



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 07:51 am BST

PDB ID : 7R4Q
EMDB ID : EMD-14314
Title : The SARS-CoV-2 spike in complex with the 1.29 neutralizing nanobody
Authors : Casasnovas, J.M.; Melero, R.; Arranz, R.; Fernandez, L.A.
Deposited on : 2022-02-09
Resolution : 3.60 Å (reported)
Based on initial models : 3TPK, 6ZXN

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

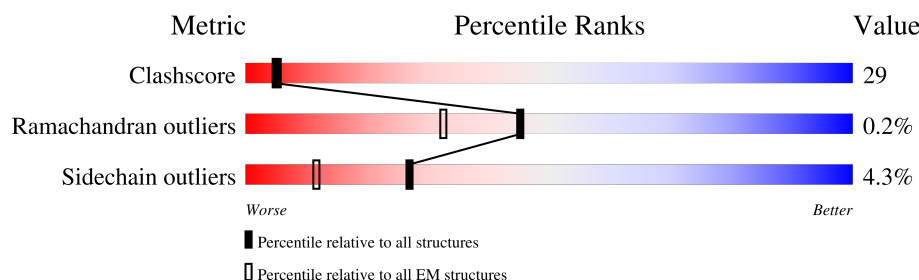
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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





| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1264 | <div> <div>21%</div> <div>51%</div> <div>25%</div> <div>5%</div> <div>16%</div> </div> |
| 1 | B | 1264 | <div> <div>19%</div> <div>49%</div> <div>27%</div> <div>5%</div> <div>17%</div> </div> |
| 1 | C | 1264 | <div> <div>20%</div> <div>51%</div> <div>25%</div> <div>6%</div> <div>16%</div> </div> |
| 2 | D | 126 | <div> <div>44%</div> <div>37%</div> <div>56%</div> <div>5%</div> </div> |
| 2 | E | 126 | <div> <div>25%</div> <div>36%</div> <div>56%</div> <div>5%</div> </div> |
| 3 | F | 2 | <div> <div>50%</div> <div>50%</div> </div> |
| 3 | G | 2 | <div> <div>100%</div> </div> |
| 3 | H | 2 | <div> <div>100%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | I | 2 |  |
| 3 | J | 2 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4 | NAG | B | 1307 | - | - | X | - |
| 4 | NAG | B | 1310 | - | - | X | - |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51957 atoms, of which 24719 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 1 | A | 1060 | Total | C | H | N | O | S | 3 | 0 |
| | | | 16380 | 5297 | 8079 | 1383 | 1583 | 38 | | |
| 1 | B | 1054 | Total | C | H | N | O | S | 3 | 0 |
| | | | 16287 | 5268 | 8034 | 1376 | 1571 | 38 | | |
| 1 | C | 1060 | Total | C | H | N | O | S | 1 | 0 |
| | | | 16361 | 5292 | 8069 | 1382 | 1580 | 38 | | |

There are 186 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 682 | GLY | ARG | variant | UNP P0DTC2 |
| A | 683 | SER | ARG | variant | UNP P0DTC2 |
| A | 685 | SER | ARG | variant | UNP P0DTC2 |
| A | 942 | PRO | ALA | variant | UNP P0DTC2 |
| A | 986 | PRO | LYS | engineered mutation | UNP P0DTC2 |
| A | 987 | PRO | VAL | engineered mutation | UNP P0DTC2 |
| A | 1209 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1210 | SER | - | expression tag | UNP P0DTC2 |
| A | 1211 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1212 | SER | - | expression tag | UNP P0DTC2 |
| A | 1213 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1214 | TYR | - | expression tag | UNP P0DTC2 |
| A | 1215 | ILE | - | expression tag | UNP P0DTC2 |
| A | 1216 | PRO | - | expression tag | UNP P0DTC2 |
| A | 1217 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1218 | ALA | - | expression tag | UNP P0DTC2 |
| A | 1219 | PRO | - | expression tag | UNP P0DTC2 |
| A | 1220 | ARG | - | expression tag | UNP P0DTC2 |
| A | 1221 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1222 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1223 | GLN | - | expression tag | UNP P0DTC2 |
| A | 1224 | ALA | - | expression tag | UNP P0DTC2 |
| A | 1225 | TYR | - | expression tag | UNP P0DTC2 |
| A | 1226 | VAL | - | expression tag | UNP P0DTC2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1227 | ARG | - | expression tag | UNP P0DTC2 |
| A | 1228 | LYS | - | expression tag | UNP P0DTC2 |
| A | 1229 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1230 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1231 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1232 | TRP | - | expression tag | UNP P0DTC2 |
| A | 1233 | VAL | - | expression tag | UNP P0DTC2 |
| A | 1234 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1235 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1236 | SER | - | expression tag | UNP P0DTC2 |
| A | 1237 | THR | - | expression tag | UNP P0DTC2 |
| A | 1238 | PHE | - | expression tag | UNP P0DTC2 |
| A | 1239 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1240 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1241 | THR | - | expression tag | UNP P0DTC2 |
| A | 1242 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1243 | ASN | - | expression tag | UNP P0DTC2 |
| A | 1244 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1245 | TYR | - | expression tag | UNP P0DTC2 |
| A | 1246 | PHE | - | expression tag | UNP P0DTC2 |
| A | 1247 | GLN | - | expression tag | UNP P0DTC2 |
| A | 1248 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1249 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1250 | TYR | - | expression tag | UNP P0DTC2 |
| A | 1251 | LYS | - | expression tag | UNP P0DTC2 |
| A | 1252 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1253 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1254 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1255 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1256 | LYS | - | expression tag | UNP P0DTC2 |
| A | 1257 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1258 | SER | - | expression tag | UNP P0DTC2 |
| A | 1259 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1260 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1261 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1262 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1263 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1264 | HIS | - | expression tag | UNP P0DTC2 |
| B | 682 | GLY | ARG | variant | UNP P0DTC2 |
| B | 683 | SER | ARG | variant | UNP P0DTC2 |
| B | 685 | SER | ARG | variant | UNP P0DTC2 |
| B | 942 | PRO | ALA | variant | UNP P0DTC2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 986 | PRO | LYS | engineered mutation | UNP P0DTC2 |
| B | 987 | PRO | VAL | engineered mutation | UNP P0DTC2 |
| B | 1209 | GLY | - | expression tag | UNP P0DTC2 |
| B | 1210 | SER | - | expression tag | UNP P0DTC2 |
| B | 1211 | GLY | - | expression tag | UNP P0DTC2 |
| B | 1212 | SER | - | expression tag | UNP P0DTC2 |
| B | 1213 | GLY | - | expression tag | UNP P0DTC2 |
| B | 1214 | TYR | - | expression tag | UNP P0DTC2 |
| B | 1215 | ILE | - | expression tag | UNP P0DTC2 |
| B | 1216 | PRO | - | expression tag | UNP P0DTC2 |
| B | 1217 | GLU | - | expression tag | UNP P0DTC2 |
| B | 1218 | ALA | - | expression tag | UNP P0DTC2 |
| B | 1219 | PRO | - | expression tag | UNP P0DTC2 |
| B | 1220 | ARG | - | expression tag | UNP P0DTC2 |
| B | 1221 | ASP | - | expression tag | UNP P0DTC2 |
| B | 1222 | GLY | - | expression tag | UNP P0DTC2 |
| B | 1223 | GLN | - | expression tag | UNP P0DTC2 |
| B | 1224 | ALA | - | expression tag | UNP P0DTC2 |
| B | 1225 | TYR | - | expression tag | UNP P0DTC2 |
| B | 1226 | VAL | - | expression tag | UNP P0DTC2 |
| B | 1227 | ARG | - | expression tag | UNP P0DTC2 |
| B | 1228 | LYS | - | expression tag | UNP P0DTC2 |
| B | 1229 | ASP | - | expression tag | UNP P0DTC2 |
| B | 1230 | GLY | - | expression tag | UNP P0DTC2 |
| B | 1231 | GLU | - | expression tag | UNP P0DTC2 |
| B | 1232 | TRP | - | expression tag | UNP P0DTC2 |
| B | 1233 | VAL | - | expression tag | UNP P0DTC2 |
| B | 1234 | LEU | - | expression tag | UNP P0DTC2 |
| B | 1235 | LEU | - | expression tag | UNP P0DTC2 |
| B | 1236 | SER | - | expression tag | UNP P0DTC2 |
| B | 1237 | THR | - | expression tag | UNP P0DTC2 |
| B | 1238 | PHE | - | expression tag | UNP P0DTC2 |
| B | 1239 | LEU | - | expression tag | UNP P0DTC2 |
| B | 1240 | GLY | - | expression tag | UNP P0DTC2 |
| B | 1241 | THR | - | expression tag | UNP P0DTC2 |
| B | 1242 | GLU | - | expression tag | UNP P0DTC2 |
| B | 1243 | ASN | - | expression tag | UNP P0DTC2 |
| B | 1244 | LEU | - | expression tag | UNP P0DTC2 |
| B | 1245 | TYR | - | expression tag | UNP P0DTC2 |
| B | 1246 | PHE | - | expression tag | UNP P0DTC2 |
| B | 1247 | GLN | - | expression tag | UNP P0DTC2 |
| B | 1248 | GLY | - | expression tag | UNP P0DTC2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 1249 | ASP | - | expression tag | UNP P0DTC2 |
| B | 1250 | TYR | - | expression tag | UNP P0DTC2 |
| B | 1251 | LYS | - | expression tag | UNP P0DTC2 |
| B | 1252 | ASP | - | expression tag | UNP P0DTC2 |
| B | 1253 | ASP | - | expression tag | UNP P0DTC2 |
| B | 1254 | ASP | - | expression tag | UNP P0DTC2 |
| B | 1255 | ASP | - | expression tag | UNP P0DTC2 |
| B | 1256 | LYS | - | expression tag | UNP P0DTC2 |
| B | 1257 | GLY | - | expression tag | UNP P0DTC2 |
| B | 1258 | SER | - | expression tag | UNP P0DTC2 |
| B | 1259 | HIS | - | expression tag | UNP P0DTC2 |
| B | 1260 | HIS | - | expression tag | UNP P0DTC2 |
| B | 1261 | HIS | - | expression tag | UNP P0DTC2 |
| B | 1262 | HIS | - | expression tag | UNP P0DTC2 |
| B | 1263 | HIS | - | expression tag | UNP P0DTC2 |
| B | 1264 | HIS | - | expression tag | UNP P0DTC2 |
| C | 682 | GLY | ARG | variant | UNP P0DTC2 |
| C | 683 | SER | ARG | variant | UNP P0DTC2 |
| C | 685 | SER | ARG | variant | UNP P0DTC2 |
| C | 942 | PRO | ALA | variant | UNP P0DTC2 |
| C | 986 | PRO | LYS | engineered mutation | UNP P0DTC2 |
| C | 987 | PRO | VAL | engineered mutation | UNP P0DTC2 |
| C | 1209 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1210 | SER | - | expression tag | UNP P0DTC2 |
| C | 1211 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1212 | SER | - | expression tag | UNP P0DTC2 |
| C | 1213 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1214 | TYR | - | expression tag | UNP P0DTC2 |
| C | 1215 | ILE | - | expression tag | UNP P0DTC2 |
| C | 1216 | PRO | - | expression tag | UNP P0DTC2 |
| C | 1217 | GLU | - | expression tag | UNP P0DTC2 |
| C | 1218 | ALA | - | expression tag | UNP P0DTC2 |
| C | 1219 | PRO | - | expression tag | UNP P0DTC2 |
| C | 1220 | ARG | - | expression tag | UNP P0DTC2 |
| C | 1221 | ASP | - | expression tag | UNP P0DTC2 |
| C | 1222 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1223 | GLN | - | expression tag | UNP P0DTC2 |
| C | 1224 | ALA | - | expression tag | UNP P0DTC2 |
| C | 1225 | TYR | - | expression tag | UNP P0DTC2 |
| C | 1226 | VAL | - | expression tag | UNP P0DTC2 |
| C | 1227 | ARG | - | expression tag | UNP P0DTC2 |
| C | 1228 | LYS | - | expression tag | UNP P0DTC2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 1229 | ASP | - | expression tag | UNP P0DTC2 |
| C | 1230 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1231 | GLU | - | expression tag | UNP P0DTC2 |
| C | 1232 | TRP | - | expression tag | UNP P0DTC2 |
| C | 1233 | VAL | - | expression tag | UNP P0DTC2 |
| C | 1234 | LEU | - | expression tag | UNP P0DTC2 |
| C | 1235 | LEU | - | expression tag | UNP P0DTC2 |
| C | 1236 | SER | - | expression tag | UNP P0DTC2 |
| C | 1237 | THR | - | expression tag | UNP P0DTC2 |
| C | 1238 | PHE | - | expression tag | UNP P0DTC2 |
| C | 1239 | LEU | - | expression tag | UNP P0DTC2 |
| C | 1240 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1241 | THR | - | expression tag | UNP P0DTC2 |
| C | 1242 | GLU | - | expression tag | UNP P0DTC2 |
| C | 1243 | ASN | - | expression tag | UNP P0DTC2 |
| C | 1244 | LEU | - | expression tag | UNP P0DTC2 |
| C | 1245 | TYR | - | expression tag | UNP P0DTC2 |
| C | 1246 | PHE | - | expression tag | UNP P0DTC2 |
| C | 1247 | GLN | - | expression tag | UNP P0DTC2 |
| C | 1248 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1249 | ASP | - | expression tag | UNP P0DTC2 |
| C | 1250 | TYR | - | expression tag | UNP P0DTC2 |
| C | 1251 | LYS | - | expression tag | UNP P0DTC2 |
| C | 1252 | ASP | - | expression tag | UNP P0DTC2 |
| C | 1253 | ASP | - | expression tag | UNP P0DTC2 |
| C | 1254 | ASP | - | expression tag | UNP P0DTC2 |
| C | 1255 | ASP | - | expression tag | UNP P0DTC2 |
| C | 1256 | LYS | - | expression tag | UNP P0DTC2 |
| C | 1257 | GLY | - | expression tag | UNP P0DTC2 |
| C | 1258 | SER | - | expression tag | UNP P0DTC2 |
| C | 1259 | HIS | - | expression tag | UNP P0DTC2 |
| C | 1260 | HIS | - | expression tag | UNP P0DTC2 |
| C | 1261 | HIS | - | expression tag | UNP P0DTC2 |
| C | 1262 | HIS | - | expression tag | UNP P0DTC2 |
| C | 1263 | HIS | - | expression tag | UNP P0DTC2 |
| C | 1264 | HIS | - | expression tag | UNP P0DTC2 |

