.95 | 0.48 |
| 2:E:2005:EDO:C2 | 3:E:513:HOH:O | 2.62 | 0.48 |
| 2:J:2123:EDO:O1 | 2:J:2123:EDO:O2 | 2.23 | 0.48 |
| 1:A:243:GLU:C | 1:A:245:ALA:N | 2.65 | 0.48 |
| 1:I:84:LYS:HD2 | 1:I:87:GLU:OE1 | 2.14 | 0.48 |
| 1:E:240:LEU:HD11 | 2:F:2043:EDO:H21 | 1.94 | 0.48 |
| 1:F:14:GLU:HG3 | 1:F:25:LYS:CE | 2.44 | 0.48 |
| 1:I:66:ARG:HB3 | 1:I:66:ARG:CZ | 2.44 | 0.48 |
| 1:I:205:TYR:H | 2:I:2051:EDO:C2 | 2.20 | 0.48 |
| 1:A:117:HIS:CD2 | 1:B:8:ILE:H | 2.16 | 0.48 |
| 1:I:126:ARG:HH22 | 2:I:2121:EDO:C1 | 2.26 | 0.48 |
| 1:A:214:TRP:CH2 | 3:A:2219:HOH:O | 2.55 | 0.48 |
| 1:F:163:LEU:O | 1:F:167:LEU:HB2 | 2.14 | 0.48 |
| 1:A:174:ASP:HB3 | 3:B:2222:HOH:O | 2.13 | 0.47 |
| 1:A:200:MSE:HE2 | 2:A:2065:EDO:H11 | 1.95 | 0.47 |
| 1:C:235:GLU:O | 2:C:2004:EDO:O2 | 2.32 | 0.47 |
| 1:B:5:ILE:HB | 1:B:140:MSE:HE1 | 1.96 | 0.47 |
| 1:H:117:HIS:HB2 | 1:H:125:VAL:HG11 | 1.96 | 0.47 |
| 1:D:111:ARG:HH22 | 1:E:111:ARG:NH2 | 2.10 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:200:MSE:HE1 | 2:H:2060:EDO:H22 | 1.96 | 0.47 |
| 1:A:159:LYS:HE2 | 1:A:225:GLU:OE2 | 2.15 | 0.47 |
| 2:G:2050:EDO:HO2 | 2:G:2050:EDO:C2 | 2.09 | 0.47 |
| 1:H:232:ARG:O | 2:H:2010:EDO:O2 | 2.31 | 0.47 |
| 2:F:2098:EDO:HO2 | 2:F:2098:EDO:C2 | 2.15 | 0.47 |
| 1:F:123:HIS:HD2 | 2:F:2086:EDO:H22 | 1.80 | 0.47 |
| 1:H:74:LEU:HD13 | 1:H:75:SER:N | 2.28 | 0.47 |
| 1:C:178:ASN:HD21 | 1:D:52:THR:HB | 1.79 | 0.47 |
| 1:H:235:GLU:HB3 | 2:H:2010:EDO:H21 | 1.97 | 0.47 |
| 2:I:2103:EDO:HO2 | 1:J:236:LYS:HZ1 | 1.54 | 0.47 |
| 1:F:199:ARG:HG2 | 1:F:200:MSE:HE3 | 1.96 | 0.47 |
| 1:C:92:HIS:O | 1:C:245:ALA:HB1 | 2.14 | 0.47 |
| 1:I:163:LEU:O | 1:I:167:LEU:HB2 | 2.15 | 0.47 |
| 1:E:121:ALA:N | 1:E:121:ALA:CB | 2.67 | 0.47 |
| 1:B:67:LEU:HB2 | 1:B:69:VAL:HG23 | 1.96 | 0.47 |
| 1:C:215:ASP:OD2 | 1:C:217:PRO:HD3 | 2.13 | 0.47 |
| 1:E:3:GLY:HA3 | 1:F:7:LEU:HD21 | 1.96 | 0.47 |
| 1:D:159:LYS:HE2 | 1:D:225:GLU:OE2 | 2.15 | 0.47 |
| 1:G:197:ARG:HA | 2:G:2050:EDO:H22 | 1.95 | 0.47 |
| 1:C:36:TRP:CD1 | 1:C:162:LYS:NZ | 2.82 | 0.47 |
| 1:E:10:GLU:OE2 | 1:F:2:PRO:CB | 2.62 | 0.47 |
| 1:H:69:VAL:CG2 | 1:H:158:VAL:HG11 | 2.43 | 0.47 |
| 1:H:215:ASP:OD2 | 1:H:217:PRO:HD3 | 2.15 | 0.47 |
| 1:G:100:PRO:HD3 | 2:G:2093:EDO:H21 | 1.96 | 0.47 |
| 1:C:91:ARG:NH1 | 2:C:2126:EDO:H12 | 2.30 | 0.47 |
| 3:E:290:HOH:O | 1:F:174:ASP:HB3 | 2.13 | 0.47 |
| 1:G:175:TRP:CG | 1:G:176:PRO:HA | 2.49 | 0.47 |
| 1:D:96:ARG:HH12 | 1:F:197:ARG:NH1 | 2.13 | 0.47 |
| 1:B:54:PHE:HE2 | 1:B:101:ILE:HG12 | 1.80 | 0.47 |
| 1:B:7:LEU:O | 1:B:10:GLU:HB2 | 2.14 | 0.47 |
| 1:J:199:ARG:HG2 | 2:J:2104:EDO:H12 | 1.97 | 0.47 |
| 1:D:189:PRO:HA | 1:D:190:PRO:HD3 | 1.72 | 0.47 |
| 1:A:105:PRO:HG2 | 1:J:122:THR:OG1 | 2.14 | 0.47 |
| 1:C:219:SER:HB3 | 1:C:222:ASP:H | 1.79 | 0.47 |
| 1:I:5:ILE:CD1 | 1:J:5:ILE:HD13 | 2.38 | 0.47 |
| 1:J:86:LYS:HB3 | 2:J:2109:EDO:C2 | 2.31 | 0.47 |
| 1:B:86:LYS:HE3 | 1:B:101:ILE:CD1 | 2.45 | 0.47 |
| 1:I:92:HIS:O | 1:I:245:ALA:HB1 | 2.15 | 0.47 |
| 2:C:2024:EDO:O2 | 2:C:2024:EDO:C1 | 2.57 | 0.46 |
| 2:D:2031:EDO:O2 | 2:D:2031:EDO:C1 | 2.57 | 0.46 |
| 2:B:2023:EDO:C1 | 2:B:2023:EDO:O2 | 2.55 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:123:HIS:CD2 | 2:F:2086:EDO:H21 | 2.48 | 0.46 |
| 1:C:193:GLU:O | 2:C:2075:EDO:O1 | 2.33 | 0.46 |
| 1:I:144:PRO:HD3 | 1:J:139:THR:OG1 | 2.14 | 0.46 |
| 1:G:202:SER:OG | 1:G:204:GLN:HG2 | 2.15 | 0.46 |
| 1:C:186:ILE:HG21 | 1:D:48:PRO:CG | 2.45 | 0.46 |
| 1:J:228:ARG:HE | 2:J:2049:EDO:C1 | 2.27 | 0.46 |
| 1:A:49:VAL:H | 2:A:2012:EDO:C2 | 2.22 | 0.46 |
| 2:C:2004:EDO:O1 | 2:C:2004:EDO:C2 | 2.56 | 0.46 |
| 1:H:48:PRO:O | 1:H:52:THR:HG23 | 2.15 | 0.46 |
| 1:H:79:VAL:O | 1:H:83:ILE:HG13 | 2.15 | 0.46 |
| 2:A:2012:EDO:C2 | 2:A:2012:EDO:HO2 | 2.13 | 0.46 |
| 1:E:236:LYS:NZ | 2:F:2043:EDO:C2 | 2.69 | 0.46 |
| 1:C:235:GLU:OE1 | 2:C:2080:EDO:C2 | 2.63 | 0.46 |
| 2:I:2007:EDO:HO1 | 2:I:2007:EDO:C1 | 2.11 | 0.46 |
| 1:J:86:LYS:O | 2:J:2109:EDO:O1 | 2.16 | 0.46 |
| 1:D:191:THR:H | 1:D:195:GLN:HE22 | 1.59 | 0.46 |
| 1:H:207:SER:HB2 | 2:H:2060:EDO:H11 | 1.97 | 0.46 |
| 1:C:145:MSE:CB | 1:C:145:MSE:CE | 2.93 | 0.46 |
| 1:C:129:PHE:HE2 | 1:C:140:MSE:CE | 2.16 | 0.46 |
| 1:F:90:GLU:HG2 | 1:F:96:ARG:HA | 1.97 | 0.46 |
| 1:A:214:TRP:HH2 | 3:A:2219:HOH:O | 1.94 | 0.46 |
| 1:C:224:GLU:CD | 1:C:231:ARG:HH22 | 2.19 | 0.46 |
| 1:J:109:VAL:HG21 | 2:J:2061:EDO:H22 | 1.98 | 0.46 |
| 1:A:47:THR:HG23 | 2:A:2012:EDO:C2 | 2.45 | 0.46 |
| 1:H:183:GLU:HG2 | 2:H:2058:EDO:C1 | 2.39 | 0.46 |
| 2:H:2058:EDO:O2 | 2:H:2058:EDO:O1 | 2.33 | 0.46 |
| 1:I:128:VAL:O | 1:I:140:MSE:HA | 2.16 | 0.46 |
| 1:B:65:GLN:HE21 | 1:B:65:GLN:HA | 1.81 | 0.46 |
| 1:G:236:LYS:NZ | 1:G:236:LYS:CD | 2.68 | 0.46 |
| 1:D:74:LEU:C | 1:D:74:LEU:HD13 | 2.36 | 0.46 |
| 1:I:238:ALA:C | 1:I:239:LYS:HD2 | 2.36 | 0.46 |
| 2:J:2123:EDO:O1 | 2:J:2123:EDO:C2 | 2.58 | 0.46 |
| 1:D:204:GLN:H | 2:D:2035:EDO:H21 | 1.81 | 0.46 |
| 1:F:106:GLN:H | 1:G:106:GLN:H | 1.64 | 0.46 |
| 1:F:239:LYS:HD2 | 1:F:244:GLU:OE2 | 2.16 | 0.46 |
| 1:B:222:ASP:OD2 | 2:B:2018:EDO:H11 | 2.16 | 0.46 |
| 1:H:74:LEU:C | 1:H:74:LEU:HD13 | 2.36 | 0.46 |
| 1:D:153:GLU:OE1 | 1:D:153:GLU:HA | 2.16 | 0.46 |
| 1:A:47:THR:CG2 | 1:A:50:CYS:SG | 3.04 | 0.46 |
| 1:C:232:ARG:O | 2:C:2004:EDO:O2 | 2.16 | 0.46 |
| 1:E:88:TRP:HA | 2:E:2076:EDO:C1 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:96:ARG:O | 1:B:98:PRO:HD3 | 2.15 | 0.46 |
| 1:I:69:VAL:HG21 | 1:I:158:VAL:HG21 | 1.98 | 0.46 |
| 1:H:36:TRP:CD2 | 1:H:132:ASP:HA | 2.52 | 0.46 |
| 1:E:194:ASP:OD1 | 1:E:194:ASP:C | 2.54 | 0.46 |
| 1:E:159:LYS:HZ2 | 2:E:2088:EDO:C2 | 2.28 | 0.45 |
| 1:J:208:LEU:HA | 1:J:208:LEU:HD12 | 1.74 | 0.45 |
| 1:C:55:VAL:O | 1:C:59:ARG:HG3 | 2.16 | 0.45 |
| 1:E:185:LEU:O | 1:E:214:TRP:HB2 | 2.16 | 0.45 |
| 1:I:5:ILE:HD11 | 1:J:5:ILE:HG21 | 1.98 | 0.45 |
| 1:G:5:ILE:HG21 | 1:H:5:ILE:HD13 | 1.98 | 0.45 |
| 1:E:186:ILE:HG21 | 1:F:48:PRO:HG2 | 1.97 | 0.45 |
| 1:C:48:PRO:CG | 2:C:2024:EDO:H11 | 2.45 | 0.45 |
| 1:C:235:GLU:OE1 | 2:C:2004:EDO:H22 | 2.15 | 0.45 |
| 1:C:91:ARG:CD | 2:C:2126:EDO:O1 | 2.62 | 0.45 |
| 1:E:18:THR:HG21 | 2:E:2077:EDO:H12 | 1.97 | 0.45 |
| 1:J:228:ARG:HH21 | 2:J:2049:EDO:C2 | 2.26 | 0.45 |
| 2:A:2124:EDO:C1 | 2:A:2124:EDO:HO1 | 2.13 | 0.45 |
| 2:I:2007:EDO:H12 | 3:I:2207:HOH:O | 2.17 | 0.45 |
| 1:A:214:TRP:CZ3 | 3:A:2219:HOH:O | 2.68 | 0.45 |
| 1:B:243:GLU:C | 1:B:244:GLU:OE1 | 2.55 | 0.45 |
| 1:F:207:SER:HB2 | 2:F:2034:EDO:H22 | 1.98 | 0.45 |
| 1:G:74:LEU:HD13 | 1:G:75:SER:N | 2.31 | 0.45 |
| 1:F:208:LEU:HD12 | 1:F:208:LEU:HA | 1.83 | 0.45 |
| 1:J:200:MSE:SE | 2:J:2105:EDO:H21 | 2.66 | 0.45 |
| 1:H:235:GLU:O | 2:H:2010:EDO:O2 | 2.33 | 0.45 |
| 1:B:106:GLN:HG2 | 1:C:122:THR:HA | 1.99 | 0.45 |
| 1:A:186:ILE:HG21 | 1:B:48:PRO:HG2 | 1.98 | 0.45 |
| 1:B:67:LEU:HD13 | 1:B:158:VAL:HG23 | 1.99 | 0.45 |
| 1:E:205:TYR:O | 2:E:2042:EDO:H12 | 2.16 | 0.45 |
| 2:F:2038:EDO:H11 | 1:H:191:THR:HG22 | 1.98 | 0.45 |
| 1:I:84:LYS:HA | 1:I:84:LYS:HD2 | 1.83 | 0.45 |
| 1:H:215:ASP:C | 1:H:217:PRO:HD3 | 2.37 | 0.45 |
| 1:G:10:GLU:OE2 | 1:H:2:PRO:N | 2.49 | 0.45 |
| 1:B:104:ASP:N | 1:B:104:ASP:OD2 | 2.37 | 0.45 |
| 1:A:59:ARG:HD3 | 1:A:59:ARG:HH11 | 1.62 | 0.45 |
| 1:E:159:LYS:NZ | 1:E:225:GLU:OE2 | 2.50 | 0.45 |
| 1:C:235:GLU:HB3 | 2:C:2004:EDO:H21 | 1.99 | 0.45 |
| 1:J:169:ARG:HE | 1:J:215:ASP:HB2 | 1.81 | 0.45 |
| 1:D:134:ARG:HG3 | 2:D:2031:EDO:H11 | 1.99 | 0.45 |
| 1:B:220:ARG:CD | 1:B:224:GLU:OE2 | 2.65 | 0.45 |
| 1:B:111:ARG:HH21 | 1:C:106:GLN:NE2 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:203:GLY:C | 2:I:2051:EDO:H21 | 2.37 | 0.45 |
| 1:F:239:LYS:NZ | 1:F:244:GLU:OE1 | 2.47 | 0.45 |
| 1:G:189:PRO:HA | 1:G:190:PRO:HD3 | 1.82 | 0.45 |
| 1:F:203:GLY:O | 2:F:2098:EDO:H12 | 2.16 | 0.45 |