- Molecule 2 is a protein called Camel-derived nanobody 1.29.

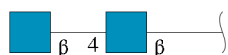
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | D | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 895 | 554 | 154 | 184 | 3 | | |

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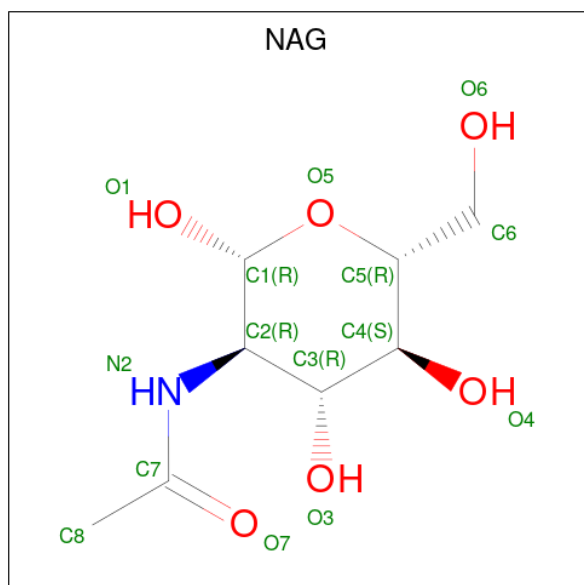
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | E | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 895 | 554 | 154 | 184 | 3 | | |

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|---|----|---------|-------|
| 3 | F | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 53 | 16 | 25 | 2 | 10 | | |
| 3 | G | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 53 | 16 | 25 | 2 | 10 | | |
| 3 | H | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 53 | 16 | 25 | 2 | 10 | | |
| 3 | I | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 53 | 16 | 25 | 2 | 10 | | |
| 3 | J | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 53 | 16 | 25 | 2 | 10 | | |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 26 | 8 | 12 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | A | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 26 | 8 | 12 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 26 | 8 | 12 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |

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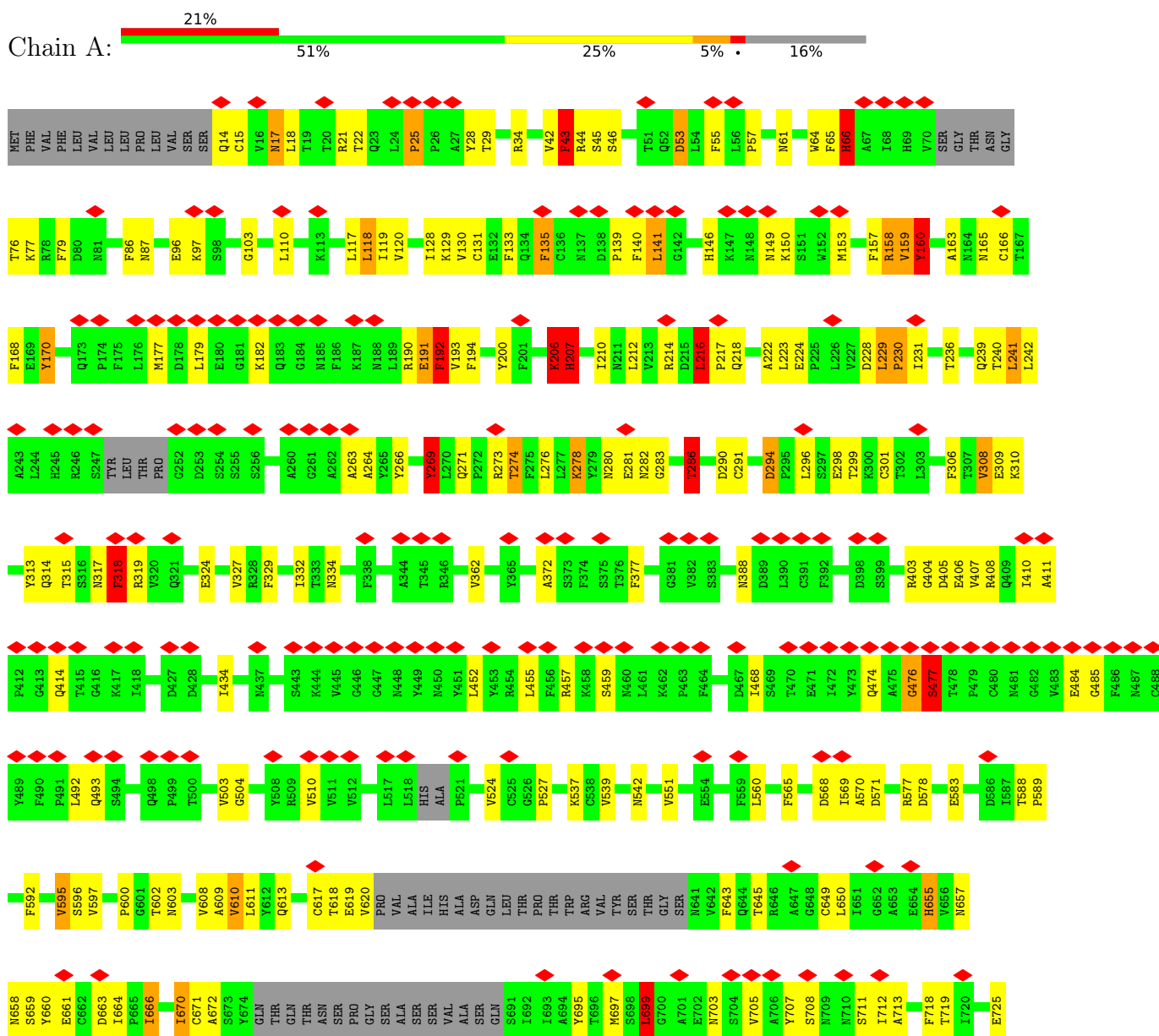
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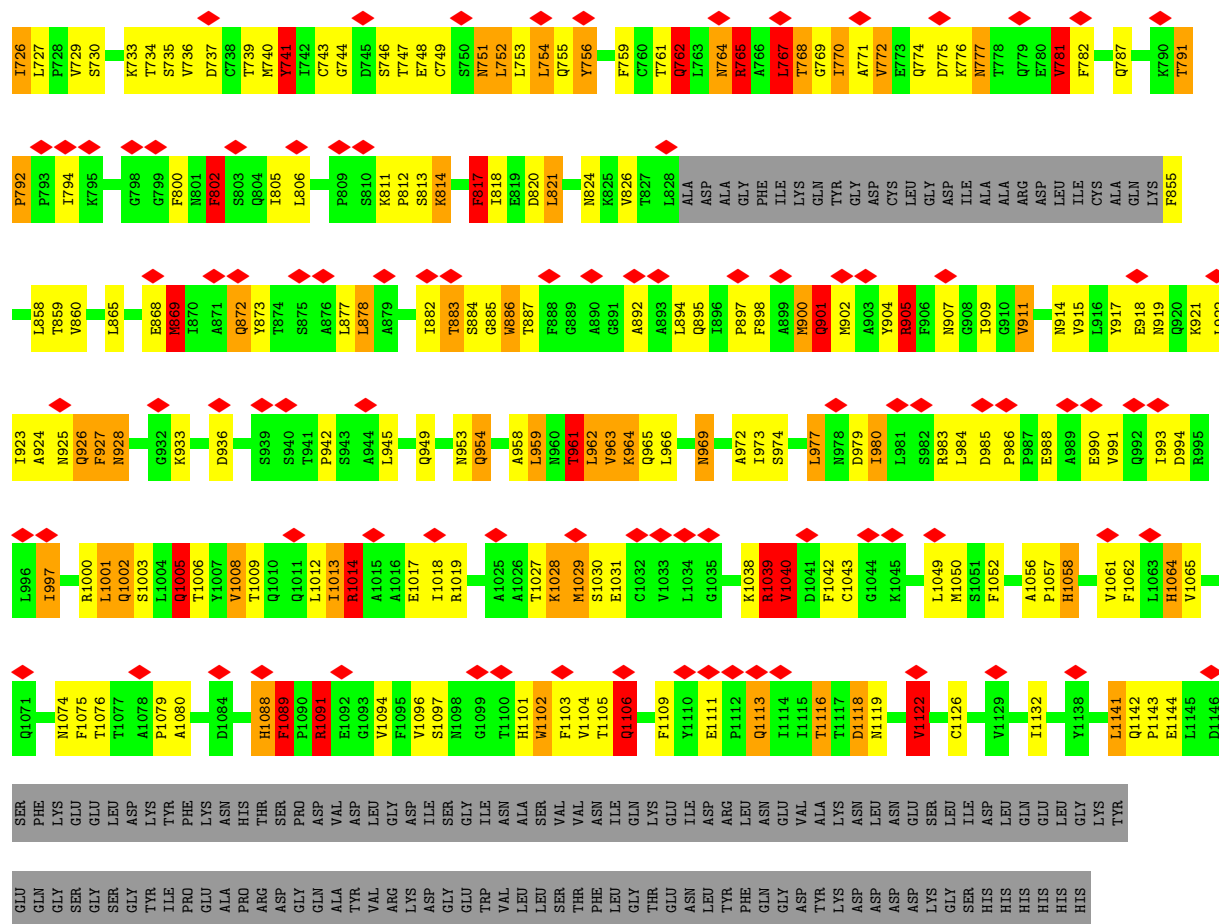
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | B | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | C | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | C | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | C | 1 | Total | C | H | N | O | 0 |
| | | | 26 | 8 | 12 | 1 | 5 | |
| 4 | C | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | C | 1 | Total | C | H | N | O | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | |
| 4 | C | 1 | Total | C | N | O | | 0 |
| | | | 14 | 8 | 1 | 5 | | |