| 1:F:206:ARG:NH1 | 1:F:214:TRP:CH2 | 2.85 | 0.45 |
| 1:I:184:GLY:HA2 | 1:I:216:THR:HG22 | 1.99 | 0.45 |
| 1:I:174:ASP:HB3 | 3:J:2219:HOH:O | 2.16 | 0.45 |
| 1:C:189:PRO:HA | 1:C:190:PRO:HD3 | 1.83 | 0.45 |
| 1:J:15:MSE:HG3 | 1:J:15:MSE:O | 2.17 | 0.45 |
| 1:C:47:THR:HA | 1:C:48:PRO:HD3 | 1.89 | 0.44 |
| 1:F:218:ALA:HA | 2:F:2097:EDO:O2 | 2.18 | 0.44 |
| 1:I:19:THR:HG22 | 1:I:102:ILE:HG12 | 2.00 | 0.44 |
| 1:A:5:ILE:HG22 | 1:A:114:GLY:HA3 | 1.98 | 0.44 |
| 1:F:114:GLY:O | 1:F:117:HIS:HE1 | 1.99 | 0.44 |
| 1:D:114:GLY:O | 1:D:117:HIS:CE1 | 2.70 | 0.44 |
| 1:G:106:GLN:O | 1:G:111:ARG:NH2 | 2.50 | 0.44 |
| 1:B:244:GLU:N | 1:B:244:GLU:CD | 2.71 | 0.44 |
| 2:J:2108:EDO:C1 | 3:J:2191:HOH:O | 2.65 | 0.44 |
| 1:E:92:HIS:NE2 | 2:E:2076:EDO:C2 | 2.80 | 0.44 |
| 1:G:41:SER:HB2 | 1:G:124:THR:HG21 | 1.99 | 0.44 |
| 1:F:239:LYS:CE | 1:F:244:GLU:OE1 | 2.65 | 0.44 |
| 1:B:130:ILE:HD13 | 1:B:157:ILE:HG21 | 1.98 | 0.44 |
| 1:D:163:LEU:HD21 | 1:D:222:ASP:CG | 2.38 | 0.44 |
| 1:J:157:ILE:HG22 | 1:J:161:LEU:HD22 | 1.98 | 0.44 |
| 2:C:2004:EDO:HO2 | 2:C:2004:EDO:C2 | 2.16 | 0.44 |
| 1:D:215:ASP:OD2 | 1:D:217:PRO:HD3 | 2.17 | 0.44 |
| 1:A:33:GLN:HB2 | 1:A:35:LYS:HG3 | 1.99 | 0.44 |
| 1:A:126:ARG:HB3 | 1:A:149:ARG:CZ | 2.47 | 0.44 |
| 1:A:174:ASP:HA | 1:B:150:LEU:HD23 | 1.98 | 0.44 |
| 1:D:126:ARG:HB3 | 1:D:149:ARG:CZ | 2.47 | 0.44 |
| 1:J:21:HIS:CB | 2:J:2068:EDO:H21 | 2.47 | 0.44 |
| 1:I:140:MSE:CE | 1:I:142:TYR:OH | 2.65 | 0.44 |
| 1:D:244:GLU:HG3 | 1:D:244:GLU:H | 1.64 | 0.44 |
| 1:B:239:LYS:HA | 1:B:243:GLU:OE1 | 2.16 | 0.44 |
| 1:G:239:LYS:HG2 | 1:G:244:GLU:CG | 2.47 | 0.44 |
| 1:J:48:PRO:O | 1:J:52:THR:HG23 | 2.17 | 0.44 |
| 1:I:157:ILE:HG23 | 1:J:147:LEU:CD1 | 2.47 | 0.44 |
| 1:E:171:VAL:HB | 1:F:147:LEU:HD12 | 2.00 | 0.44 |
| 1:A:232:ARG:O | 2:A:2001:EDO:O2 | 2.35 | 0.44 |
| 1:E:206:ARG:HA | 2:E:2090:EDO:C2 | 2.44 | 0.44 |
| 1:I:17:VAL:HA | 2:I:2100:EDO:C1 | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:2115:EDO:C1 | 2:I:2115:EDO:O2 | 2.55 | 0.44 |
| 1:J:169:ARG:HB3 | 1:J:185:LEU:HB3 | 1.99 | 0.44 |
| 1:J:114:GLY:O | 1:J:117:HIS:HE1 | 2.00 | 0.44 |
| 1:C:241:LEU:HA | 1:C:241:LEU:HD23 | 1.72 | 0.44 |
| 1:D:39:LEU:HD12 | 1:D:40:PHE:N | 2.33 | 0.44 |
| 1:I:42:HIS:CE1 | 1:I:75:SER:HB3 | 2.53 | 0.44 |
| 1:E:236:LYS:NZ | 1:F:183:GLU:OE2 | 2.50 | 0.44 |
| 1:B:65:GLN:O | 1:B:67:LEU:O | 2.36 | 0.44 |
| 1:D:129:PHE:CZ | 1:D:140:MSE:HE3 | 2.50 | 0.44 |
| 1:A:242:TYR:CE1 | 1:B:214:TRP:HH2 | 2.35 | 0.44 |
| 1:H:200:MSE:HE1 | 1:H:213:CYS:SG | 2.58 | 0.44 |
| 1:G:205:TYR:H | 2:G:2047:EDO:C1 | 2.31 | 0.44 |
| 1:G:186:ILE:HG21 | 1:H:48:PRO:HG2 | 2.00 | 0.44 |
| 1:J:109:VAL:CG2 | 2:J:2061:EDO:H22 | 2.47 | 0.44 |
| 1:E:53:GLU:HG2 | 1:F:173:ALA:HB2 | 2.00 | 0.44 |
| 1:A:163:LEU:HD22 | 1:A:167:LEU:CD2 | 2.44 | 0.43 |
| 1:I:199:ARG:HD3 | 3:I:2153:HOH:O | 2.17 | 0.43 |
| 1:E:112:ARG:HH11 | 2:E:2079:EDO:H12 | 1.83 | 0.43 |
| 1:F:182:GLY:HA3 | 2:F:2043:EDO:H21 | 1.98 | 0.43 |
| 2:D:2119:EDO:H22 | 3:D:2205:HOH:O | 2.17 | 0.43 |
| 1:I:150:LEU:HD12 | 1:J:174:ASP:CB | 2.33 | 0.43 |
| 1:E:5:ILE:HD11 | 1:F:5:ILE:HG21 | 2.00 | 0.43 |
| 1:C:112:ARG:HH11 | 1:C:112:ARG:CA | 2.31 | 0.43 |
| 1:E:24:ILE:HD13 | 1:E:24:ILE:HG21 | 1.62 | 0.43 |
| 2:I:2007:EDO:C1 | 3:I:2207:HOH:O | 2.65 | 0.43 |
| 1:C:36:TRP:CD2 | 1:C:132:ASP:HA | 2.52 | 0.43 |
| 1:E:147:LEU:HD23 | 1:F:171:VAL:HB | 2.00 | 0.43 |
| 1:J:76:VAL:O | 1:J:105:PRO:HA | 2.19 | 0.43 |
| 1:A:207:SER:HB2 | 1:A:213:CYS:SG | 2.58 | 0.43 |
| 1:A:157:ILE:HG22 | 1:A:161:LEU:HD22 | 2.01 | 0.43 |
| 1:I:163:LEU:HD22 | 1:I:167:LEU:HD22 | 2.00 | 0.43 |
| 1:H:5:ILE:HG13 | 1:H:6:PRO:O | 2.19 | 0.43 |
| 1:B:28:ASP:O | 1:B:32:SER:HB2 | 2.18 | 0.43 |
| 1:F:237:PRO:HG2 | 1:F:240:LEU:HD21 | 2.00 | 0.43 |
| 1:I:203:GLY:N | 2:I:2051:EDO:H21 | 2.33 | 0.43 |
| 1:C:103:ALA:C | 1:C:105:PRO:HD3 | 2.37 | 0.43 |
| 1:I:122:THR:HG23 | 1:I:123:HIS:CD2 | 2.53 | 0.43 |
| 1:B:24:ILE:HG21 | 1:B:24:ILE:HD13 | 1.75 | 0.43 |
| 1:J:235:GLU:O | 2:J:2008:EDO:O1 | 2.37 | 0.43 |
| 1:H:183:GLU:H | 2:H:2058:EDO:H12 | 1.82 | 0.43 |
| 1:I:192:THR:HG21 | 2:I:2115:EDO:C2 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:235:GLU:CG | 2:H:2010:EDO:H21 | 2.48 | 0.43 |
| 1:I:39:LEU:C | 1:I:39:LEU:HD12 | 2.38 | 0.43 |
| 1:J:67:LEU:CD2 | 1:J:159:LYS:HD3 | 2.49 | 0.43 |
| 1:B:240:LEU:HA | 1:B:240:LEU:HD23 | 1.75 | 0.43 |
| 2:G:2093:EDO:O1 | 2:G:2093:EDO:O2 | 2.34 | 0.43 |
| 2:E:2089:EDO:C2 | 2:E:2089:EDO:HO2 | 2.12 | 0.43 |
| 1:D:47:THR:CG2 | 1:D:50:CYS:SG | 3.06 | 0.43 |
| 1:G:179:GLU:HG2 | 1:H:59:ARG:NH1 | 2.23 | 0.43 |
| 1:D:143:TYR:HD2 | 1:D:147:LEU:HD13 | 1.84 | 0.43 |
| 1:J:21:HIS:CG | 2:J:2068:EDO:H21 | 2.54 | 0.43 |
| 1:J:157:ILE:CG2 | 1:J:161:LEU:HD22 | 2.49 | 0.43 |
| 1:D:112:ARG:HD2 | 3:D:2218:HOH:O | 2.18 | 0.43 |
| 1:C:21:HIS:HB2 | 2:C:2064:EDO:H22 | 2.00 | 0.43 |
| 1:G:139:THR:OG1 | 1:H:144:PRO:HD3 | 2.19 | 0.43 |
| 1:D:175:TRP:CG | 1:D:176:PRO:HA | 2.54 | 0.43 |
| 1:H:117:HIS:HB2 | 1:H:125:VAL:CG1 | 2.48 | 0.43 |
| 1:D:228:ARG:HG3 | 2:D:2072:EDO:C1 | 2.47 | 0.43 |
| 1:H:76:VAL:HG11 | 1:I:106:GLN:NE2 | 2.34 | 0.43 |
| 1:G:146:GLU:HB3 | 2:H:2111:EDO:H21 | 2.01 | 0.43 |
| 1:C:188:PRO:HA | 1:C:189:PRO:HD3 | 1.94 | 0.43 |
| 1:G:235:GLU:HB2 | 2:G:2009:EDO:C1 | 2.46 | 0.42 |
| 1:G:8:ILE:N | 1:H:117:HIS:CD2 | 2.66 | 0.42 |
| 1:D:111:ARG:NH2 | 1:E:106:GLN:HE21 | 2.16 | 0.42 |
| 1:E:88:TRP:HA | 2:E:2076:EDO:H12 | 2.01 | 0.42 |
| 1:F:111:ARG:NH2 | 1:G:106:GLN:NE2 | 2.64 | 0.42 |
| 1:D:239:LYS:CE | 1:D:244:GLU:OE2 | 2.55 | 0.42 |
| 1:A:14:GLU:O | 1:A:112:ARG:NH2 | 2.51 | 0.42 |
| 1:J:42:HIS:HB2 | 1:J:50:CYS:SG | 2.58 | 0.42 |
| 1:B:189:PRO:HA | 1:B:190:PRO:HD3 | 1.94 | 0.42 |
| 1:H:200:MSE:HE2 | 1:H:200:MSE:HA | 2.01 | 0.42 |
| 1:E:15:MSE:CE | 1:E:112:ARG:HG2 | 2.49 | 0.42 |
| 1:F:36:TRP:CD2 | 1:F:132:ASP:HA | 2.54 | 0.42 |
| 1:H:12:PHE:CZ | 1:H:39:LEU:HD23 | 2.54 | 0.42 |
| 2:J:2008:EDO:C1 | 2:J:2008:EDO:HO2 | 2.31 | 0.42 |
| 1:D:191:THR:N | 1:D:195:GLN:NE2 | 2.57 | 0.42 |
| 1:D:104:ASP:N | 1:D:105:PRO:CD | 2.82 | 0.42 |
| 1:E:106:GLN:O | 1:E:111:ARG:NH2 | 2.53 | 0.42 |
| 1:G:132:ASP:OD1 | 1:G:132:ASP:C | 2.58 | 0.42 |
| 1:B:210:TRP:CZ3 | 1:B:211:TRP:HB3 | 2.54 | 0.42 |
| 1:H:145:MSE:HB3 | 1:H:145:MSE:CE | 2.48 | 0.42 |
| 2:C:2024:EDO:H21 | 2:C:2067:EDO:O1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:2029:EDO:O2 | 2:A:2029:EDO:C1 | 2.54 | 0.42 |
| 1:E:122:THR:HG23 | 1:E:123:HIS:HD2 | 1.83 | 0.42 |
| 1:J:5:ILE:HB | 1:J:6:PRO:HD2 | 2.02 | 0.42 |
| 1:A:7:LEU:HA | 1:A:140:MSE:HE1 | 2.00 | 0.42 |
| 1:I:199:ARG:HD2 | 1:I:205:TYR:CE1 | 2.55 | 0.42 |
| 1:C:67:LEU:O | 1:C:162:LYS:CE | 2.62 | 0.42 |
| 1:H:76:VAL:HG11 | 1:I:106:GLN:HE22 | 1.83 | 0.42 |
| 1:I:180:ILE:HA | 1:J:241:LEU:HB2 | 2.01 | 0.42 |
| 1:E:174:ASP:HB3 | 3:E:505:HOH:O | 2.19 | 0.42 |
| 1:J:190:PRO:HG3 | 1:J:199:ARG:HG3 | 2.01 | 0.42 |
| 1:E:200:MSE:HE1 | 1:E:213:CYS:SG | 2.59 | 0.42 |
| 1:G:146:GLU:CB | 2:H:2111:EDO:H21 | 2.49 | 0.42 |
| 1:H:132:ASP:C | 1:H:132:ASP:OD1 | 2.58 | 0.42 |
| 1:G:5:ILE:HD13 | 1:H:5:ILE:HD13 | 2.00 | 0.42 |
| 1:C:139:THR:OG1 | 1:D:144:PRO:HD3 | 2.19 | 0.42 |
| 1:A:61:TYR:HD1 | 1:A:71:LEU:HD12 | 1.85 | 0.42 |
| 1:D:235:GLU:CB | 2:D:2003:EDO:H11 | 2.31 | 0.42 |
| 1:F:140:MSE:HB3 | 1:F:140:MSE:HE2 | 1.71 | 0.42 |
| 1:E:91:ARG:NH1 | 2:E:2076:EDO:O2 | 2.53 | 0.42 |
| 1:F:204:GLN:HB2 | 1:F:204:GLN:HE21 | 1.42 | 0.42 |
| 1:E:134:ARG:HG3 | 2:E:2039:EDO:H11 | 2.01 | 0.42 |
| 1:G:242:TYR:CD2 | 1:G:243:GLU:HG3 | 2.55 | 0.42 |
| 1:I:146:GLU:HG3 | 3:J:2159:HOH:O | 2.20 | 0.42 |
| 1:E:25:LYS:HD2 | 1:E:25:LYS:NZ | 2.28 | 0.42 |
| 2:A:2124:EDO:C2 | 2:A:2124:EDO:HO2 | 2.13 | 0.42 |
| 1:E:208:LEU:HD13 | 1:F:242:TYR:CD1 | 2.55 | 0.42 |
| 1:E:214:TRP:CH2 | 1:F:242:TYR:CG | 3.04 | 0.42 |
| 1:F:79:VAL:HG22 | 2:F:2038:EDO:H12 | 2.02 | 0.42 |
| 1:B:36:TRP:CD2 | 1:B:132:ASP:HA | 2.54 | 0.42 |
| 1:F:185:LEU:HA | 1:F:185:LEU:HD23 | 1.87 | 0.42 |
| 1:E:208:LEU:HA | 1:E:208:LEU:HD12 | 1.78 | 0.42 |
| 1:E:139:THR:C | 1:E:140:MSE:HG3 | 2.40 | 0.42 |
| 1:J:97:ILE:N | 2:J:2109:EDO:C1 | 2.55 | 0.42 |
| 1:F:79:VAL:CG2 | 2:F:2038:EDO:H12 | 2.50 | 0.42 |
| 1:A:189:PRO:HA | 1:A:190:PRO:HD3 | 1.78 | 0.42 |
| 1:F:106:GLN:HG2 | 1:G:122:THR:HA | 2.02 | 0.41 |
| 1:G:8:ILE:HG13 | 1:H:117:HIS:CD2 | 2.55 | 0.41 |
| 2:F:2087:EDO:H11 | 3:F:998:HOH:O | 2.20 | 0.41 |
| 1:I:157:ILE:HG23 | 1:J:147:LEU:HD11 | 2.01 | 0.41 |
| 1:J:67:LEU:HD21 | 1:J:159:LYS:HD3 | 2.01 | 0.41 |
| 1:J:163:LEU:HD22 | 1:J:167:LEU:HD22 | 2.00 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:99:PHE:HB2 | 1:F:100:PRO:HD2 | 2.01 | 0.41 |
| 1:B:105:PRO:HG2 | 1:C:122:THR:OG1 | 2.21 | 0.41 |
| 1:A:242:TYR:HD1 | 1:B:208:LEU:CD1 | 2.33 | 0.41 |
| 1:F:42:HIS:HB2 | 1:F:50:CYS:SG | 2.60 | 0.41 |
| 1:J:225:GLU:HG3 | 2:J:2049:EDO:C2 | 2.50 | 0.41 |
| 1:I:192:THR:CG2 | 2:I:2115:EDO:H22 | 2.50 | 0.41 |
| 1:B:204:GLN:N | 2:B:2030:EDO:H21 | 2.35 | 0.41 |
| 1:J:96:ARG:CG | 2:J:2109:EDO:O2 | 2.59 | 0.41 |
| 1:C:111:ARG:HG3 | 1:C:116:LEU:HD12 | 2.02 | 0.41 |
| 2:J:2108:EDO:H11 | 3:J:2191:HOH:O | 2.20 | 0.41 |
| 1:E:91:ARG:HD3 | 2:E:2076:EDO:C1 | 2.50 | 0.41 |
| 1:A:45:ASP:O | 1:A:46:PHE:HB2 | 2.20 | 0.41 |
| 1:C:14:GLU:OE1 | 1:C:25:LYS:HE2 | 2.20 | 0.41 |
| 1:B:87:GLU:HG2 | 1:B:91:ARG:NH2 | 2.35 | 0.41 |
| 1:B:185:LEU:O | 1:B:214:TRP:HB2 | 2.21 | 0.41 |
| 1:F:41:SER:HA | 1:F:74:LEU:O | 2.20 | 0.41 |
| 1:G:42:HIS:CE1 | 1:G:75:SER:HB3 | 2.55 | 0.41 |
| 1:B:231:ARG:HH11 | 1:B:231:ARG:HD2 | 1.62 | 0.41 |
| 1:I:86:LYS:HE3 | 1:I:101:ILE:CD1 | 2.50 | 0.41 |
| 1:I:19:THR:HA | 1:I:102:ILE:HA | 2.02 | 0.41 |
| 1:B:91:ARG:NE | 2:B:2125:EDO:O2 | 2.53 | 0.41 |
| 1:G:19:THR:HG22 | 1:G:102:ILE:HG12 | 2.02 | 0.41 |
| 1:B:173:ALA:O | 1:B:174:ASP:HB2 | 2.19 | 0.41 |
| 1:A:91:ARG:HG2 | 1:A:92:HIS:CD2 | 2.54 | 0.41 |
| 1:F:128:VAL:O | 1:F:140:MSE:HA | 2.20 | 0.41 |
| 1:J:35:LYS:CD | 1:J:70:ASP:OD2 | 2.67 | 0.41 |
| 1:F:13:PRO:O | 1:F:15:MSE:HG2 | 2.21 | 0.41 |
| 1:C:179:GLU:CD | 1:D:59:ARG:HH12 | 2.24 | 0.41 |
| 1:I:11:ARG:HD3 | 3:I:2167:HOH:O | 2.20 | 0.41 |
| 1:H:35:LYS:NZ | 1:H:65:GLN:HE22 | 2.19 | 0.41 |
| 1:G:145:MSE:HE2 | 1:G:145:MSE:CB | 2.51 | 0.41 |
| 1:E:36:TRP:CD1 | 1:E:162:LYS:HE2 | 2.56 | 0.41 |
| 1:I:242:TYR:HA | 1:I:245:ALA:HB3 | 2.03 | 0.41 |
| 1:H:235:GLU:OE1 | 2:H:2010:EDO:C2 | 2.69 | 0.41 |
| 1:E:128:VAL:O | 1:E:140:MSE:HA | 2.21 | 0.41 |
| 1:B:67:LEU:CB | 1:B:69:VAL:HG23 | 2.51 | 0.41 |
| 1:G:183:GLU:HG2 | 2:G:2057:EDO:C2 | 2.50 | 0.41 |
| 1:G:239:LYS:HG2 | 1:G:244:GLU:OE2 | 2.20 | 0.41 |
| 1:E:15:MSE:SE | 1:E:109:VAL:HG13 | 2.71 | 0.41 |
| 1:E:15:MSE:HE1 | 1:E:112:ARG:HG2 | 2.02 | 0.41 |
| 1:G:5:ILE:O | 1:H:2:PRO:HB3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:227:ARG:HH11 | 1:B:227:ARG:HD2 | 1.62 | 0.41 |
| 1:E:150:LEU:HD12 | 1:E:150:LEU:HA | 1.86 | 0.41 |
| 1:E:236:LYS:CE | 2:F:2043:EDO:H22 | 2.50 | 0.41 |
| 1:A:244:GLU:OE2 | 2:A:2066:EDO:H22 | 2.21 | 0.41 |
| 1:D:5:ILE:HG22 | 1:D:114:GLY:HA3 | 2.03 | 0.40 |
| 1:F:112:ARG:CB | 1:F:112:ARG:NH1 | 2.79 | 0.40 |
| 1:C:36:TRP:HB2 | 1:C:69:VAL:HG22 | 2.04 | 0.40 |
| 1:E:191:THR:H | 1:E:195:GLN:NE2 | 2.18 | 0.40 |
| 1:J:183:GLU:H | 1:J:183:GLU:HG2 | 1.45 | 0.40 |
| 1:C:15:MSE:HG3 | 1:C:15:MSE:O | 2.21 | 0.40 |
| 1:B:216:THR:HA | 3:B:2200:HOH:O | 2.20 | 0.40 |
| 1:D:43:PRO:HG3 | 1:D:145:MSE:HG2 | 2.01 | 0.40 |
| 1:F:168:LYS:HE3 | 3:F:1011:HOH:O | 2.20 | 0.40 |
| 3:A:2219:HOH:O | 1:B:242:TYR:HB2 | 2.21 | 0.40 |
| 1:B:169:ARG:HB3 | 1:B:185:LEU:HB3 | 2.03 | 0.40 |
| 1:H:132:ASP:OD2 | 1:H:138:ARG:HD3 | 2.21 | 0.40 |
| 1:E:52:THR:HB | 1:F:178:ASN:HD21 | 1.85 | 0.40 |
| 1:C:35:LYS:HG3 | 2:C:2084:EDO:H11 | 2.02 | 0.40 |
| 1:B:68:GLY:HA3 | 3:B:2242:HOH:O | 2.21 | 0.40 |
| 1:H:227:ARG:HH11 | 1:H:227:ARG:HD2 | 1.55 | 0.40 |
| 1:J:189:PRO:HA | 1:J:190:PRO:HD3 | 1.73 | 0.40 |
| 1:D:106:GLN:O | 1:D:111:ARG:NH1 | 2.54 | 0.40 |
| 1:D:231:ARG:HD2 | 1:D:231:ARG:HH11 | 1.56 | 0.40 |
| 1:E:5:ILE:HD13 | 1:F:5:ILE:HG21 | 2.03 | 0.40 |
| 1:D:74:LEU:HD23 | 1:D:102:ILE:HB | 2.03 | 0.40 |
| 1:B:104:ASP:OD1 | 1:B:107:GLY:HA2 | 2.22 | 0.40 |
| 1:G:199:ARG:HH11 | 1:G:199:ARG:HD2 | 1.56 | 0.40 |
| 1:A:231:ARG:NH2 | 3:A:2260:HOH:O | 2.28 | 0.40 |
| 1:E:104:ASP:HB2 | 3:E:336:HOH:O | 2.22 | 0.40 |
| 1:A:171:VAL:HA | 1:A:172:PRO:HD2 | 1.88 | 0.40 |
| 1:J:240:LEU:H | 1:J:243:GLU:CD | 2.22 | 0.40 |
| 1:E:52:THR:HG22 | 1:F:180:ILE:HD12 | 2.03 | 0.40 |
| 1:B:187:VAL:O | 1:B:188:PRO:C | 2.60 | 0.40 |
| 1:G:240:LEU:HD23 | 1:G:240:LEU:HA | 1.88 | 0.40 |
| 1:J:216:THR:N | 1:J:217:PRO:CD | 2.85 | 0.40 |
| 1:B:244:GLU:H | 1:B:244:GLU:CD | 2.25 | 0.40 |
| 1:F:219:SER:N | 2:F:2097:EDO:O2 | 2.36 | 0.40 |
| 1:H:42:HIS:HB2 | 1:H:50:CYS:SG | 2.62 | 0.40 |
| 1:H:231:ARG:NH2 | 3:H:1081:HOH:O | 2.50 | 0.40 |
| 1:I:143:TYR:CD2 | 1:I:147:LEU:HD13 | 2.57 | 0.40 |
| 1:E:84:LYS:HD2 | 1:E:84:LYS:HA | 1.94 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 2:H:2114:EDO:O1 | 3:C:2190:HOH:O[1_556] | 2.16 | 0.04 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1 | A | 242/249 (97%) | 229 (95%) | 10 (4%) | 3 (1%) | 16 | 8 |
| 1 | B | 242/249 (97%) | 234 (97%) | 6 (2%) | 2 (1%) | 24 | 15 |
| 1 | C | 242/249 (97%) | 235 (97%) | 6 (2%) | 1 (0%) | 39 | 33 |
| 1 | D | 242/249 (97%) | 231 (96%) | 9 (4%) | 2 (1%) | 24 | 15 |
| 1 | E | 242/249 (97%) | 233 (96%) | 6 (2%) | 3 (1%) | 16 | 8 |
| 1 | F | 242/249 (97%) | 235 (97%) | 6 (2%) | 1 (0%) | 39 | 33 |
| 1 | G | 242/249 (97%) | 232 (96%) | 7 (3%) | 3 (1%) | 16 | 8 |
| 1 | H | 242/249 (97%) | 233 (96%) | 7 (3%) | 2 (1%) | 24 | 15 |
| 1 | I | 242/249 (97%) | 234 (97%) | 7 (3%) | 1 (0%) | 39 | 33 |
| 1 | J | 242/249 (97%) | 236 (98%) | 3 (1%) | 3 (1%) | 16 | 8 |
| All | All | 2420/2490 (97%) | 2332 (96%) | 67 (3%) | 21 (1%) | 21 | 13 |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 176 | PRO |
| 1 | G | 27 | PRO |
| 1 | J | 27 | PRO |
| 1 | A | 106 | GLN |
| 1 | A | 244 | GLU |
| 1 | B | 106 | GLN |
| 1 | E | 106 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 106 | GLN |
| 1 | J | 106 | GLN |
| 1 | G | 106 | GLN |
| 1 | I | 119 | GLU |
| 1 | D | 105 | PRO |
| 1 | E | 239 | LYS |
| 1 | G | 239 | LYS |
| 1 | F | 106 | GLN |
| 1 | C | 125 | VAL |
| 1 | H | 125 | VAL |
| 1 | A | 203 | GLY |
| 1 | B | 125 | VAL |
| 1 | D | 125 | VAL |
| 1 | J | 125 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 1 | A | 210/211 (100%) | 190 (90%) | 20 (10%) | 11 | 6 |
| 1 | B | 210/211 (100%) | 193 (92%) | 17 (8%) | 15 | 9 |
| 1 | C | 210/211 (100%) | 189 (90%) | 21 (10%) | 9 | 5 |
| 1 | D | 210/211 (100%) | 193 (92%) | 17 (8%) | 15 | 9 |
| 1 | E | 210/211 (100%) | 197 (94%) | 13 (6%) | 23 | 16 |
| 1 | F | 210/211 (100%) | 193 (92%) | 17 (8%) | 15 | 9 |
| 1 | G | 210/211 (100%) | 195 (93%) | 15 (7%) | 18 | 12 |
| 1 | H | 210/211 (100%) | 197 (94%) | 13 (6%) | 23 | 16 |
| 1 | I | 210/211 (100%) | 190 (90%) | 20 (10%) | 11 | 6 |
| 1 | J | 210/211 (100%) | 190 (90%) | 20 (10%) | 11 | 6 |
| All | All | 2100/2110 (100%) | 1927 (92%) | 173 (8%) | 14 | 9 |

All (173) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | ARG |
| 1 | A | 14 | GLU |
| 1 | A | 16 | GLU |
| 1 | A | 28 | ASP |
| 1 | A | 47 | THR |
| 1 | A | 147 | LEU |
| 1 | A | 159 | LYS |
| 1 | A | 161 | LEU |
| 1 | A | 162 | LYS |
| 1 | A | 166 | SER |
| 1 | A | 167 | LEU |
| 1 | A | 176 | PRO |
| 1 | A | 194 | ASP |
| 1 | A | 197 | ARG |
| 1 | A | 202 | SER |
| 1 | A | 207 | SER |
| 1 | A | 208 | LEU |
| 1 | A | 212 | PHE |
| 1 | A | 214 | TRP |
| 1 | A | 244 | GLU |
| 1 | B | 4 | SER |