3 Residue-property plots

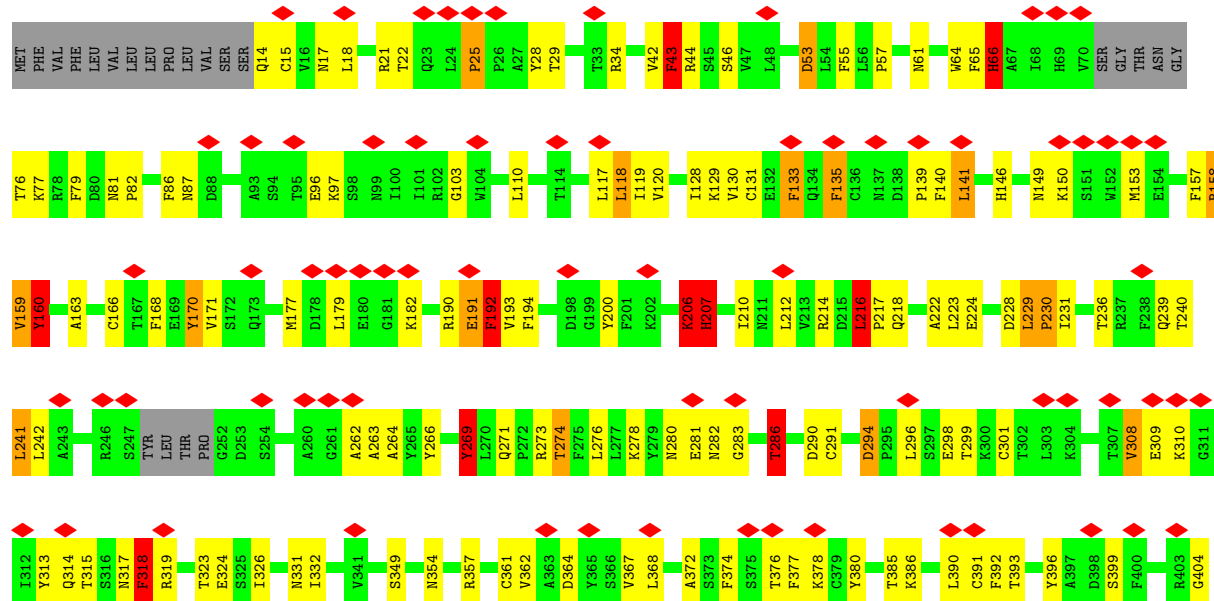
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein



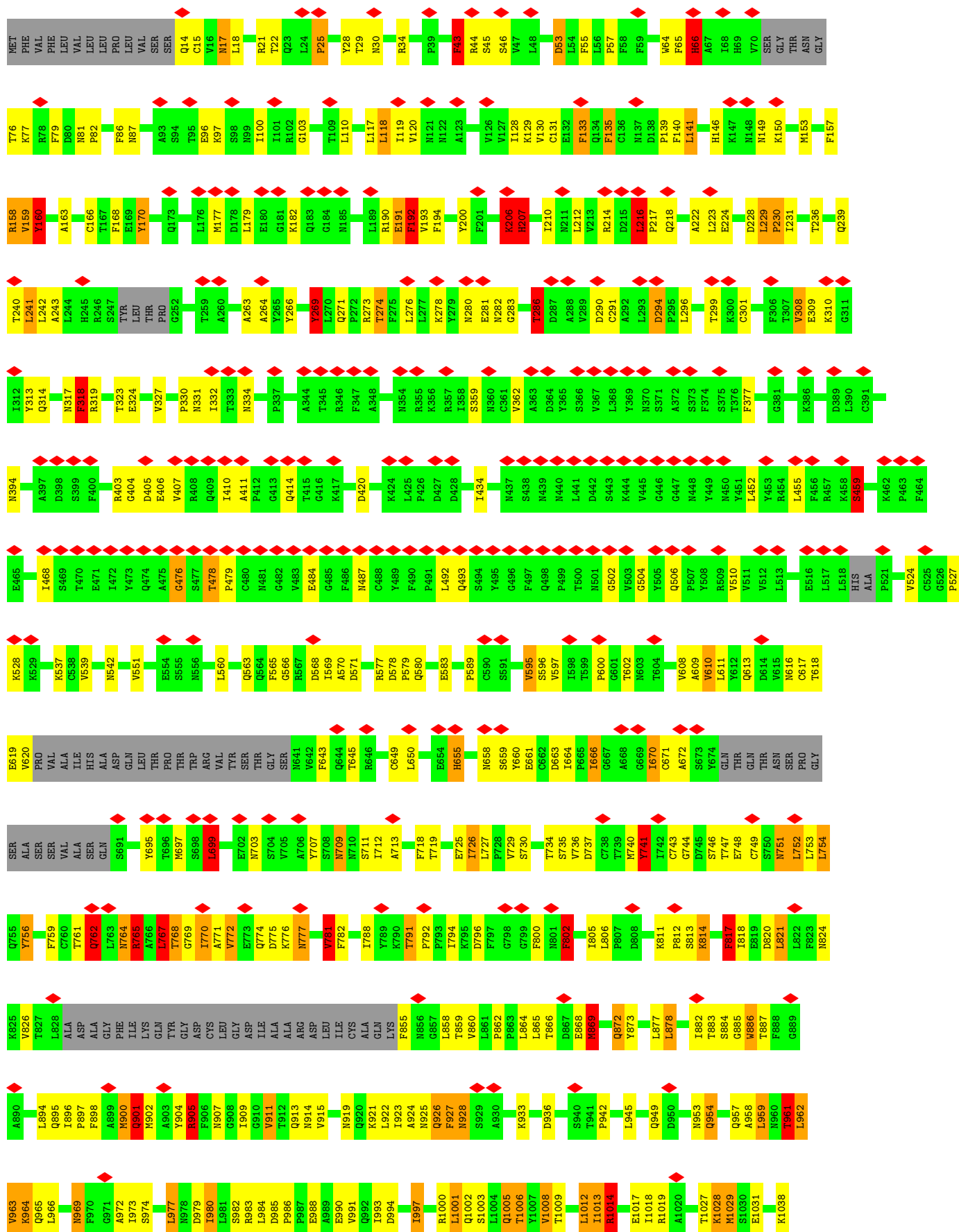


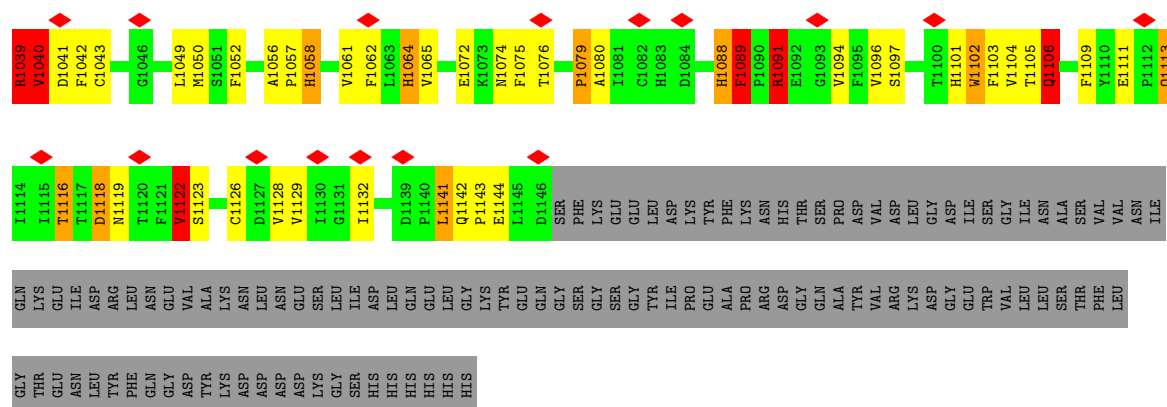
• Molecule 1: Spike glycoprotein



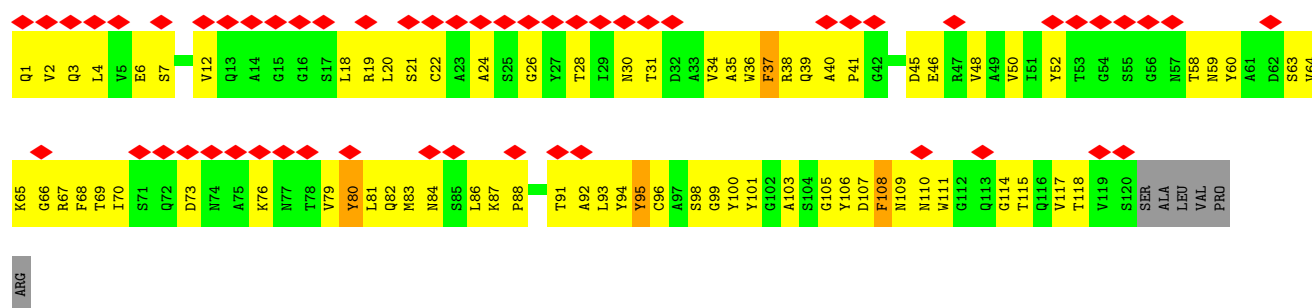


- Chain C: 