| 1 | B | 11 | ARG |
| 1 | B | 39 | LEU |
| 1 | B | 59 | ARG |
| 1 | B | 65 | GLN |
| 1 | B | 112 | ARG |
| 1 | B | 147 | LEU |
| 1 | B | 150 | LEU |
| 1 | B | 159 | LYS |
| 1 | B | 161 | LEU |
| 1 | B | 162 | LYS |
| 1 | B | 167 | LEU |
| 1 | B | 199 | ARG |
| 1 | B | 208 | LEU |
| 1 | B | 212 | PHE |
| 1 | B | 228 | ARG |
| 1 | B | 244 | GLU |
| 1 | C | 5 | ILE |
| 1 | C | 11 | ARG |
| 1 | C | 17 | VAL |
| 1 | C | 28 | ASP |
| 1 | C | 39 | LEU |
| 1 | C | 47 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 66 | ARG |
| 1 | C | 74 | LEU |
| 1 | C | 112 | ARG |
| 1 | C | 147 | LEU |
| 1 | C | 161 | LEU |
| 1 | C | 167 | LEU |
| 1 | C | 199 | ARG |
| 1 | C | 204 | GLN |
| 1 | C | 208 | LEU |
| 1 | C | 212 | PHE |
| 1 | C | 217 | PRO |
| 1 | C | 219 | SER |
| 1 | C | 220 | ARG |
| 1 | C | 224 | GLU |
| 1 | C | 239 | LYS |
| 1 | D | 28 | ASP |
| 1 | D | 47 | THR |
| 1 | D | 48 | PRO |
| 1 | D | 96 | ARG |
| 1 | D | 112 | ARG |
| 1 | D | 122 | THR |
| 1 | D | 147 | LEU |
| 1 | D | 161 | LEU |
| 1 | D | 163 | LEU |
| 1 | D | 167 | LEU |
| 1 | D | 197 | ARG |
| 1 | D | 208 | LEU |
| 1 | D | 212 | PHE |
| 1 | D | 217 | PRO |
| 1 | D | 225 | GLU |
| 1 | D | 242 | TYR |
| 1 | D | 244 | GLU |
| 1 | E | 2 | PRO |
| 1 | E | 11 | ARG |
| 1 | E | 28 | ASP |
| 1 | E | 70 | ASP |
| 1 | E | 112 | ARG |
| 1 | E | 147 | LEU |
| 1 | E | 159 | LYS |
| 1 | E | 167 | LEU |
| 1 | E | 191 | THR |
| 1 | E | 194 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 201 | GLU |
| 1 | E | 208 | LEU |
| 1 | E | 212 | PHE |
| 1 | F | 2 | PRO |
| 1 | F | 11 | ARG |
| 1 | F | 24 | ILE |
| 1 | F | 28 | ASP |
| 1 | F | 95 | VAL |
| 1 | F | 112 | ARG |
| 1 | F | 119 | GLU |
| 1 | F | 159 | LYS |
| 1 | F | 161 | LEU |
| 1 | F | 167 | LEU |
| 1 | F | 197 | ARG |
| 1 | F | 204 | GLN |
| 1 | F | 208 | LEU |
| 1 | F | 212 | PHE |
| 1 | F | 217 | PRO |
| 1 | F | 220 | ARG |
| 1 | F | 239 | LYS |
| 1 | G | 11 | ARG |
| 1 | G | 17 | VAL |
| 1 | G | 28 | ASP |
| 1 | G | 96 | ARG |
| 1 | G | 106 | GLN |
| 1 | G | 112 | ARG |
| 1 | G | 124 | THR |
| 1 | G | 144 | PRO |
| 1 | G | 147 | LEU |
| 1 | G | 150 | LEU |
| 1 | G | 161 | LEU |
| 1 | G | 167 | LEU |
| 1 | G | 199 | ARG |
| 1 | G | 208 | LEU |
| 1 | G | 242 | TYR |
| 1 | H | 28 | ASP |
| 1 | H | 39 | LEU |
| 1 | H | 59 | ARG |
| 1 | H | 93 | ILE |
| 1 | H | 119 | GLU |
| 1 | H | 144 | PRO |
| 1 | H | 147 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 159 | LYS |
| 1 | H | 161 | LEU |
| 1 | H | 167 | LEU |
| 1 | H | 201 | GLU |
| 1 | H | 204 | GLN |
| 1 | H | 208 | LEU |
| 1 | I | 4 | SER |
| 1 | I | 11 | ARG |
| 1 | I | 28 | ASP |
| 1 | I | 39 | LEU |
| 1 | I | 59 | ARG |
| 1 | I | 62 | GLU |
| 1 | I | 66 | ARG |
| 1 | I | 112 | ARG |
| 1 | I | 119 | GLU |
| 1 | I | 125 | VAL |
| 1 | I | 128 | VAL |
| 1 | I | 144 | PRO |
| 1 | I | 147 | LEU |
| 1 | I | 158 | VAL |
| 1 | I | 167 | LEU |
| 1 | I | 199 | ARG |
| 1 | I | 212 | PHE |
| 1 | I | 235 | GLU |
| 1 | I | 239 | LYS |
| 1 | I | 244 | GLU |
| 1 | J | 2 | PRO |
| 1 | J | 28 | ASP |
| 1 | J | 48 | PRO |
| 1 | J | 70 | ASP |
| 1 | J | 74 | LEU |
| 1 | J | 106 | GLN |
| 1 | J | 122 | THR |
| 1 | J | 147 | LEU |
| 1 | J | 161 | LEU |
| 1 | J | 162 | LYS |
| 1 | J | 166 | SER |
| 1 | J | 167 | LEU |
| 1 | J | 174 | ASP |
| 1 | J | 183 | GLU |
| 1 | J | 199 | ARG |
| 1 | J | 208 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 212 | PHE |
| 1 | J | 215 | ASP |
| 1 | J | 228 | ARG |
| 1 | J | 244 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 106 | GLN |
| 1 | A | 117 | HIS |
| 1 | A | 123 | HIS |
| 1 | A | 204 | GLN |
| 1 | B | 65 | GLN |
| 1 | B | 106 | GLN |
| 1 | B | 117 | HIS |
| 1 | C | 106 | GLN |
| 1 | C | 117 | HIS |
| 1 | C | 195 | GLN |
| 1 | C | 204 | GLN |
| 1 | D | 106 | GLN |
| 1 | D | 117 | HIS |
| 1 | D | 195 | GLN |
| 1 | E | 65 | GLN |
| 1 | E | 106 | GLN |
| 1 | E | 117 | HIS |
| 1 | E | 123 | HIS |
| 1 | E | 195 | GLN |
| 1 | F | 117 | HIS |
| 1 | F | 123 | HIS |
| 1 | F | 195 | GLN |
| 1 | F | 204 | GLN |
| 1 | G | 92 | HIS |
| 1 | G | 106 | GLN |
| 1 | H | 65 | GLN |
| 1 | H | 117 | HIS |
| 1 | H | 195 | GLN |
| 1 | I | 92 | HIS |
| 1 | I | 117 | HIS |
| 1 | I | 195 | GLN |
| 1 | J | 92 | HIS |
| 1 | J | 117 | HIS |
| 1 | J | 195 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

128 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | EDO | A | 2001 | - | 3,3,3 | 2.44 | 2 (66%) | 2,2,2 | 0.23 | 0 |
| 2 | EDO | A | 2011 | - | 3,3,3 | 2.59 | 2 (66%) | 2,2,2 | 1.39 | 0 |
| 2 | EDO | A | 2012 | - | 3,3,3 | 3.86 | 2 (66%) | 2,2,2 | 0.35 | 0 |
| 2 | EDO | A | 2016 | - | 3,3,3 | 2.09 | 2 (66%) | 2,2,2 | 0.62 | 0 |
| 2 | EDO | A | 2017 | - | 3,3,3 | 1.97 | 2 (66%) | 2,2,2 | 1.02 | 0 |
| 2 | EDO | A | 2019 | - | 3,3,3 | 2.60 | 2 (66%) | 2,2,2 | 0.81 | 0 |
| 2 | EDO | A | 2022 | - | 3,3,3 | 1.97 | 1 (33%) | 2,2,2 | 1.08 | 0 |
| 2 | EDO | A | 2029 | - | 3,3,3 | 3.11 | 2 (66%) | 2,2,2 | 0.76 | 0 |
| 2 | EDO | A | 2063 | - | 3,3,3 | 3.25 | 2 (66%) | 2,2,2 | 1.05 | 0 |
| 2 | EDO | A | 2065 | - | 3,3,3 | 2.50 | 2 (66%) | 2,2,2 | 0.71 | 0 |
| 2 | EDO | A | 2066 | - | 3,3,3 | 2.87 | 2 (66%) | 2,2,2 | 0.53 | 0 |
| 2 | EDO | A | 2116 | - | 3,3,3 | 2.93 | 2 (66%) | 2,2,2 | 0.47 | 0 |
| 2 | EDO | A | 2122 | - | 3,3,3 | 2.99 | 1 (33%) | 2,2,2 | 1.35 | 0 |
| 2 | EDO | A | 2124 | - | 3,3,3 | 4.22 | 2 (66%) | 2,2,2 | 0.81 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | EDO | B | 2002 | - | 3,3,3 | 4.43 | 2 (66%) | 2,2,2 | 1.29 | 0 |
| 2 | EDO | B | 2013 | - | 3,3,3 | 2.35 | 2 (66%) | 2,2,2 | 0.79 | 0 |
| 2 | EDO | B | 2015 | - | 3,3,3 | 2.28 | 2 (66%) | 2,2,2 | 0.73 | 0 |
| 2 | EDO | B | 2018 | - | 3,3,3 | 2.07 | 2 (66%) | 2,2,2 | 0.85 | 0 |
| 2 | EDO | B | 2020 | - | 3,3,3 | 2.85 | 2 (66%) | 2,2,2 | 0.80 | 0 |
| 2 | EDO | B | 2021 | - | 3,3,3 | 3.86 | 2 (66%) | 2,2,2 | 0.13 | 0 |
| 2 | EDO | B | 2023 | - | 3,3,3 | 3.10 | 2 (66%) | 2,2,2 | 1.05 | 0 |
| 2 | EDO | B | 2025 | - | 3,3,3 | 2.81 | 2 (66%) | 2,2,2 | 0.72 | 0 |
| 2 | EDO | B | 2027 | - | 3,3,3 | 1.65 | 1 (33%) | 2,2,2 | 1.21 | 0 |
| 2 | EDO | B | 2028 | - | 3,3,3 | 2.21 | 2 (66%) | 2,2,2 | 1.20 | 0 |
| 2 | EDO | B | 2030 | - | 3,3,3 | 1.00 | 0 | 2,2,2 | 0.37 | 0 |
| 2 | EDO | B | 2062 | - | 3,3,3 | 1.80 | 1 (33%) | 2,2,2 | 1.11 | 0 |
| 2 | EDO | B | 2070 | - | 3,3,3 | 2.71 | 2 (66%) | 2,2,2 | 0.95 | 0 |
| 2 | EDO | B | 2125 | - | 3,3,3 | 2.70 | 3 (100%) | 2,2,2 | 1.02 | 0 |
| 2 | EDO | C | 2004 | - | 3,3,3 | 4.28 | 2 (66%) | 2,2,2 | 0.53 | 0 |
| 2 | EDO | C | 2024 | - | 3,3,3 | 3.29 | 2 (66%) | 2,2,2 | 0.86 | 0 |
| 2 | EDO | C | 2026 | - | 3,3,3 | 1.03 | 0 | 2,2,2 | 0.83 | 0 |
| 2 | EDO | C | 2036 | - | 3,3,3 | 2.59 | 2 (66%) | 2,2,2 | 1.17 | 0 |
| 2 | EDO | C | 2064 | - | 3,3,3 | 2.60 | 2 (66%) | 2,2,2 | 0.63 | 0 |
| 2 | EDO | C | 2067 | - | 3,3,3 | 2.72 | 1 (33%) | 2,2,2 | 0.47 | 0 |
| 2 | EDO | C | 2075 | - | 3,3,3 | 2.09 | 2 (66%) | 2,2,2 | 1.27 | 0 |
| 2 | EDO | C | 2080 | - | 3,3,3 | 2.64 | 2 (66%) | 2,2,2 | 0.45 | 0 |
| 2 | EDO | C | 2081 | - | 3,3,3 | 2.75 | 3 (100%) | 2,2,2 | 0.97 | 0 |
| 2 | EDO | C | 2082 | - | 3,3,3 | 3.15 | 1 (33%) | 2,2,2 | 0.67 | 0 |
| 2 | EDO | C | 2083 | - | 3,3,3 | 2.66 | 2 (66%) | 2,2,2 | 1.31 | 0 |
| 2 | EDO | C | 2084 | - | 3,3,3 | 3.03 | 2 (66%) | 2,2,2 | 1.30 | 0 |
| 2 | EDO | C | 2085 | - | 3,3,3 | 3.85 | 2 (66%) | 2,2,2 | 1.45 | 1 (50%) |
| 2 | EDO | C | 2117 | - | 3,3,3 | 2.31 | 2 (66%) | 2,2,2 | 0.52 | 0 |
| 2 | EDO | C | 2126 | - | 3,3,3 | 3.17 | 3 (100%) | 2,2,2 | 0.59 | 0 |
| 2 | EDO | C | 2128 | - | 3,3,3 | 3.27 | 2 (66%) | 2,2,2 | 1.02 | 0 |
| 2 | EDO | D | 2003 | - | 3,3,3 | 2.68 | 2 (66%) | 2,2,2 | 0.93 | 0 |
| 2 | EDO | D | 2031 | - | 3,3,3 | 2.87 | 2 (66%) | 2,2,2 | 0.62 | 0 |
| 2 | EDO | D | 2033 | - | 3,3,3 | 2.22 | 2 (66%) | 2,2,2 | 1.08 | 0 |
| 2 | EDO | D | 2035 | - | 3,3,3 | 1.24 | 0 | 2,2,2 | 0.34 | 0 |
| 2 | EDO | D | 2071 | - | 3,3,3 | 2.81 | 2 (66%) | 2,2,2 | 0.56 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | EDO | D | 2072 | - | 3,3,3 | 2.55 | 2 (66%) | 2,2,2 | 0.66 | 0 |
| 2 | EDO | D | 2073 | - | 3,3,3 | 2.01 | 2 (66%) | 2,2,2 | 0.70 | 0 |
| 2 | EDO | D | 2074 | - | 3,3,3 | 3.61 | 2 (66%) | 2,2,2 | 1.44 | 0 |
| 2 | EDO | D | 2118 | - | 3,3,3 | 3.05 | 2 (66%) | 2,2,2 | 0.30 | 0 |
| 2 | EDO | D | 2119 | - | 3,3,3 | 2.48 | 2 (66%) | 2,2,2 | 0.98 | 0 |
| 2 | EDO | E | 2005 | - | 3,3,3 | 4.29 | 2 (66%) | 2,2,2 | 0.54 | 0 |
| 2 | EDO | E | 2032 | - | 3,3,3 | 2.93 | 1 (33%) | 2,2,2 | 0.89 | 0 |
| 2 | EDO | E | 2039 | - | 3,3,3 | 2.04 | 2 (66%) | 2,2,2 | 0.36 | 0 |
| 2 | EDO | E | 2040 | - | 3,3,3 | 2.54 | 2 (66%) | 2,2,2 | 0.88 | 0 |
| 2 | EDO | E | 2041 | - | 3,3,3 | 1.64 | 1 (33%) | 2,2,2 | 1.09 | 0 |
| 2 | EDO | E | 2042 | - | 3,3,3 | 2.10 | 2 (66%) | 2,2,2 | 0.89 | 0 |
| 2 | EDO | E | 2076 | - | 3,3,3 | 2.48 | 2 (66%) | 2,2,2 | 1.00 | 0 |
| 2 | EDO | E | 2077 | - | 3,3,3 | 2.61 | 2 (66%) | 2,2,2 | 0.98 | 0 |
| 2 | EDO | E | 2078 | - | 3,3,3 | 2.32 | 1 (33%) | 2,2,2 | 1.41 | 0 |
| 2 | EDO | E | 2079 | - | 3,3,3 | 2.60 | 2 (66%) | 2,2,2 | 1.23 | 0 |
| 2 | EDO | E | 2088 | - | 3,3,3 | 2.72 | 2 (66%) | 2,2,2 | 1.26 | 0 |
| 2 | EDO | E | 2089 | - | 3,3,3 | 3.34 | 2 (66%) | 2,2,2 | 0.23 | 0 |
| 2 | EDO | E | 2090 | - | 3,3,3 | 2.58 | 2 (66%) | 2,2,2 | 0.65 | 0 |
| 2 | EDO | E | 2091 | - | 3,3,3 | 3.15 | 2 (66%) | 2,2,2 | 1.34 | 0 |
| 2 | EDO | E | 2092 | - | 3,3,3 | 1.75 | 1 (33%) | 2,2,2 | 1.32 | 0 |
| 2 | EDO | E | 2120 | - | 3,3,3 | 2.86 | 2 (66%) | 2,2,2 | 0.78 | 0 |
| 2 | EDO | E | 2127 | - | 3,3,3 | 2.52 | 2 (66%) | 2,2,2 | 1.53 | 1 (50%) |
| 2 | EDO | F | 2006 | - | 3,3,3 | 3.42 | 3 (100%) | 2,2,2 | 0.93 | 0 |
| 2 | EDO | F | 2034 | - | 3,3,3 | 2.11 | 1 (33%) | 2,2,2 | 0.31 | 0 |
| 2 | EDO | F | 2037 | - | 3,3,3 | 2.39 | 2 (66%) | 2,2,2 | 1.12 | 0 |
| 2 | EDO | F | 2038 | - | 3,3,3 | 2.38 | 2 (66%) | 2,2,2 | 0.74 | 0 |
| 2 | EDO | F | 2043 | - | 3,3,3 | 2.92 | 2 (66%) | 2,2,2 | 1.43 | 1 (50%) |
| 2 | EDO | F | 2086 | - | 3,3,3 | 2.38 | 2 (66%) | 2,2,2 | 1.53 | 1 (50%) |
| 2 | EDO | F | 2087 | - | 3,3,3 | 1.59 | 1 (33%) | 2,2,2 | 0.84 | 0 |
| 2 | EDO | F | 2094 | - | 3,3,3 | 2.88 | 2 (66%) | 2,2,2 | 1.48 | 1 (50%) |
| 2 | EDO | F | 2095 | - | 3,3,3 | 2.94 | 2 (66%) | 2,2,2 | 1.06 | 0 |
| 2 | EDO | F | 2096 | - | 3,3,3 | 2.31 | 2 (66%) | 2,2,2 | 1.04 | 0 |
| 2 | EDO | F | 2097 | - | 3,3,3 | 2.84 | 2 (66%) | 2,2,2 | 0.15 | 0 |
| 2 | EDO | F | 2098 | - | 3,3,3 | 4.00 | 2 (66%) | 2,2,2 | 0.83 | 0 |
| 2 | EDO | G | 2009 | - | 3,3,3 | 3.59 | 2 (66%) | 2,2,2 | 1.23 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | EDO | G | 2047 | - | 3,3,3 | 2.70 | 2 (66%) | 2,2,2 | 0.79 | 0 |
| 2 | EDO | G | 2050 | - | 3,3,3 | 2.86 | 1 (33%) | 2,2,2 | 0.29 | 0 |
| 2 | EDO | G | 2056 | - | 3,3,3 | 3.04 | 2 (66%) | 2,2,2 | 0.91 | 0 |
| 2 | EDO | G | 2057 | - | 3,3,3 | 1.40 | 1 (33%) | 2,2,2 | 0.92 | 0 |
| 2 | EDO | G | 2093 | - | 3,3,3 | 2.91 | 2 (66%) | 2,2,2 | 1.23 | 0 |
| 2 | EDO | G | 2101 | - | 3,3,3 | 2.18 | 2 (66%) | 2,2,2 | 1.96 | 1 (50%) |
| 2 | EDO | G | 2102 | - | 3,3,3 | 2.95 | 2 (66%) | 2,2,2 | 0.83 | 0 |
| 2 | EDO | G | 2112 | - | 3,3,3 | 2.57 | 2 (66%) | 2,2,2 | 0.48 | 0 |
| 2 | EDO | H | 2010 | - | 3,3,3 | 3.80 | 2 (66%) | 2,2,2 | 0.45 | 0 |
| 2 | EDO | H | 2044 | - | 3,3,3 | 2.11 | 1 (33%) | 2,2,2 | 0.30 | 0 |
| 2 | EDO | H | 2054 | - | 3,3,3 | 2.16 | 2 (66%) | 2,2,2 | 0.99 | 0 |
| 2 | EDO | H | 2058 | - | 3,3,3 | 3.19 | 2 (66%) | 2,2,2 | 1.58 | 1 (50%) |
| 2 | EDO | H | 2059 | - | 3,3,3 | 3.89 | 3 (100%) | 2,2,2 | 0.53 | 0 |
| 2 | EDO | H | 2060 | - | 3,3,3 | 0.98 | 0 | 2,2,2 | 0.22 | 0 |
| 2 | EDO | H | 2111 | - | 3,3,3 | 2.47 | 3 (100%) | 2,2,2 | 1.07 | 0 |
| 2 | EDO | H | 2113 | - | 3,3,3 | 2.42 | 1 (33%) | 2,2,2 | 0.85 | 0 |
| 2 | EDO | H | 2114 | - | 3,3,3 | 3.06 | 2 (66%) | 2,2,2 | 0.97 | 0 |
| 2 | EDO | I | 2007 | - | 3,3,3 | 3.64 | 2 (66%) | 2,2,2 | 1.50 | 1 (50%) |
| 2 | EDO | I | 2045 | - | 3,3,3 | 2.86 | 2 (66%) | 2,2,2 | 0.49 | 0 |
| 2 | EDO | I | 2046 | - | 3,3,3 | 2.14 | 1 (33%) | 2,2,2 | 1.11 | 0 |
| 2 | EDO | I | 2051 | - | 3,3,3 | 1.93 | 1 (33%) | 2,2,2 | 1.18 | 0 |
| 2 | EDO | I | 2052 | - | 3,3,3 | 2.49 | 2 (66%) | 2,2,2 | 1.08 | 0 |
| 2 | EDO | I | 2099 | - | 3,3,3 | 2.41 | 2 (66%) | 2,2,2 | 1.93 | 1 (50%) |
| 2 | EDO | I | 2100 | - | 3,3,3 | 1.75 | 1 (33%) | 2,2,2 | 0.84 | 0 |
| 2 | EDO | I | 2103 | - | 3,3,3 | 2.72 | 2 (66%) | 2,2,2 | 1.96 | 1 (50%) |
| 2 | EDO | I | 2107 | - | 3,3,3 | 1.48 | 1 (33%) | 2,2,2 | 0.60 | 0 |
| 2 | EDO | I | 2115 | - | 3,3,3 | 3.53 | 2 (66%) | 2,2,2 | 1.01 | 0 |
| 2 | EDO | I | 2121 | - | 3,3,3 | 1.21 | 0 | 2,2,2 | 0.84 | 0 |
| 2 | EDO | J | 2008 | - | 3,3,3 | 4.76 | 2 (66%) | 2,2,2 | 1.27 | 0 |
| 2 | EDO | J | 2014 | - | 3,3,3 | 3.28 | 2 (66%) | 2,2,2 | 0.74 | 0 |
| 2 | EDO | J | 2048 | - | 3,3,3 | 2.95 | 2 (66%) | 2,2,2 | 0.97 | 0 |
| 2 | EDO | J | 2049 | - | 3,3,3 | 2.83 | 2 (66%) | 2,2,2 | 0.93 | 0 |
| 2 | EDO | J | 2053 | - | 3,3,3 | 3.24 | 2 (66%) | 2,2,2 | 0.32 | 0 |
| 2 | EDO | J | 2055 | - | 3,3,3 | 2.02 | 1 (33%) | 2,2,2 | 0.90 | 0 |
| 2 | EDO | J | 2061 | - | 3,3,3 | 2.14 | 1 (33%) | 2,2,2 | 1.04 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | EDO | J | 2068 | - | 3,3,3 | 2.76 | 2 (66%) | 2,2,2 | 0.07 | 0 |
| 2 | EDO | J | 2069 | - | 3,3,3 | 2.74 | 2 (66%) | 2,2,2 | 0.50 | 0 |
| 2 | EDO | J | 2104 | - | 3,3,3 | 3.64 | 2 (66%) | 2,2,2 | 2.14 | 1 (50%) |
| 2 | EDO | J | 2105 | - | 3,3,3 | 2.90 | 2 (66%) | 2,2,2 | 0.56 | 0 |
| 2 | EDO | J | 2106 | - | 3,3,3 | 2.29 | 1 (33%) | 2,2,2 | 1.04 | 0 |
| 2 | EDO | J | 2108 | - | 3,3,3 | 1.57 | 1 (33%) | 2,2,2 | 0.88 | 0 |
| 2 | EDO | J | 2109 | - | 3,3,3 | 1.24 | 1 (33%) | 2,2,2 | 1.23 | 0 |
| 2 | EDO | J | 2110 | - | 3,3,3 | 2.39 | 2 (66%) | 2,2,2 | 1.14 | 0 |
| 2 | EDO | J | 2123 | - | 3,3,3 | 3.31 | 2 (66%) | 2,2,2 | 2.04 | 1 (50%) |

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 |
|-----|------|-------|------|------|---------|----------|---------|
| 2 | EDO | A | 2001 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2011 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2012 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2016 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2017 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2019 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2022 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2029 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2063 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2065 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2066 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2116 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2122 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | A | 2124 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2002 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2013 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2015 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2018 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2020 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2021 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2023 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2025 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2027 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2028 