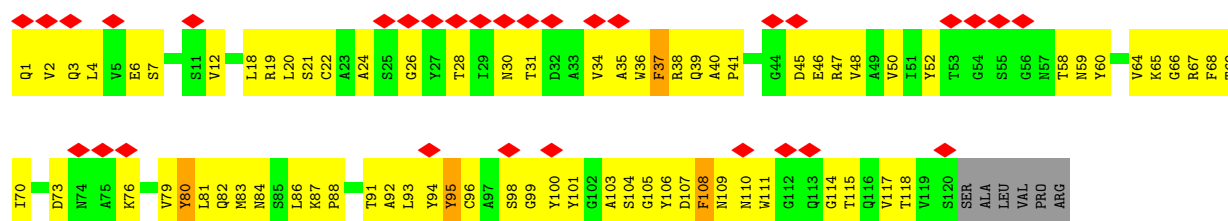




• Molecule 2: Camel-derived nanobody 1.29



• Molecule 2: Camel-derived nanobody 1.29



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 40000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 1.963 | Depositor |
| Minimum map value | -0.002 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.022 | Depositor |
| Recommended contour level | 0.025 | Depositor |
| Map size (Å) | 418.2, 418.2, 418.2 | wwPDB |
| Map dimensions | 492, 492, 492 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.85, 0.85, 0.85 | Depositor |

5 Model quality

5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 1.05 | 65/8501 (0.8%) | 2.07 | 240/11563 (2.1%) |
| 1 | B | 1.06 | 66/8452 (0.8%) | 2.08 | 238/11495 (2.1%) |
| 1 | C | 1.05 | 66/8488 (0.8%) | 2.07 | 239/11544 (2.1%) |
| 2 | D | 0.34 | 0/912 | 0.54 | 0/1238 |
| 2 | E | 0.34 | 0/912 | 0.54 | 0/1238 |
| All | All | 1.02 | 197/27265 (0.7%) | 2.01 | 717/37078 (1.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 11 | 40 |
| 1 | B | 11 | 38 |
| 1 | C | 11 | 38 |
| All | All | 33 | 116 |

All (197) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | C | 192 | PHE | CE1-CZ | -24.11 | 0.91 | 1.37 |
| 1 | A | 192 | PHE | CE1-CZ | -24.04 | 0.91 | 1.37 |
| 1 | B | 192 | PHE | CE1-CZ | -24.04 | 0.91 | 1.37 |
| 1 | B | 741 | TYR | CG-CD1 | -17.29 | 1.16 | 1.39 |
| 1 | C | 741 | TYR | CG-CD1 | -17.27 | 1.16 | 1.39 |
| 1 | A | 741 | TYR | CG-CD1 | -17.26 | 1.16 | 1.39 |
| 1 | B | 741 | TYR | CD2-CE2 | 17.03 | 1.65 | 1.39 |
| 1 | C | 741 | TYR | CD2-CE2 | 16.99 | 1.64 | 1.39 |
| 1 | A | 741 | TYR | CD2-CE2 | 16.98 | 1.64 | 1.39 |
| 1 | A | 741 | TYR | CE1-CZ | -16.46 | 1.17 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1 | C | 741 | TYR | CE1-CZ | -16.44 | 1.17 | 1.38 |
| 1 | B | 741 | TYR | CE1-CZ | -16.44 | 1.17 | 1.38 |
| 1 | B | 1106 | GLN | CB-CG | -15.74 | 1.10 | 1.52 |
| 1 | C | 1106 | GLN | CB-CG | -15.74 | 1.10 | 1.52 |
| 1 | A | 1106 | GLN | CB-CG | -15.73 | 1.10 | 1.52 |
| 1 | A | 741 | TYR | CE2-CZ | -13.41 | 1.21 | 1.38 |
| 1 | B | 741 | TYR | CE2-CZ | -13.37 | 1.21 | 1.38 |
| 1 | C | 741 | TYR | CE2-CZ | -13.36 | 1.21 | 1.38 |
| 1 | C | 43 | PHE | CE1-CZ | -12.71 | 1.13 | 1.37 |
| 1 | A | 43 | PHE | CE1-CZ | -12.69 | 1.13 | 1.37 |
| 1 | B | 43 | PHE | CE1-CZ | -12.68 | 1.13 | 1.37 |
| 1 | A | 772 | VAL | CB-CG2 | -12.36 | 1.26 | 1.52 |
| 1 | B | 772 | VAL | CB-CG2 | -12.36 | 1.26 | 1.52 |
| 1 | C | 772 | VAL | CB-CG2 | -12.34 | 1.26 | 1.52 |
| 1 | C | 911 | VAL | CB-CG2 | 12.02 | 1.78 | 1.52 |
| 1 | A | 911 | VAL | CB-CG2 | 12.01 | 1.78 | 1.52 |
| 1 | B | 911 | VAL | CB-CG2 | 12.01 | 1.78 | 1.52 |
| 1 | C | 911 | VAL | CB-CG1 | -12.00 | 1.27 | 1.52 |
| 1 | A | 911 | VAL | CB-CG1 | -11.98 | 1.27 | 1.52 |
| 1 | B | 911 | VAL | CB-CG1 | -11.96 | 1.27 | 1.52 |
| 1 | B | 170 | TYR | CG-CD2 | -11.39 | 1.24 | 1.39 |
| 1 | A | 170 | TYR | CG-CD2 | -11.38 | 1.24 | 1.39 |
| 1 | C | 170 | TYR | CG-CD2 | -11.36 | 1.24 | 1.39 |
| 1 | C | 230 | PRO | CG-CD | -11.32 | 1.13 | 1.50 |
| 1 | A | 230 | PRO | CG-CD | -11.32 | 1.13 | 1.50 |
| 1 | B | 230 | PRO | CG-CD | -11.32 | 1.13 | 1.50 |
| 1 | B | 756 | TYR | CD1-CE1 | -11.30 | 1.22 | 1.39 |
| 1 | C | 756 | TYR | CD1-CE1 | -11.29 | 1.22 | 1.39 |
| 1 | A | 756 | TYR | CD1-CE1 | -11.27 | 1.22 | 1.39 |
| 1 | A | 817 | PHE | CG-CD1 | -10.85 | 1.22 | 1.38 |
| 1 | C | 817 | PHE | CG-CD1 | -10.82 | 1.22 | 1.38 |
| 1 | B | 817 | PHE | CG-CD1 | -10.81 | 1.22 | 1.38 |
| 1 | A | 170 | TYR | CD2-CE2 | -9.75 | 1.24 | 1.39 |
| 1 | B | 43 | PHE | CD1-CE1 | -9.71 | 1.19 | 1.39 |
| 1 | B | 170 | TYR | CD2-CE2 | -9.69 | 1.24 | 1.39 |
| 1 | C | 43 | PHE | CD1-CE1 | -9.69 | 1.19 | 1.39 |
| 1 | C | 170 | TYR | CD2-CE2 | -9.68 | 1.24 | 1.39 |
| 1 | A | 43 | PHE | CD1-CE1 | -9.67 | 1.20 | 1.39 |
| 1 | A | 43 | PHE | CG-CD1 | -8.92 | 1.25 | 1.38 |
| 1 | B | 43 | PHE | CG-CD1 | -8.87 | 1.25 | 1.38 |
| 1 | C | 43 | PHE | CG-CD1 | -8.85 | 1.25 | 1.38 |
| 1 | B | 1106 | GLN | CD-OE1 | -8.45 | 1.05 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 1106 | GLN | CD-OE1 | -8.42 | 1.05 | 1.24 |
| 1 | C | 1106 | GLN | CD-OE1 | -8.39 | 1.05 | 1.24 |
| 1 | C | 756 | TYR | CD2-CE2 | -8.33 | 1.26 | 1.39 |
| 1 | A | 756 | TYR | CD2-CE2 | -8.31 | 1.26 | 1.39 |
| 1 | B | 756 | TYR | CD2-CE2 | -8.31 | 1.26 | 1.39 |
| 1 | A | 308 | VAL | CB-CG1 | -8.14 | 1.35 | 1.52 |
| 1 | C | 308 | VAL | CB-CG1 | -8.10 | 1.35 | 1.52 |
| 1 | B | 308 | VAL | CB-CG1 | -8.09 | 1.35 | 1.52 |
| 1 | A | 308 | VAL | CB-CG2 | 7.95 | 1.69 | 1.52 |
| 1 | B | 308 | VAL | CB-CG2 | 7.93 | 1.69 | 1.52 |
| 1 | C | 308 | VAL | CB-CG2 | 7.93 | 1.69 | 1.52 |
| 1 | B | 269 | TYR | CG-CD1 | -7.91 | 1.28 | 1.39 |
| 1 | C | 269 | TYR | CG-CD1 | -7.90 | 1.28 | 1.39 |
| 1 | A | 269 | TYR | CG-CD1 | -7.88 | 1.28 | 1.39 |
| 1 | B | 192 | PHE | CG-CD1 | -7.73 | 1.27 | 1.38 |
| 1 | C | 192 | PHE | CG-CD1 | -7.71 | 1.27 | 1.38 |
| 1 | A | 192 | PHE | CG-CD1 | -7.67 | 1.27 | 1.38 |
| 1 | A | 770 | ILE | CB-CG2 | 7.54 | 1.76 | 1.52 |
| 1 | B | 770 | ILE | CB-CG2 | 7.53 | 1.76 | 1.52 |
| 1 | C | 741 | TYR | CG-CD2 | 7.51 | 1.49 | 1.39 |
| 1 | C | 770 | ILE | CB-CG2 | 7.51 | 1.76 | 1.52 |
| 1 | A | 741 | TYR | CG-CD2 | 7.51 | 1.49 | 1.39 |
| 1 | B | 741 | TYR | CG-CD2 | 7.46 | 1.48 | 1.39 |
| 1 | B | 595 | VAL | CB-CG2 | 7.39 | 1.68 | 1.52 |
| 1 | A | 595 | VAL | CB-CG2 | 7.35 | 1.68 | 1.52 |
| 1 | C | 595 | VAL | CB-CG2 | 7.34 | 1.68 | 1.52 |
| 1 | C | 802 | PHE | CG-CD1 | -7.23 | 1.27 | 1.38 |
| 1 | A | 595 | VAL | CB-CG1 | -7.22 | 1.37 | 1.52 |
| 1 | C | 595 | VAL | CB-CG1 | -7.21 | 1.37 | 1.52 |
| 1 | B | 595 | VAL | CB-CG1 | -7.20 | 1.37 | 1.52 |
| 1 | A | 802 | PHE | CG-CD1 | -7.20 | 1.27 | 1.38 |
| 1 | B | 802 | PHE | CG-CD1 | -7.17 | 1.27 | 1.38 |
| 1 | A | 959 | LEU | CG-CD2 | 6.95 | 1.77 | 1.51 |
| 1 | C | 959 | LEU | CG-CD2 | 6.95 | 1.77 | 1.51 |
| 1 | B | 959 | LEU | CG-CD2 | 6.93 | 1.77 | 1.51 |
| 1 | C | 802 | PHE | CG-CD2 | 6.86 | 1.49 | 1.38 |
| 1 | B | 802 | PHE | CG-CD2 | 6.85 | 1.49 | 1.38 |
| 1 | A | 802 | PHE | CG-CD2 | 6.82 | 1.49 | 1.38 |
| 1 | A | 28 | TYR | CD1-CE1 | -6.76 | 1.29 | 1.39 |
| 1 | B | 699 | LEU | CG-CD2 | 6.68 | 1.76 | 1.51 |
| 1 | A | 699 | LEU | CG-CD2 | 6.66 | 1.76 | 1.51 |
| 1 | C | 699 | LEU | CG-CD2 | 6.66 | 1.76 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | B | 28 | TYR | CD1-CE1 | -6.64 | 1.29 | 1.39 |
| 1 | C | 28 | TYR | CD1-CE1 | -6.64 | 1.29 | 1.39 |
| 1 | C | 909 | ILE | CB-CG2 | 6.63 | 1.73 | 1.52 |
| 1 | A | 909 | ILE | CB-CG2 | 6.63 | 1.73 | 1.52 |
| 1 | B | 909 | ILE | CB-CG2 | 6.60 | 1.73 | 1.52 |
| 1 | B | 699 | LEU | CG-CD1 | -6.46 | 1.27 | 1.51 |
| 1 | C | 699 | LEU | CG-CD1 | -6.46 | 1.27 | 1.51 |
| 1 | A | 699 | LEU | CG-CD1 | -6.46 | 1.27 | 1.51 |
| 1 | B | 160 | TYR | CG-CD1 | -6.42 | 1.30 | 1.39 |
| 1 | A | 901 | GLN | CD-NE2 | -6.42 | 1.16 | 1.32 |
| 1 | B | 901 | GLN | CD-NE2 | -6.40 | 1.16 | 1.32 |
| 1 | C | 901 | GLN | CD-NE2 | -6.39 | 1.16 | 1.32 |
| 1 | A | 18 | LEU | CG-CD1 | -6.38 | 1.28 | 1.51 |
| 1 | C | 18 | LEU | CG-CD1 | -6.37 | 1.28 | 1.51 |
| 1 | A | 905 | ARG | CG-CD | 6.37 | 1.67 | 1.51 |
| 1 | B | 18 | LEU | CG-CD1 | -6.36 | 1.28 | 1.51 |
| 1 | C | 160 | TYR | CG-CD1 | -6.35 | 1.30 | 1.39 |
| 1 | C | 905 | ARG | CG-CD | 6.35 | 1.67 | 1.51 |
| 1 | B | 905 | ARG | CG-CD | 6.33 | 1.67 | 1.51 |
| 1 | A | 160 | TYR | CG-CD1 | -6.32 | 1.30 | 1.39 |
| 1 | C | 170 | TYR | CE1-CZ | -6.32 | 1.30 | 1.38 |
| 1 | B | 170 | TYR | CE1-CZ | -6.26 | 1.30 | 1.38 |
| 1 | A | 170 | TYR | CE1-CZ | -6.24 | 1.30 | 1.38 |
| 1 | C | 1106 | GLN | CD-NE2 | -6.20 | 1.17 | 1.32 |
| 1 | B | 1106 | GLN | CD-NE2 | -6.17 | 1.17 | 1.32 |
| 1 | A | 1106 | GLN | CD-NE2 | -6.16 | 1.17 | 1.32 |
| 1 | A | 610 | VAL | CB-CG1 | -6.12 | 1.40 | 1.52 |
| 1 | C | 802 | PHE | CE1-CZ | -6.12 | 1.25 | 1.37 |
| 1 | A | 802 | PHE | CE1-CZ | -6.11 | 1.25 | 1.37 |
| 1 | B | 610 | VAL | CB-CG1 | -6.09 | 1.40 | 1.52 |
| 1 | B | 802 | PHE | CE1-CZ | -6.08 | 1.25 | 1.37 |
| 1 | C | 610 | VAL | CB-CG1 | -6.06 | 1.40 | 1.52 |
| 1 | B | 821 | LEU | CG-CD2 | 6.01 | 1.74 | 1.51 |
| 1 | A | 28 | TYR | CD2-CE2 | -5.99 | 1.30 | 1.39 |
| 1 | C | 776 | LYS | CG-CD | 5.99 | 1.72 | 1.52 |
| 1 | A | 821 | LEU | CG-CD2 | 5.98 | 1.74 | 1.51 |
| 1 | B | 776 | LYS | CG-CD | 5.98 | 1.72 | 1.52 |
| 1 | C | 821 | LEU | CG-CD2 | 5.98 | 1.74 | 1.51 |
| 1 | A | 776 | LYS | CG-CD | 5.97 | 1.72 | 1.52 |
| 1 | B | 28 | TYR | CD2-CE2 | -5.96 | 1.30 | 1.39 |
| 1 | C | 28 | TYR | CD2-CE2 | -5.96 | 1.30 | 1.39 |
| 1 | A | 18 | LEU | CG-CD2 | -5.92 | 1.29 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | C | 18 | LEU | CG-CD2 | -5.90 | 1.30 | 1.51 |
| 1 | B | 18 | LEU | CG-CD2 | -5.90 | 1.30 | 1.51 |
| 1 | A | 901 | GLN | CG-CD | 5.76 | 1.64 | 1.51 |
| 1 | B | 997 | ILE | CB-CG1 | -5.76 | 1.38 | 1.54 |
| 1 | B | 901 | GLN | CG-CD | 5.76 | 1.64 | 1.51 |
| 1 | C | 997 | ILE | CB-CG1 | -5.75 | 1.38 | 1.54 |
| 1 | C | 901 | GLN | CG-CD | 5.75 | 1.64 | 1.51 |
| 1 | A | 997 | ILE | CB-CG1 | -5.75 | 1.38 | 1.54 |
| 1 | B | 168 | PHE | CD2-CE2 | -5.55 | 1.28 | 1.39 |
| 1 | A | 168 | PHE | CD2-CE2 | -5.53 | 1.28 | 1.39 |
| 1 | C | 168 | PHE | CD2-CE2 | -5.52 | 1.28 | 1.39 |
| 1 | B | 1013 | ILE | CB-CG2 | -5.48 | 1.35 | 1.52 |
| 1 | B | 170 | TYR | CD1-CE1 | -5.48 | 1.31 | 1.39 |
| 1 | C | 1013 | ILE | CB-CG2 | -5.47 | 1.35 | 1.52 |
| 1 | A | 1013 | ILE | CB-CG2 | -5.44 | 1.35 | 1.52 |
| 1 | C | 135 | PHE | CD1-CE1 | -5.44 | 1.28 | 1.39 |
| 1 | C | 170 | TYR | CD1-CE1 | -5.43 | 1.31 | 1.39 |
| 1 | A | 135 | PHE | CD1-CE1 | -5.42 | 1.28 | 1.39 |
| 1 | A | 170 | TYR | CD1-CE1 | -5.41 | 1.31 | 1.39 |
| 1 | B | 135 | PHE | CD1-CE1 | -5.41 | 1.28 | 1.39 |
| 1 | B | 299 | THR | CB-CG2 | -5.31 | 1.34 | 1.52 |
| 1 | A | 299 | THR | CB-CG2 | -5.31 | 1.34 | 1.52 |
| 1 | C | 299 | THR | CB-CG2 | -5.31 | 1.34 | 1.52 |
| 1 | C | 991 | VAL | CB-CG1 | -5.31 | 1.41 | 1.52 |
| 1 | A | 991 | VAL | CB-CG1 | -5.27 | 1.41 | 1.52 |
| 1 | B | 991 | VAL | CB-CG1 | -5.24 | 1.41 | 1.52 |
| 1 | B | 160 | TYR | CE2-CZ | -5.23 | 1.31 | 1.38 |
| 1 | C | 719 | THR | CB-CG2 | -5.20 | 1.35 | 1.52 |
| 1 | A | 719 | THR | CB-CG2 | -5.19 | 1.35 | 1.52 |
| 1 | B | 877 | LEU | CG-CD2 | -5.19 | 1.32 | 1.51 |
| 1 | B | 1089 | PHE | CG-CD1 | -5.19 | 1.30 | 1.38 |
| 1 | C | 802 | PHE | CE2-CZ | -5.19 | 1.27 | 1.37 |
| 1 | B | 719 | THR | CB-CG2 | -5.18 | 1.35 | 1.52 |
| 1 | C | 877 | LEU | CG-CD2 | -5.18 | 1.32 | 1.51 |
| 1 | B | 802 | PHE | CE2-CZ | -5.17 | 1.27 | 1.37 |
| 1 | A | 877 | LEU | CG-CD2 | -5.17 | 1.32 | 1.51 |
| 1 | C | 160 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | A | 160 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | B | 160 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | A | 802 | PHE | CE2-CZ | -5.14 | 1.27 | 1.37 |
| 1 | A | 160 | TYR | CE2-CZ | -5.13 | 1.31 | 1.38 |
| 1 | C | 1089 | PHE | CG-CD1 | -5.13 | 1.31 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 269 | TYR | CE2-CZ | -5.12 | 1.31 | 1.38 |
| 1 | C | 160 | TYR | CE2-CZ | -5.11 | 1.31 | 1.38 |
| 1 | B | 141 | LEU | CB-CG | 5.11 | 1.67 | 1.52 |
| 1 | A | 1089 | PHE | CG-CD1 | -5.11 | 1.31 | 1.38 |
| 1 | C | 141 | LEU | CB-CG | 5.10 | 1.67 | 1.52 |
| 1 | B | 269 | TYR | CE2-CZ | -5.09 | 1.31 | 1.38 |
| 1 | A | 141 | LEU | CB-CG | 5.09 | 1.67 | 1.52 |
| 1 | C | 133 | PHE | CD1-CE1 | -5.09 | 1.29 | 1.39 |
| 1 | C | 741 | TYR | CZ-OH | -5.09 | 1.29 | 1.37 |
| 1 | B | 741 | TYR | CZ-OH | -5.08 | 1.29 | 1.37 |
| 1 | B | 133 | PHE | CD1-CE1 | -5.07 | 1.29 | 1.39 |
| 1 | A | 741 | TYR | CZ-OH | -5.06 | 1.29 | 1.37 |
| 1 | C | 269 | TYR | CE2-CZ | -5.05 | 1.31 | 1.38 |
| 1 | B | 230 | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 1 | A | 1065 | VAL | CB-CG2 | 5.04 | 1.63 | 1.52 |
| 1 | C | 1065 | VAL | CB-CG2 | 5.03 | 1.63 | 1.52 |
| 1 | C | 230 | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 1 | A | 135 | PHE | CD2-CE2 | -5.01 | 1.29 | 1.39 |
| 1 | B | 1065 | VAL | CB-CG2 | 5.00 | 1.63 | 1.52 |