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2030 | - | - | 0/1/1/1 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 2 | EDO | B | 2062 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2070 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | B | 2125 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2004 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2024 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2026 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2036 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2064 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2067 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2075 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2080 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2081 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2082 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2083 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2084 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2085 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2117 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2126 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | C | 2128 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2003 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2031 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2033 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2035 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2071 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2072 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2073 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2074 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2118 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | D | 2119 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2005 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2032 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2039 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2040 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2041 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2042 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2076 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2077 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2078 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2079 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2088 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2089 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2090 | - | - | 0/1/1/1 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 2 | EDO | E | 2091 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2092 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2120 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | E | 2127 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2006 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2034 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2037 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2038 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2043 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2086 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2087 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2094 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2095 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2096 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2097 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | F | 2098 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2009 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2047 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2050 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2056 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2057 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2093 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2101 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2102 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | G | 2112 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2010 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2044 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2054 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2058 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2059 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2060 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2111 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2113 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | H | 2114 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2007 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2045 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2046 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2051 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2052 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2099 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2100 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2103 | - | - | 0/1/1/1 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 2 | EDO | I | 2107 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2115 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | I | 2121 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2008 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2014 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2048 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2049 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2053 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2055 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2061 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2068 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2069 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2104 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2105 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2106 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2108 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2109 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2110 | - | - | 0/1/1/1 | 0/0/0/0 |
| 2 | EDO | J | 2123 | - | - | 0/1/1/1 | 0/0/0/0 |

All (227) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | F | 2006 | EDO | C2-C1 | 2.01 | 1.62 | 1.47 |
| 2 | A | 2065 | EDO | O2-C2 | 2.01 | 1.52 | 1.42 |
| 2 | B | 2023 | EDO | O1-C1 | 2.03 | 1.53 | 1.42 |
| 2 | I | 2107 | EDO | O1-C1 | 2.04 | 1.53 | 1.42 |
| 2 | B | 2027 | EDO | O1-C1 | 2.07 | 1.53 | 1.42 |
| 2 | J | 2109 | EDO | O2-C2 | 2.07 | 1.53 | 1.42 |
| 2 | C | 2075 | EDO | O2-C2 | 2.07 | 1.53 | 1.42 |
| 2 | F | 2096 | EDO | O1-C1 | 2.09 | 1.53 | 1.42 |
| 2 | D | 2033 | EDO | O1-C1 | 2.10 | 1.53 | 1.42 |
| 2 | H | 2111 | EDO | O1-C1 | 2.12 | 1.53 | 1.42 |
| 2 | B | 2028 | EDO | O1-C1 | 2.12 | 1.53 | 1.42 |
| 2 | D | 2072 | EDO | O1-C1 | 2.14 | 1.53 | 1.42 |
| 2 | C | 2126 | EDO | C2-C1 | 2.17 | 1.63 | 1.47 |
| 2 | B | 2018 | EDO | O1-C1 | 2.17 | 1.53 | 1.42 |
| 2 | G | 2057 | EDO | O1-C1 | 2.20 | 1.53 | 1.42 |
| 2 | F | 2086 | EDO | O2-C2 | 2.22 | 1.54 | 1.42 |
| 2 | C | 2081 | EDO | C2-C1 | 2.25 | 1.64 | 1.47 |
| 2 | H | 2111 | EDO | C2-C1 | 2.25 | 1.64 | 1.47 |
| 2 | E | 2039 | EDO | O1-C1 | 2.31 | 1.54 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | E | 2092 | EDO | O1-C1 | 2.33 | 1.54 | 1.42 |
| 2 | C | 2081 | EDO | O1-C1 | 2.34 | 1.54 | 1.42 |
| 2 | A | 2017 | EDO | O1-C1 | 2.35 | 1.54 | 1.42 |
| 2 | J | 2068 | EDO | O1-C1 | 2.35 | 1.54 | 1.42 |
| 2 | E | 2127 | EDO | O1-C1 | 2.35 | 1.54 | 1.42 |