All (717) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | B | 192 | PHE | CB-CG-CD1 | 56.88 | 160.62 | 120.80 |
| 1 | C | 192 | PHE | CB-CG-CD1 | 56.85 | 160.60 | 120.80 |
| 1 | A | 192 | PHE | CB-CG-CD1 | 56.80 | 160.56 | 120.80 |
| 1 | B | 192 | PHE | CB-CG-CD2 | -51.66 | 84.64 | 120.80 |
| 1 | A | 192 | PHE | CB-CG-CD2 | -51.65 | 84.65 | 120.80 |
| 1 | C | 192 | PHE | CB-CG-CD2 | -51.61 | 84.67 | 120.80 |
| 1 | B | 741 | TYR | CB-CG-CD1 | 48.82 | 150.29 | 121.00 |
| 1 | A | 741 | TYR | CB-CG-CD1 | 48.78 | 150.27 | 121.00 |
| 1 | C | 741 | TYR | CB-CG-CD1 | 48.71 | 150.23 | 121.00 |
| 1 | B | 741 | TYR | CB-CG-CD2 | -42.21 | 95.67 | 121.00 |
| 1 | C | 741 | TYR | CB-CG-CD2 | -42.21 | 95.67 | 121.00 |
| 1 | A | 741 | TYR | CB-CG-CD2 | -42.18 | 95.69 | 121.00 |
| 1 | A | 741 | TYR | CD1-CG-CD2 | -38.91 | 75.09 | 117.90 |
| 1 | C | 741 | TYR | CD1-CG-CD2 | -38.91 | 75.10 | 117.90 |
| 1 | B | 741 | TYR | CD1-CG-CD2 | -38.87 | 75.14 | 117.90 |
| 1 | A | 802 | PHE | CB-CG-CD2 | -34.93 | 96.35 | 120.80 |
| 1 | C | 802 | PHE | CB-CG-CD2 | -34.89 | 96.38 | 120.80 |
| 1 | B | 802 | PHE | CB-CG-CD2 | -34.87 | 96.39 | 120.80 |
| 1 | B | 1106 | GLN | CA-CB-CG | 30.26 | 179.98 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | A | 1106 | GLN | CA-CB-CG | 30.25 | 179.96 | 113.40 |
| 1 | C | 1106 | GLN | CA-CB-CG | 30.24 | 179.93 | 113.40 |
| 1 | B | 959 | LEU | CB-CG-CD1 | 28.16 | 158.87 | 111.00 |
| 1 | C | 959 | LEU | CB-CG-CD1 | 28.14 | 158.84 | 111.00 |
| 1 | A | 959 | LEU | CB-CG-CD1 | 28.13 | 158.83 | 111.00 |
| 1 | A | 1012 | LEU | CB-CG-CD1 | 27.59 | 157.91 | 111.00 |
| 1 | B | 1012 | LEU | CB-CG-CD1 | 27.57 | 157.86 | 111.00 |
| 1 | C | 1012 | LEU | CB-CG-CD1 | 27.55 | 157.83 | 111.00 |
| 1 | B | 911 | VAL | CG1-CB-CG2 | -26.16 | 69.05 | 110.90 |
| 1 | C | 911 | VAL | CG1-CB-CG2 | -26.14 | 69.07 | 110.90 |
| 1 | A | 911 | VAL | CG1-CB-CG2 | -26.14 | 69.08 | 110.90 |
| 1 | C | 909 | ILE | CG1-CB-CG2 | -25.02 | 56.34 | 111.40 |
| 1 | A | 909 | ILE | CG1-CB-CG2 | -25.02 | 56.36 | 111.40 |
| 1 | B | 909 | ILE | CG1-CB-CG2 | -25.02 | 56.36 | 111.40 |
| 1 | B | 802 | PHE | CB-CG-CD1 | 23.88 | 137.51 | 120.80 |
| 1 | A | 192 | PHE | CD1-CG-CD2 | -23.85 | 87.29 | 118.30 |
| 1 | B | 192 | PHE | CD1-CG-CD2 | -23.84 | 87.31 | 118.30 |
| 1 | C | 192 | PHE | CD1-CG-CD2 | -23.84 | 87.31 | 118.30 |
| 1 | C | 802 | PHE | CB-CG-CD1 | 23.82 | 137.47 | 120.80 |
| 1 | A | 802 | PHE | CB-CG-CD1 | 23.80 | 137.46 | 120.80 |
| 1 | A | 43 | PHE | CB-CG-CD2 | -22.98 | 104.71 | 120.80 |
| 1 | C | 43 | PHE | CB-CG-CD2 | -22.98 | 104.72 | 120.80 |
| 1 | B | 43 | PHE | CB-CG-CD2 | -22.97 | 104.72 | 120.80 |
| 1 | A | 1065 | VAL | CG1-CB-CG2 | -22.78 | 74.45 | 110.90 |
| 1 | B | 595 | VAL | CG1-CB-CG2 | -22.78 | 74.46 | 110.90 |
| 1 | C | 1065 | VAL | CG1-CB-CG2 | -22.77 | 74.47 | 110.90 |
| 1 | B | 1065 | VAL | CG1-CB-CG2 | -22.76 | 74.48 | 110.90 |
| 1 | A | 595 | VAL | CG1-CB-CG2 | -22.75 | 74.50 | 110.90 |
| 1 | C | 595 | VAL | CG1-CB-CG2 | -22.74 | 74.51 | 110.90 |
| 1 | C | 927 | PHE | CB-CG-CD2 | -21.31 | 105.88 | 120.80 |
| 1 | A | 927 | PHE | CB-CG-CD2 | -21.30 | 105.89 | 120.80 |
| 1 | B | 927 | PHE | CB-CG-CD2 | -21.30 | 105.89 | 120.80 |
| 1 | C | 160 | TYR | CB-CG-CD2 | -20.82 | 108.51 | 121.00 |
| 1 | A | 160 | TYR | CB-CG-CD2 | -20.81 | 108.52 | 121.00 |
| 1 | B | 160 | TYR | CB-CG-CD2 | -20.80 | 108.52 | 121.00 |
| 1 | C | 959 | LEU | CB-CG-CD2 | -19.97 | 77.05 | 111.00 |
| 1 | A | 959 | LEU | CB-CG-CD2 | -19.95 | 77.09 | 111.00 |
| 1 | B | 959 | LEU | CB-CG-CD2 | -19.93 | 77.11 | 111.00 |
| 1 | A | 770 | ILE | CG1-CB-CG2 | -19.82 | 67.80 | 111.40 |
| 1 | B | 770 | ILE | CG1-CB-CG2 | -19.82 | 67.80 | 111.40 |
| 1 | C | 770 | ILE | CG1-CB-CG2 | -19.82 | 67.81 | 111.40 |
| 1 | A | 962 | LEU | CB-CG-CD1 | -19.74 | 77.44 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | B | 962 | LEU | CB-CG-CD1 | -19.74 | 77.45 | 111.00 |
| 1 | C | 962 | LEU | CB-CG-CD1 | -19.74 | 77.45 | 111.00 |
| 1 | B | 192 | PHE | CG-CD1-CE1 | 19.60 | 142.36 | 120.80 |
| 1 | A | 192 | PHE | CG-CD1-CE1 | 19.58 | 142.34 | 120.80 |
| 1 | C | 192 | PHE | CG-CD1-CE1 | 19.57 | 142.33 | 120.80 |
| 1 | A | 802 | PHE | CD1-CG-CD2 | -19.55 | 92.88 | 118.30 |
| 1 | C | 802 | PHE | CD1-CG-CD2 | -19.55 | 92.89 | 118.30 |
| 1 | B | 802 | PHE | CD1-CG-CD2 | -19.53 | 92.92 | 118.30 |
| 1 | C | 1012 | LEU | CB-CG-CD2 | -18.38 | 79.76 | 111.00 |
| 1 | B | 1012 | LEU | CB-CG-CD2 | -18.37 | 79.78 | 111.00 |
| 1 | A | 1012 | LEU | CB-CG-CD2 | -18.36 | 79.80 | 111.00 |
| 1 | A | 776 | LYS | CD-CE-NZ | 18.35 | 153.91 | 111.70 |
| 1 | C | 776 | LYS | CD-CE-NZ | 18.33 | 153.86 | 111.70 |
| 1 | B | 776 | LYS | CD-CE-NZ | 18.33 | 153.85 | 111.70 |
| 1 | C | 610 | VAL | CG1-CB-CG2 | -18.28 | 81.65 | 110.90 |
| 1 | B | 610 | VAL | CG1-CB-CG2 | -18.26 | 81.68 | 110.90 |
| 1 | A | 610 | VAL | CG1-CB-CG2 | -18.25 | 81.70 | 110.90 |
| 1 | B | 308 | VAL | CG1-CB-CG2 | -17.91 | 82.24 | 110.90 |
| 1 | A | 308 | VAL | CG1-CB-CG2 | -17.91 | 82.24 | 110.90 |
| 1 | C | 308 | VAL | CG1-CB-CG2 | -17.91 | 82.25 | 110.90 |
| 1 | B | 765 | ARG | CD-NE-CZ | 16.86 | 147.20 | 123.60 |
| 1 | C | 765 | ARG | CD-NE-CZ | 16.85 | 147.19 | 123.60 |
| 1 | A | 765 | ARG | CD-NE-CZ | 16.82 | 147.15 | 123.60 |
| 1 | C | 905 | ARG | NE-CZ-NH2 | -16.42 | 112.09 | 120.30 |
| 1 | A | 905 | ARG | NE-CZ-NH2 | -16.38 | 112.11 | 120.30 |
| 1 | B | 905 | ARG | NE-CZ-NH2 | -16.35 | 112.12 | 120.30 |
| 1 | B | 741 | TYR | CG-CD1-CE1 | 16.05 | 134.14 | 121.30 |
| 1 | A | 741 | TYR | CG-CD1-CE1 | 16.00 | 134.10 | 121.30 |
| 1 | C | 741 | TYR | CG-CD1-CE1 | 15.97 | 134.08 | 121.30 |
| 1 | A | 905 | ARG | CG-CD-NE | 15.84 | 145.06 | 111.80 |
| 1 | B | 905 | ARG | CG-CD-NE | 15.83 | 145.04 | 111.80 |
| 1 | C | 905 | ARG | CG-CD-NE | 15.82 | 145.02 | 111.80 |
| 1 | B | 1116 | THR | OG1-CB-CG2 | -15.16 | 75.12 | 110.00 |
| 1 | A | 1116 | THR | OG1-CB-CG2 | -15.16 | 75.13 | 110.00 |
| 1 | C | 1116 | THR | OG1-CB-CG2 | -15.14 | 75.18 | 110.00 |
| 1 | C | 814 | LYS | CD-CE-NZ | 15.02 | 146.25 | 111.70 |
| 1 | A | 814 | LYS | CD-CE-NZ | 15.02 | 146.25 | 111.70 |
| 1 | B | 814 | LYS | CD-CE-NZ | 15.02 | 146.24 | 111.70 |
| 1 | B | 43 | PHE | CB-CG-CD1 | 14.47 | 130.93 | 120.80 |
| 1 | A | 821 | LEU | CB-CG-CD1 | 14.46 | 135.59 | 111.00 |
| 1 | A | 43 | PHE | CB-CG-CD1 | 14.46 | 130.92 | 120.80 |
| 1 | C | 821 | LEU | CB-CG-CD1 | 14.45 | 135.56 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | B | 821 | LEU | CB-CG-CD1 | 14.44 | 135.54 | 111.00 |
| 1 | C | 43 | PHE | CB-CG-CD1 | 14.37 | 130.86 | 120.80 |
| 1 | A | 1012 | LEU | CA-CB-CG | 14.29 | 148.16 | 115.30 |
| 1 | B | 1012 | LEU | CA-CB-CG | 14.29 | 148.16 | 115.30 |
| 1 | C | 1012 | LEU | CA-CB-CG | 14.28 | 148.15 | 115.30 |
| 1 | A | 962 | LEU | CB-CG-CD2 | 14.28 | 135.28 | 111.00 |
| 1 | C | 962 | LEU | CB-CG-CD2 | 14.28 | 135.28 | 111.00 |
| 1 | B | 962 | LEU | CB-CG-CD2 | 14.25 | 135.22 | 111.00 |
| 1 | C | 741 | TYR | CD1-CE1-CZ | -14.23 | 106.99 | 119.80 |
| 1 | A | 741 | TYR | CD1-CE1-CZ | -14.23 | 107.00 | 119.80 |
| 1 | B | 741 | TYR | CD1-CE1-CZ | -14.18 | 107.04 | 119.80 |
| 1 | C | 927 | PHE | CB-CG-CD1 | 13.97 | 130.58 | 120.80 |
| 1 | A | 927 | PHE | CB-CG-CD1 | 13.95 | 130.56 | 120.80 |
| 1 | B | 927 | PHE | CB-CG-CD1 | 13.94 | 130.56 | 120.80 |
| 1 | A | 230 | PRO | CA-N-CD | -13.94 | 91.99 | 111.50 |
| 1 | B | 230 | PRO | CA-N-CD | -13.92 | 92.01 | 111.50 |
| 1 | C | 230 | PRO | CA-N-CD | -13.92 | 92.01 | 111.50 |
| 1 | C | 1141 | LEU | CB-CG-CD2 | 13.75 | 134.37 | 111.00 |
| 1 | B | 1141 | LEU | CB-CG-CD2 | 13.73 | 134.35 | 111.00 |
| 1 | A | 1141 | LEU | CB-CG-CD2 | 13.73 | 134.34 | 111.00 |
| 1 | B | 141 | LEU | CA-CB-CG | -13.33 | 84.64 | 115.30 |
| 1 | C | 141 | LEU | CA-CB-CG | -13.32 | 84.67 | 115.30 |
| 1 | A | 141 | LEU | CA-CB-CG | -13.32 | 84.67 | 115.30 |
| 1 | B | 699 | LEU | CD1-CG-CD2 | -12.91 | 71.76 | 110.50 |
| 1 | C | 699 | LEU | CD1-CG-CD2 | -12.91 | 71.78 | 110.50 |
| 1 | A | 699 | LEU | CD1-CG-CD2 | -12.90 | 71.78 | 110.50 |
| 1 | C | 821 | LEU | CB-CG-CD2 | -12.71 | 89.39 | 111.00 |
| 1 | B | 821 | LEU | CB-CG-CD2 | -12.71 | 89.39 | 111.00 |
| 1 | A | 821 | LEU | CB-CG-CD2 | -12.68 | 89.44 | 111.00 |
| 1 | A | 991 | VAL | CG1-CB-CG2 | -12.65 | 90.66 | 110.90 |
| 1 | C | 991 | VAL | CG1-CB-CG2 | -12.64 | 90.68 | 110.90 |
| 1 | B | 991 | VAL | CG1-CB-CG2 | -12.63 | 90.69 | 110.90 |
| 1 | A | 911 | VAL | CA-CB-CG1 | 12.62 | 129.83 | 110.90 |
| 1 | B | 911 | VAL | CA-CB-CG1 | 12.60 | 129.80 | 110.90 |
| 1 | C | 911 | VAL | CA-CB-CG1 | 12.60 | 129.79 | 110.90 |
| 1 | B | 997 | ILE | CA-CB-CG1 | 12.51 | 134.77 | 111.00 |
| 1 | A | 821 | LEU | CD1-CG-CD2 | -12.50 | 73.00 | 110.50 |
| 1 | B | 821 | LEU | CD1-CG-CD2 | -12.50 | 73.00 | 110.50 |
| 1 | C | 821 | LEU | CD1-CG-CD2 | -12.50 | 73.01 | 110.50 |
| 1 | C | 997 | ILE | CA-CB-CG1 | 12.50 | 134.74 | 111.00 |
| 1 | A | 997 | ILE | CA-CB-CG1 | 12.49 | 134.72 | 111.00 |
| 1 | A | 909 | ILE | CA-CB-CG2 | -12.44 | 86.03 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | B | 909 | ILE | CA-CB-CG2 | -12.43 | 86.05 | 110.90 |
| 1 | C | 909 | ILE | CA-CB-CG2 | -12.42 | 86.07 | 110.90 |
| 1 | B | 909 | ILE | CA-CB-CG1 | 12.37 | 134.51 | 111.00 |
| 1 | C | 909 | ILE | CA-CB-CG1 | 12.37 | 134.51 | 111.00 |
| 1 | A | 909 | ILE | CA-CB-CG1 | 12.36 | 134.48 | 111.00 |
| 1 | A | 216 | LEU | CA-CB-CG | 12.21 | 143.38 | 115.30 |
| 1 | C | 216 | LEU | CA-CB-CG | 12.19 | 143.33 | 115.30 |
| 1 | B | 216 | LEU | CA-CB-CG | 12.18 | 143.32 | 115.30 |
| 1 | B | 902 | MET | CB-CG-SD | 12.09 | 148.66 | 112.40 |
| 1 | C | 902 | MET | CB-CG-SD | 12.07 | 148.62 | 112.40 |
| 1 | A | 902 | MET | CB-CG-SD | 12.07 | 148.61 | 112.40 |
| 1 | C | 1079 | PRO | CA-N-CD | -11.98 | 94.73 | 111.50 |
| 1 | B | 1079 | PRO | CA-N-CD | -11.95 | 94.78 | 111.50 |
| 1 | A | 1079 | PRO | CA-N-CD | -11.93 | 94.80 | 111.50 |
| 1 | C | 1141 | LEU | CA-CB-CG | 11.87 | 142.60 | 115.30 |
| 1 | B | 1141 | LEU | CA-CB-CG | 11.86 | 142.58 | 115.30 |
| 1 | A | 1141 | LEU | CA-CB-CG | 11.84 | 142.54 | 115.30 |
| 1 | A | 1116 | THR | CA-CB-OG1 | 11.62 | 133.39 | 109.00 |
| 1 | C | 1116 | THR | CA-CB-OG1 | 11.61 | 133.38 | 109.00 |
| 1 | A | 278 | LYS | CD-CE-NZ | 11.61 | 138.40 | 111.70 |
| 1 | B | 1116 | THR | CA-CB-OG1 | 11.59 | 133.35 | 109.00 |
| 1 | C | 278 | LYS | CD-CE-NZ | 11.59 | 138.35 | 111.70 |
| 1 | A | 43 | PHE | CD1-CG-CD2 | -11.57 | 103.25 | 118.30 |
| 1 | B | 278 | LYS | CD-CE-NZ | 11.57 | 138.32 | 111.70 |
| 1 | C | 43 | PHE | CD1-CG-CD2 | -11.54 | 103.29 | 118.30 |
| 1 | B | 43 | PHE | CD1-CG-CD2 | -11.53 | 103.31 | 118.30 |
| 1 | B | 927 | PHE | CD1-CG-CD2 | -11.52 | 103.32 | 118.30 |
| 1 | A | 927 | PHE | CD1-CG-CD2 | -11.51 | 103.33 | 118.30 |
| 1 | C | 927 | PHE | CD1-CG-CD2 | -11.51 | 103.34 | 118.30 |
| 1 | B | 1091 | ARG | CA-CB-CG | 11.45 | 138.58 | 113.40 |
| 1 | C | 1091 | ARG | CA-CB-CG | 11.42 | 138.52 | 113.40 |
| 1 | A | 1091 | ARG | CA-CB-CG | 11.41 | 138.51 | 113.40 |
| 1 | B | 762 | GLN | CG-CD-OE1 | 11.40 | 144.39 | 121.60 |
| 1 | C | 762 | GLN | CG-CD-OE1 | 11.38 | 144.36 | 121.60 |
| 1 | A | 762 | GLN | CG-CD-OE1 | 11.37 | 144.34 | 121.60 |
| 1 | B | 1005 | GLN | CA-CB-CG | 11.36 | 138.39 | 113.40 |
| 1 | C | 1005 | GLN | CA-CB-CG | 11.36 | 138.38 | 113.40 |
| 1 | A | 1005 | GLN | CA-CB-CG | 11.35 | 138.37 | 113.40 |
| 1 | A | 762 | GLN | CG-CD-NE2 | -11.27 | 89.64 | 116.70 |
| 1 | B | 762 | GLN | CG-CD-NE2 | -11.27 | 89.66 | 116.70 |
| 1 | C | 762 | GLN | CG-CD-NE2 | -11.26 | 89.68 | 116.70 |
| 1 | B | 817 | PHE | CD1-CG-CD2 | -10.97 | 104.03 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | C | 817 | PHE | CD1-CG-CD2 | -10.94 | 104.08 | 118.30 |
| 1 | A | 1013 | ILE | CA-CB-CG1 | 10.93 | 131.76 | 111.00 |
| 1 | A | 817 | PHE | CD1-CG-CD2 | -10.92 | 104.10 | 118.30 |
| 1 | C | 901 | GLN | CG-CD-OE1 | 10.91 | 143.41 | 121.60 |
| 1 | C | 1013 | ILE | CA-CB-CG1 | 10.90 | 131.72 | 111.00 |
| 1 | A | 901 | GLN | CG-CD-OE1 | 10.90 | 143.40 | 121.60 |
| 1 | B | 1013 | ILE | CA-CB-CG1 | 10.90 | 131.70 | 111.00 |
| 1 | A | 170 | TYR | CD1-CE1-CZ | -10.89 | 110.00 | 119.80 |
| 1 | B | 901 | GLN | CG-CD-OE1 | 10.88 | 143.37 | 121.60 |