| 2 | B | 2125 | EDO | C2-C1 | 2.36 | 1.64 | 1.47 |
| 2 | D | 2031 | EDO | O1-C1 | 2.37 | 1.54 | 1.42 |
| 2 | E | 2088 | EDO | O2-C2 | 2.37 | 1.54 | 1.42 |
| 2 | B | 2018 | EDO | O2-C2 | 2.37 | 1.54 | 1.42 |
| 2 | F | 2037 | EDO | O1-C1 | 2.37 | 1.54 | 1.42 |
| 2 | B | 2015 | EDO | O2-C2 | 2.38 | 1.54 | 1.42 |
| 2 | D | 2073 | EDO | O2-C2 | 2.40 | 1.54 | 1.42 |
| 2 | D | 2003 | EDO | O1-C1 | 2.40 | 1.55 | 1.42 |
| 2 | G | 2056 | EDO | O1-C1 | 2.40 | 1.55 | 1.42 |
| 2 | D | 2073 | EDO | O1-C1 | 2.40 | 1.55 | 1.42 |
| 2 | A | 2016 | EDO | O2-C2 | 2.42 | 1.55 | 1.42 |
| 2 | E | 2076 | EDO | O1-C1 | 2.42 | 1.55 | 1.42 |
| 2 | G | 2101 | EDO | O1-C1 | 2.42 | 1.55 | 1.42 |
| 2 | J | 2108 | EDO | O2-C2 | 2.42 | 1.55 | 1.42 |
| 2 | A | 2017 | EDO | O2-C2 | 2.43 | 1.55 | 1.42 |
| 2 | E | 2042 | EDO | O1-C1 | 2.43 | 1.55 | 1.42 |
| 2 | E | 2039 | EDO | O2-C2 | 2.44 | 1.55 | 1.42 |
| 2 | D | 2071 | EDO | O1-C1 | 2.44 | 1.55 | 1.42 |
| 2 | H | 2059 | EDO | C2-C1 | 2.46 | 1.65 | 1.47 |
| 2 | J | 2110 | EDO | O1-C1 | 2.47 | 1.55 | 1.42 |
| 2 | H | 2054 | EDO | O1-C1 | 2.47 | 1.55 | 1.42 |
| 2 | A | 2011 | EDO | O1-C1 | 2.49 | 1.55 | 1.42 |
| 2 | C | 2036 | EDO | O2-C2 | 2.50 | 1.55 | 1.42 |
| 2 | D | 2118 | EDO | O1-C1 | 2.54 | 1.55 | 1.42 |
| 2 | E | 2042 | EDO | O2-C2 | 2.55 | 1.55 | 1.42 |
| 2 | A | 2016 | EDO | O1-C1 | 2.58 | 1.55 | 1.42 |
| 2 | J | 2049 | EDO | O1-C1 | 2.58 | 1.55 | 1.42 |
| 2 | F | 2038 | EDO | O2-C2 | 2.59 | 1.56 | 1.42 |
| 2 | G | 2102 | EDO | O1-C1 | 2.59 | 1.56 | 1.42 |
| 2 | I | 2103 | EDO | O2-C2 | 2.62 | 1.56 | 1.42 |
| 2 | B | 2020 | EDO | O2-C2 | 2.63 | 1.56 | 1.42 |
| 2 | E | 2120 | EDO | O2-C2 | 2.66 | 1.56 | 1.42 |
| 2 | A | 2001 | EDO | O2-C2 | 2.67 | 1.56 | 1.42 |
| 2 | C | 2117 | EDO | O1-C1 | 2.67 | 1.56 | 1.42 |
| 2 | F | 2043 | EDO | O1-C1 | 2.67 | 1.56 | 1.42 |
| 2 | I | 2051 | EDO | O2-C2 | 2.68 | 1.56 | 1.42 |
| 2 | F | 2006 | EDO | O2-C2 | 2.68 | 1.56 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | C | 2126 | EDO | O1-C1 | 2.71 | 1.56 | 1.42 |
| 2 | I | 2045 | EDO | O2-C2 | 2.73 | 1.56 | 1.42 |
| 2 | F | 2087 | EDO | O1-C1 | 2.74 | 1.56 | 1.42 |
| 2 | E | 2041 | EDO | O1-C1 | 2.75 | 1.56 | 1.42 |
| 2 | I | 2100 | EDO | O2-C2 | 2.76 | 1.56 | 1.42 |
| 2 | E | 2079 | EDO | O1-C1 | 2.77 | 1.57 | 1.42 |
| 2 | G | 2093 | EDO | O1-C1 | 2.78 | 1.57 | 1.42 |
| 2 | B | 2013 | EDO | O1-C1 | 2.80 | 1.57 | 1.42 |
| 2 | H | 2054 | EDO | O2-C2 | 2.81 | 1.57 | 1.42 |
| 2 | B | 2125 | EDO | O2-C2 | 2.81 | 1.57 | 1.42 |
| 2 | E | 2089 | EDO | O1-C1 | 2.81 | 1.57 | 1.42 |
| 2 | G | 2101 | EDO | O2-C2 | 2.81 | 1.57 | 1.42 |
| 2 | I | 2099 | EDO | O1-C1 | 2.84 | 1.57 | 1.42 |
| 2 | B | 2062 | EDO | O1-C1 | 2.85 | 1.57 | 1.42 |
| 2 | C | 2117 | EDO | O2-C2 | 2.85 | 1.57 | 1.42 |
| 2 | C | 2064 | EDO | O2-C2 | 2.86 | 1.57 | 1.42 |
| 2 | D | 2074 | EDO | O2-C2 | 2.87 | 1.57 | 1.42 |
| 2 | I | 2052 | EDO | O2-C2 | 2.88 | 1.57 | 1.42 |
| 2 | B | 2013 | EDO | O2-C2 | 2.88 | 1.57 | 1.42 |
| 2 | A | 2019 | EDO | O2-C2 | 2.88 | 1.57 | 1.42 |
| 2 | E | 2040 | EDO | O2-C2 | 2.89 | 1.57 | 1.42 |
| 2 | B | 2125 | EDO | O1-C1 | 2.90 | 1.57 | 1.42 |
| 2 | C | 2080 | EDO | O1-C1 | 2.90 | 1.57 | 1.42 |
| 2 | C | 2075 | EDO | O1-C1 | 2.91 | 1.57 | 1.42 |
| 2 | B | 2070 | EDO | O2-C2 | 2.91 | 1.57 | 1.42 |
| 2 | A | 2001 | EDO | O1-C1 | 2.92 | 1.57 | 1.42 |
| 2 | A | 2022 | EDO | O1-C1 | 2.92 | 1.57 | 1.42 |
| 2 | D | 2119 | EDO | O1-C1 | 2.93 | 1.57 | 1.42 |
| 2 | G | 2112 | EDO | O2-C2 | 2.94 | 1.57 | 1.42 |
| 2 | H | 2111 | EDO | O2-C2 | 2.95 | 1.58 | 1.42 |
| 2 | I | 2099 | EDO | O2-C2 | 2.97 | 1.58 | 1.42 |
| 2 | J | 2105 | EDO | O1-C1 | 3.00 | 1.58 | 1.42 |
| 2 | H | 2059 | EDO | O1-C1 | 3.02 | 1.58 | 1.42 |
| 2 | B | 2015 | EDO | O1-C1 | 3.03 | 1.58 | 1.42 |
| 2 | H | 2044 | EDO | O1-C1 | 3.04 | 1.58 | 1.42 |
| 2 | F | 2038 | EDO | O1-C1 | 3.04 | 1.58 | 1.42 |
| 2 | E | 2090 | EDO | O1-C1 | 3.06 | 1.58 | 1.42 |
| 2 | E | 2076 | EDO | O2-C2 | 3.07 | 1.58 | 1.42 |
| 2 | B | 2025 | EDO | O2-C2 | 3.09 | 1.58 | 1.42 |
| 2 | E | 2040 | EDO | O1-C1 | 3.09 | 1.58 | 1.42 |
| 2 | J | 2048 | EDO | O1-C1 | 3.10 | 1.58 | 1.42 |
| 2 | C | 2083 | EDO | O1-C1 | 3.11 | 1.58 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | G | 2047 | EDO | O1-C1 | 3.12 | 1.58 | 1.42 |
| 2 | G | 2112 | EDO | O1-C1 | 3.13 | 1.58 | 1.42 |
| 2 | D | 2119 | EDO | O2-C2 | 3.13 | 1.58 | 1.42 |
| 2 | H | 2114 | EDO | O2-C2 | 3.14 | 1.59 | 1.42 |
| 2 | I | 2046 | EDO | O2-C2 | 3.17 | 1.59 | 1.42 |
| 2 | E | 2077 | EDO | O2-C2 | 3.18 | 1.59 | 1.42 |
| 2 | D | 2033 | EDO | O2-C2 | 3.18 | 1.59 | 1.42 |
| 2 | B | 2028 | EDO | O2-C2 | 3.18 | 1.59 | 1.42 |
| 2 | E | 2077 | EDO | O1-C1 | 3.21 | 1.59 | 1.42 |
| 2 | E | 2090 | EDO | O2-C2 | 3.21 | 1.59 | 1.42 |
| 2 | J | 2069 | EDO | O1-C1 | 3.22 | 1.59 | 1.42 |
| 2 | A | 2066 | EDO | O1-C1 | 3.22 | 1.59 | 1.42 |
| 2 | C | 2128 | EDO | O1-C1 | 3.22 | 1.59 | 1.42 |
| 2 | I | 2052 | EDO | O1-C1 | 3.22 | 1.59 | 1.42 |
| 2 | A | 2116 | EDO | O1-C1 | 3.26 | 1.59 | 1.42 |
| 2 | J | 2055 | EDO | O2-C2 | 3.29 | 1.59 | 1.42 |
| 2 | J | 2110 | EDO | O2-C2 | 3.32 | 1.59 | 1.42 |
| 2 | F | 2096 | EDO | O2-C2 | 3.32 | 1.59 | 1.42 |
| 2 | F | 2037 | EDO | O2-C2 | 3.36 | 1.60 | 1.42 |
| 2 | C | 2080 | EDO | O2-C2 | 3.36 | 1.60 | 1.42 |
| 2 | E | 2127 | EDO | O2-C2 | 3.37 | 1.60 | 1.42 |
| 2 | J | 2069 | EDO | O2-C2 | 3.37 | 1.60 | 1.42 |
| 2 | C | 2083 | EDO | O2-C2 | 3.37 | 1.60 | 1.42 |
| 2 | B | 2070 | EDO | O1-C1 | 3.39 | 1.60 | 1.42 |
| 2 | A | 2019 | EDO | O1-C1 | 3.41 | 1.60 | 1.42 |
| 2 | C | 2024 | EDO | O1-C1 | 3.43 | 1.60 | 1.42 |
| 2 | E | 2079 | EDO | O2-C2 | 3.43 | 1.60 | 1.42 |
| 2 | G | 2047 | EDO | O2-C2 | 3.44 | 1.60 | 1.42 |
| 2 | F | 2097 | EDO | O2-C2 | 3.45 | 1.60 | 1.42 |
| 2 | F | 2094 | EDO | O2-C2 | 3.47 | 1.60 | 1.42 |
| 2 | C | 2064 | EDO | O1-C1 | 3.47 | 1.60 | 1.42 |
| 2 | F | 2086 | EDO | O1-C1 | 3.47 | 1.60 | 1.42 |
| 2 | C | 2081 | EDO | O2-C2 | 3.50 | 1.60 | 1.42 |
| 2 | F | 2097 | EDO | O1-C1 | 3.51 | 1.61 | 1.42 |
| 2 | J | 2106 | EDO | O1-C1 | 3.51 | 1.61 | 1.42 |
| 2 | F | 2094 | EDO | O1-C1 | 3.53 | 1.61 | 1.42 |
| 2 | H | 2113 | EDO | O1-C1 | 3.54 | 1.61 | 1.42 |
| 2 | F | 2095 | EDO | O2-C2 | 3.54 | 1.61 | 1.42 |
| 2 | F | 2034 | EDO | O2-C2 | 3.55 | 1.61 | 1.42 |
| 2 | A | 2066 | EDO | O2-C2 | 3.56 | 1.61 | 1.42 |
| 2 | F | 2095 | EDO | O1-C1 | 3.56 | 1.61 | 1.42 |
| 2 | J | 2123 | EDO | O2-C2 | 3.57 | 1.61 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | A | 2029 | EDO | O1-C1 | 3.57 | 1.61 | 1.42 |
| 2 | I | 2115 | EDO | O1-C1 | 3.58 | 1.61 | 1.42 |
| 2 | J | 2061 | EDO | O1-C1 | 3.58 | 1.61 | 1.42 |
| 2 | C | 2084 | EDO | O1-C1 | 3.59 | 1.61 | 1.42 |
| 2 | B | 2025 | EDO | O1-C1 | 3.64 | 1.61 | 1.42 |
| 2 | A | 2011 | EDO | O2-C2 | 3.66 | 1.61 | 1.42 |
| 2 | H | 2058 | EDO | O1-C1 | 3.67 | 1.61 | 1.42 |
| 2 | C | 2036 | EDO | O1-C1 | 3.68 | 1.61 | 1.42 |
| 2 | A | 2116 | EDO | O2-C2 | 3.70 | 1.62 | 1.42 |
| 2 | E | 2005 | EDO | O1-C1 | 3.71 | 1.62 | 1.42 |
| 2 | J | 2053 | EDO | O1-C1 | 3.71 | 1.62 | 1.42 |
| 2 | F | 2098 | EDO | O1-C1 | 3.72 | 1.62 | 1.42 |
| 2 | E | 2078 | EDO | O1-C1 | 3.73 | 1.62 | 1.42 |
| 2 | G | 2009 | EDO | O2-C2 | 3.74 | 1.62 | 1.42 |
| 2 | A | 2065 | EDO | O1-C1 | 3.75 | 1.62 | 1.42 |
| 2 | I | 2103 | EDO | O1-C1 | 3.76 | 1.62 | 1.42 |
| 2 | I | 2007 | EDO | O2-C2 | 3.77 | 1.62 | 1.42 |
| 2 | E | 2091 | EDO | O1-C1 | 3.77 | 1.62 | 1.42 |
| 2 | I | 2045 | EDO | O1-C1 | 3.81 | 1.62 | 1.42 |
| 2 | C | 2084 | EDO | O2-C2 | 3.82 | 1.62 | 1.42 |
| 2 | J | 2014 | EDO | O2-C2 | 3.83 | 1.62 | 1.42 |
| 2 | D | 2003 | EDO | O2-C2 | 3.84 | 1.62 | 1.42 |
| 2 | D | 2072 | EDO | O2-C2 | 3.86 | 1.62 | 1.42 |
| 2 | A | 2063 | EDO | O2-C2 | 3.87 | 1.62 | 1.42 |
| 2 | H | 2010 | EDO | O1-C1 | 3.88 | 1.62 | 1.42 |
| 2 | J | 2048 | EDO | O2-C2 | 3.93 | 1.63 | 1.42 |
| 2 | D | 2071 | EDO | O2-C2 | 3.93 | 1.63 | 1.42 |
| 2 | E | 2091 | EDO | O2-C2 | 3.93 | 1.63 | 1.42 |
| 2 | H | 2114 | EDO | O1-C1 | 3.96 | 1.63 | 1.42 |
| 2 | A | 2029 | EDO | O2-C2 | 3.98 | 1.63 | 1.42 |
| 2 | J | 2104 | EDO | O1-C1 | 3.99 | 1.63 | 1.42 |
| 2 | J | 2053 | EDO | O2-C2 | 4.00 | 1.63 | 1.42 |
| 2 | J | 2008 | EDO | O2-C2 | 4.00 | 1.63 | 1.42 |
| 2 | A | 2012 | EDO | O1-C1 | 4.01 | 1.63 | 1.42 |
| 2 | J | 2105 | EDO | O2-C2 | 4.03 | 1.63 | 1.42 |
| 2 | E | 2088 | EDO | O1-C1 | 4.07 | 1.64 | 1.42 |
| 2 | A | 2063 | EDO | O1-C1 | 4.08 | 1.64 | 1.42 |
| 2 | B | 2020 | EDO | O1-C1 | 4.08 | 1.64 | 1.42 |
| 2 | J | 2123 | EDO | O1-C1 | 4.09 | 1.64 | 1.42 |
| 2 | E | 2120 | EDO | O1-C1 | 4.10 | 1.64 | 1.42 |
| 2 | J | 2014 | EDO | O1-C1 | 4.11 | 1.64 | 1.42 |
| 2 | H | 2058 | EDO | O2-C2 | 4.12 | 1.64 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | J | 2049 | EDO | O2-C2 | 4.14 | 1.64 | 1.42 |
| 2 | G | 2093 | EDO | O2-C2 | 4.17 | 1.64 | 1.42 |
| 2 | J | 2068 | EDO | O2-C2 | 4.17 | 1.64 | 1.42 |
| 2 | D | 2031 | EDO | O2-C2 | 4.18 | 1.64 | 1.42 |
| 2 | B | 2021 | EDO | O1-C1 | 4.25 | 1.65 | 1.42 |
| 2 | C | 2126 | EDO | O2-C2 | 4.25 | 1.65 | 1.42 |
| 2 | C | 2128 | EDO | O2-C2 | 4.27 | 1.65 | 1.42 |
| 2 | F | 2043 | EDO | O2-C2 | 4.29 | 1.65 | 1.42 |
| 2 | C | 2067 | EDO | O2-C2 | 4.32 | 1.65 | 1.42 |
| 2 | C | 2024 | EDO | O2-C2 | 4.36 | 1.65 | 1.42 |
| 2 | G | 2102 | EDO | O2-C2 | 4.38 | 1.65 | 1.42 |
| 2 | G | 2056 | EDO | O2-C2 | 4.40 | 1.65 | 1.42 |
| 2 | G | 2050 | EDO | O2-C2 | 4.44 | 1.66 | 1.42 |
| 2 | C | 2085 | EDO | O2-C2 | 4.55 | 1.66 | 1.42 |
| 2 | E | 2032 | EDO | O2-C2 | 4.57 | 1.66 | 1.42 |
| 2 | J | 2104 | EDO | O2-C2 | 4.58 | 1.66 | 1.42 |
| 2 | D | 2118 | EDO | O2-C2 | 4.60 | 1.66 | 1.42 |
| 2 | I | 2115 | EDO | O2-C2 | 4.63 | 1.67 | 1.42 |
| 2 | C | 2004 | EDO | O1-C1 | 4.65 | 1.67 | 1.42 |
| 2 | G | 2009 | EDO | O1-C1 | 4.71 | 1.67 | 1.42 |
| 2 | B | 2023 | EDO | O2-C2 | 4.78 | 1.67 | 1.42 |
| 2 | C | 2085 | EDO | O1-C1 | 4.83 | 1.68 | 1.42 |
| 2 | F | 2006 | EDO | O1-C1 | 4.88 | 1.68 | 1.42 |
| 2 | I | 2007 | EDO | O1-C1 | 4.91 | 1.68 | 1.42 |
| 2 | E | 2089 | EDO | O2-C2 | 4.92 | 1.68 | 1.42 |
| 2 | C | 2082 | EDO | O2-C2 | 4.93 | 1.68 | 1.42 |
| 2 | B | 2021 | EDO | O2-C2 | 4.96 | 1.68 | 1.42 |
| 2 | B | 2002 | EDO | O2-C2 | 5.06 | 1.69 | 1.42 |
| 2 | A | 2122 | EDO | O2-C2 | 5.12 | 1.69 | 1.42 |
| 2 | A | 2124 | EDO | O2-C2 | 5.14 | 1.69 | 1.42 |
| 2 | A | 2124 | EDO | O1-C1 | 5.15 | 1.69 | 1.42 |
| 2 | H | 2010 | EDO | O2-C2 | 5.25 | 1.70 | 1.42 |
| 2 | D | 2074 | EDO | O1-C1 | 5.26 | 1.70 | 1.42 |
| 2 | A | 2012 | EDO | O2-C2 | 5.26 | 1.70 | 1.42 |
| 2 | H | 2059 | EDO | O2-C2 | 5.51 | 1.71 | 1.42 |
| 2 | B | 2002 | EDO | O1-C1 | 5.51 | 1.71 | 1.42 |
| 2 | F | 2098 | EDO | O2-C2 | 5.57 | 1.72 | 1.42 |
| 2 | C | 2004 | EDO | O2-C2 | 5.74 | 1.73 | 1.42 |
| 2 | E | 2005 | EDO | O2-C2 | 6.19 | 1.75 | 1.42 |
| 2 | J | 2008 | EDO | O1-C1 | 7.03 | 1.80 | 1.42 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|----------|-------|------------------------|---------------------|
| 2 | G | 2101 | EDO | O2-C2-C1 | -2.74 | 92.91 | 112.54 |
| 2 | J | 2123 | EDO | O2-C2-C1 | -2.70 | 93.21 | 112.54 |
| 2 | I | 2099 | EDO | O2-C2-C1 | -2.65 | 93.54 | 112.54 |
| 2 | J | 2104 | EDO | O2-C2-C1 | -2.30 | 96.06 | 112.54 |
| 2 | H | 2058 | EDO | O2-C2-C1 | -2.23 | 96.52 | 112.54 |
| 2 | I | 2103 | EDO | O1-C1-C2 | -2.17 | 96.97 | 112.54 |
| 2 | E | 2127 | EDO | O1-C1-C2 | -2.11 | 97.45 | 112.54 |
| 2 | F | 2086 | EDO | O2-C2-C1 | -2.10 | 97.49 | 112.54 |
| 2 | F | 2094 | EDO | O2-C2-C1 | -2.09 | 97.52 | 112.54 |
| 2 | I | 2007 | EDO | O2-C2-C1 | -2.04 | 97.88 | 112.54 |
| 2 | C | 2085 | EDO | O2-C2-C1 | -2.03 | 97.95 | 112.54 |
| 2 | F | 2043 | EDO | O2-C2-C1 | -2.02 | 98.03 | 112.54 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

107 monomers are involved in 502 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | A | 2001 | EDO | 6 | 0 |
| 2 | A | 2011 | EDO | 1 | 0 |
| 2 | A | 2012 | EDO | 11 | 0 |
| 2 | A | 2017 | EDO | 2 | 0 |
| 2 | A | 2022 | EDO | 3 | 0 |
| 2 | A | 2029 | EDO | 7 | 0 |
| 2 | A | 2063 | EDO | 7 | 0 |
| 2 | A | 2065 | EDO | 5 | 0 |
| 2 | A | 2066 | EDO | 1 | 0 |
| 2 | A | 2116 | EDO | 1 | 0 |
| 2 | A | 2122 | EDO | 4 | 0 |
| 2 | A | 2124 | EDO | 7 | 0 |
| 2 | B | 2002 | EDO | 5 | 0 |
| 2 | B | 2018 | EDO | 1 | 0 |
| 2 | B | 2020 | EDO | 2 | 0 |
| 2 | B | 2021 | EDO | 4 | 0 |
| 2 | B | 2023 | EDO | 3 | 0 |
| 2 | B | 2025 | EDO | 2 | 0 |
| 2 | B | 2028 | EDO | 11 | 0 |
| 2 | B | 2030 | EDO | 10 | 0 |
| 2 | B | 2125 | EDO | 8 | 0 |
| 2 | C | 2004 | EDO | 11 | 0 |
| 2 | C | 2024 | EDO | 12 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | C | 2036 | EDO | 1 | 0 |
| 2 | C | 2064 | EDO | 2 | 0 |
| 2 | C | 2067 | EDO | 4 | 0 |
| 2 | C | 2075 | EDO | 7 | 0 |
| 2 | C | 2080 | EDO | 2 | 0 |
| 2 | C | 2082 | EDO | 2 | 0 |
| 2 | C | 2084 | EDO | 1 | 0 |
| 2 | C | 2085 | EDO | 10 | 0 |
| 2 | C | 2117 | EDO | 3 | 0 |
| 2 | C | 2126 | EDO | 6 | 0 |
| 2 | C | 2128 | EDO | 8 | 0 |
| 2 | D | 2003 | EDO | 4 | 0 |
| 2 | D | 2031 | EDO | 4 | 0 |
| 2 | D | 2035 | EDO | 11 | 0 |
| 2 | D | 2072 | EDO | 3 | 0 |
| 2 | D | 2074 | EDO | 2 | 0 |
| 2 | D | 2118 | EDO | 7 | 0 |
| 2 | D | 2119 | EDO | 2 | 0 |
| 2 | E | 2005 | EDO | 5 | 0 |
| 2 | E | 2032 | EDO | 3 | 0 |
| 2 | E | 2039 | EDO | 2 | 0 |
| 2 | E | 2040 | EDO | 1 | 0 |
| 2 | E | 2042 | EDO | 2 | 0 |
| 2 | E | 2076 | EDO | 7 | 0 |
| 2 | E | 2077 | EDO | 1 | 0 |
| 2 | E | 2078 | EDO | 1 | 0 |
| 2 | E | 2079 | EDO | 2 | 0 |
| 2 | E | 2088 | EDO | 3 | 0 |
| 2 | E | 2089 | EDO | 4 | 0 |
| 2 | E | 2090 | EDO | 5 | 0 |
| 2 | E | 2091 | EDO | 5 | 0 |
| 2 | E | 2092 | EDO | 1 | 0 |
| 2 | E | 2120 | EDO | 6 | 0 |
| 2 | E | 2127 | EDO | 9 | 0 |
| 2 | F | 2006 | EDO | 2 | 0 |
| 2 | F | 2034 | EDO | 5 | 0 |
| 2 | F | 2038 | EDO | 4 | 0 |
| 2 | F | 2043 | EDO | 13 | 0 |
| 2 | F | 2086 | EDO | 7 | 0 |
| 2 | F | 2087 | EDO | 2 | 0 |
| 2 | F | 2095 | EDO | 2 | 0 |
| 2 | F | 2097 | EDO | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | F | 2098 | EDO | 3 | 0 |
| 2 | G | 2009 | EDO | 4 | 0 |
| 2 | G | 2047 | EDO | 2 | 0 |
| 2 | G | 2050 | EDO | 5 | 0 |
| 2 | G | 2056 | EDO | 7 | 0 |
| 2 | G | 2057 | EDO | 7 | 0 |
| 2 | G | 2093 | EDO | 6 | 0 |
| 2 | G | 2102 | EDO | 3 | 0 |
| 2 | G | 2112 | EDO | 2 | 0 |
| 2 | H | 2010 | EDO | 8 | 0 |
| 2 | H | 2044 | EDO | 4 | 0 |
| 2 | H | 2054 | EDO | 1 | 0 |
| 2 | H | 2058 | EDO | 11 | 0 |
| 2 | H | 2059 | EDO | 2 | 0 |
| 2 | H | 2060 | EDO | 4 | 0 |
| 2 | H | 2111 | EDO | 3 | 0 |
| 2 | H | 2113 | EDO | 4 | 0 |
| 2 | H | 2114 | EDO | 0 | 1 |
| 2 | I | 2007 | EDO | 5 | 0 |
| 2 | I | 2045 | EDO | 2 | 0 |
| 2 | I | 2046 | EDO | 4 | 0 |
| 2 | I | 2051 | EDO | 6 | 0 |
| 2 | I | 2099 | EDO | 3 | 0 |
| 2 | I | 2100 | EDO | 2 | 0 |
| 2 | I | 2103 | EDO | 4 | 0 |
| 2 | I | 2107 | EDO | 11 | 0 |
| 2 | I | 2115 | EDO | 7 | 0 |
| 2 | I | 2121 | EDO | 12 | 0 |
| 2 | J | 2008 | EDO | 7 | 0 |
| 2 | J | 2014 | EDO | 3 | 0 |
| 2 | J | 2049 | EDO | 10 | 0 |
| 2 | J | 2053 | EDO | 3 | 0 |
| 2 | J | 2055 | EDO | 2 | 0 |
| 2 | J | 2061 | EDO | 2 | 0 |
| 2 | J | 2068 | EDO | 6 | 0 |
| 2 | J | 2104 | EDO | 14 | 0 |
| 2 | J | 2105 | EDO | 4 | 0 |
| 2 | J | 2106 | EDO | 2 | 0 |
| 2 | J | 2108 | EDO | 3 | 0 |
| 2 | J | 2109 | EDO | 14 | 0 |
| 2 | J | 2110 | EDO | 3 | 0 |
| 2 | J | 2123 | EDO | 6 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.