| 1 | C | 911 | VAL | CA-CB-CG2 | -10.87 | 94.59 | 110.90 |
| 1 | B | 911 | VAL | CA-CB-CG2 | -10.86 | 94.61 | 110.90 |
| 1 | A | 911 | VAL | CA-CB-CG2 | -10.84 | 94.64 | 110.90 |
| 1 | A | 666 | ILE | CB-CG1-CD1 | 10.83 | 144.23 | 113.90 |
| 1 | C | 170 | TYR | CD1-CE1-CZ | -10.83 | 110.05 | 119.80 |
| 1 | B | 170 | TYR | CD1-CE1-CZ | -10.81 | 110.07 | 119.80 |
| 1 | B | 666 | ILE | CB-CG1-CD1 | 10.81 | 144.16 | 113.90 |
| 1 | C | 666 | ILE | CB-CG1-CD1 | 10.80 | 144.15 | 113.90 |
| 1 | C | 1012 | LEU | CD1-CG-CD2 | -10.80 | 78.10 | 110.50 |
| 1 | B | 1012 | LEU | CD1-CG-CD2 | -10.79 | 78.12 | 110.50 |
| 1 | A | 1012 | LEU | CD1-CG-CD2 | -10.79 | 78.14 | 110.50 |
| 1 | C | 241 | LEU | CA-CB-CG | 10.71 | 139.92 | 115.30 |
| 1 | A | 241 | LEU | CA-CB-CG | 10.69 | 139.88 | 115.30 |
| 1 | B | 241 | LEU | CA-CB-CG | 10.68 | 139.85 | 115.30 |
| 1 | C | 1029 | MET | CA-CB-CG | 10.62 | 131.35 | 113.30 |
| 1 | A | 1029 | MET | CA-CB-CG | 10.61 | 131.33 | 113.30 |
| 1 | B | 1029 | MET | CA-CB-CG | 10.61 | 131.33 | 113.30 |
| 1 | A | 301 | CYS | CA-CB-SG | 10.60 | 133.08 | 114.00 |
| 1 | C | 301 | CYS | CA-CB-SG | 10.60 | 133.07 | 114.00 |
| 1 | B | 301 | CYS | CA-CB-SG | 10.58 | 133.05 | 114.00 |
| 1 | C | 977 | LEU | CA-CB-CG | 10.51 | 139.48 | 115.30 |
| 1 | A | 977 | LEU | CA-CB-CG | 10.50 | 139.46 | 115.30 |
| 1 | B | 977 | LEU | CA-CB-CG | 10.49 | 139.42 | 115.30 |
| 1 | C | 821 | LEU | CA-CB-CG | 10.27 | 138.92 | 115.30 |
| 1 | B | 821 | LEU | CA-CB-CG | 10.26 | 138.89 | 115.30 |
| 1 | A | 821 | LEU | CA-CB-CG | 10.24 | 138.86 | 115.30 |
| 1 | A | 729 | VAL | CG1-CB-CG2 | -10.19 | 94.60 | 110.90 |
| 1 | B | 729 | VAL | CG1-CB-CG2 | -10.18 | 94.62 | 110.90 |
| 1 | C | 729 | VAL | CG1-CB-CG2 | -10.17 | 94.63 | 110.90 |
| 1 | B | 756 | TYR | CB-CG-CD2 | -10.16 | 114.91 | 121.00 |
| 1 | A | 756 | TYR | CB-CG-CD2 | -10.14 | 114.92 | 121.00 |
| 1 | C | 756 | TYR | CB-CG-CD2 | -10.13 | 114.92 | 121.00 |
| 1 | B | 1089 | PHE | N-CA-CB | -10.12 | 92.39 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | A | 1089 | PHE | N-CA-CB | -10.11 | 92.40 | 110.60 |
| 1 | C | 1089 | PHE | N-CA-CB | -10.10 | 92.43 | 110.60 |
| 1 | B | 206 | LYS | CD-CE-NZ | 10.06 | 134.84 | 111.70 |
| 1 | C | 206 | LYS | CD-CE-NZ | 10.06 | 134.84 | 111.70 |
| 1 | A | 206 | LYS | CD-CE-NZ | 10.05 | 134.81 | 111.70 |
| 1 | B | 900 | MET | CG-SD-CE | 9.98 | 116.17 | 100.20 |
| 1 | A | 900 | MET | CG-SD-CE | 9.97 | 116.15 | 100.20 |
| 1 | C | 900 | MET | CG-SD-CE | 9.95 | 116.13 | 100.20 |
| 1 | C | 699 | LEU | CB-CG-CD1 | 9.93 | 127.88 | 111.00 |
| 1 | A | 859 | THR | OG1-CB-CG2 | -9.91 | 87.20 | 110.00 |
| 1 | B | 699 | LEU | CB-CG-CD1 | 9.91 | 127.85 | 111.00 |
| 1 | C | 859 | THR | OG1-CB-CG2 | -9.91 | 87.20 | 110.00 |
| 1 | A | 118 | LEU | CA-CB-CG | 9.91 | 138.09 | 115.30 |
| 1 | B | 859 | THR | OG1-CB-CG2 | -9.91 | 87.21 | 110.00 |
| 1 | C | 118 | LEU | CA-CB-CG | 9.90 | 138.08 | 115.30 |
| 1 | A | 699 | LEU | CB-CG-CD1 | 9.90 | 127.83 | 111.00 |
| 1 | B | 118 | LEU | CA-CB-CG | 9.90 | 138.06 | 115.30 |
| 1 | A | 160 | TYR | CD1-CG-CD2 | -9.80 | 107.12 | 117.90 |
| 1 | C | 160 | TYR | CD1-CG-CD2 | -9.80 | 107.12 | 117.90 |
| 1 | B | 160 | TYR | CD1-CG-CD2 | -9.73 | 107.20 | 117.90 |
| 1 | B | 1116 | THR | CA-CB-CG2 | -9.73 | 98.78 | 112.40 |
| 1 | C | 1116 | THR | CA-CB-CG2 | -9.71 | 98.81 | 112.40 |
| 1 | C | 160 | TYR | CB-CG-CD1 | 9.69 | 126.81 | 121.00 |
| 1 | A | 1116 | THR | CA-CB-CG2 | -9.68 | 98.85 | 112.40 |
| 1 | A | 160 | TYR | CB-CG-CD1 | 9.60 | 126.76 | 121.00 |
| 1 | A | 877 | LEU | CB-CG-CD2 | -9.60 | 94.69 | 111.00 |
| 1 | C | 877 | LEU | CB-CG-CD2 | -9.59 | 94.70 | 111.00 |
| 1 | B | 160 | TYR | CB-CG-CD1 | 9.58 | 126.75 | 121.00 |
| 1 | C | 1065 | VAL | CA-CB-CG1 | 9.57 | 125.25 | 110.90 |
| 1 | B | 877 | LEU | CB-CG-CD2 | -9.56 | 94.74 | 111.00 |
| 1 | B | 1065 | VAL | CA-CB-CG1 | 9.54 | 125.22 | 110.90 |
| 1 | A | 997 | ILE | CG1-CB-CG2 | -9.52 | 90.45 | 111.40 |
| 1 | A | 1065 | VAL | CA-CB-CG1 | 9.52 | 125.19 | 110.90 |
| 1 | C | 997 | ILE | CG1-CB-CG2 | -9.52 | 90.45 | 111.40 |
| 1 | A | 963 | VAL | CG1-CB-CG2 | -9.52 | 95.67 | 110.90 |
| 1 | C | 963 | VAL | CG1-CB-CG2 | -9.51 | 95.68 | 110.90 |
| 1 | B | 997 | ILE | CG1-CB-CG2 | -9.50 | 90.49 | 111.40 |
| 1 | B | 963 | VAL | CG1-CB-CG2 | -9.50 | 95.70 | 110.90 |
| 1 | B | 756 | TYR | CB-CG-CD1 | 9.40 | 126.64 | 121.00 |
| 1 | A | 756 | TYR | CB-CG-CD1 | 9.36 | 126.62 | 121.00 |
| 1 | C | 756 | TYR | CB-CG-CD1 | 9.32 | 126.59 | 121.00 |
| 1 | C | 230 | PRO | N-CD-CG | -9.31 | 89.23 | 103.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | B | 230 | PRO | N-CD-CG | -9.29 | 89.26 | 103.20 |
| 1 | A | 814 | LYS | CB-CG-CD | 9.26 | 135.67 | 111.60 |
| 1 | B | 814 | LYS | CB-CG-CD | 9.26 | 135.67 | 111.60 |
| 1 | C | 814 | LYS | CB-CG-CD | 9.26 | 135.67 | 111.60 |
| 1 | A | 230 | PRO | N-CD-CG | -9.25 | 89.32 | 103.20 |
| 1 | A | 977 | LEU | CB-CG-CD1 | -9.08 | 95.57 | 111.00 |
| 1 | C | 977 | LEU | CB-CG-CD1 | -9.06 | 95.60 | 111.00 |
| 1 | B | 977 | LEU | CB-CG-CD1 | -9.04 | 95.63 | 111.00 |
| 1 | A | 670 | ILE | CB-CG1-CD1 | 8.90 | 138.81 | 113.90 |
| 1 | B | 670 | ILE | CB-CG1-CD1 | 8.90 | 138.81 | 113.90 |
| 1 | C | 670 | ILE | CB-CG1-CD1 | 8.90 | 138.81 | 113.90 |
| 1 | A | 905 | ARG | NE-CZ-NH1 | 8.88 | 124.74 | 120.30 |
| 1 | B | 1029 | MET | CB-CG-SD | 8.88 | 139.03 | 112.40 |
| 1 | A | 1029 | MET | CB-CG-SD | 8.86 | 138.97 | 112.40 |
| 1 | C | 1029 | MET | CB-CG-SD | 8.86 | 138.97 | 112.40 |
| 1 | C | 905 | ARG | NE-CZ-NH1 | 8.82 | 124.71 | 120.30 |
| 1 | B | 595 | VAL | CA-CB-CG2 | -8.75 | 97.77 | 110.90 |
| 1 | B | 905 | ARG | NE-CZ-NH1 | 8.74 | 124.67 | 120.30 |
| 1 | C | 595 | VAL | CA-CB-CG2 | -8.74 | 97.79 | 110.90 |
| 1 | A | 595 | VAL | CA-CB-CG2 | -8.73 | 97.80 | 110.90 |
| 1 | C | 762 | GLN | CA-CB-CG | 8.68 | 132.49 | 113.40 |
| 1 | A | 762 | GLN | CA-CB-CG | 8.65 | 132.44 | 113.40 |
| 1 | C | 207 | HIS | N-CA-CB | -8.64 | 95.05 | 110.60 |
| 1 | B | 762 | GLN | CA-CB-CG | 8.64 | 132.40 | 113.40 |
| 1 | A | 207 | HIS | N-CA-CB | -8.64 | 95.06 | 110.60 |
| 1 | B | 207 | HIS | N-CA-CB | -8.64 | 95.06 | 110.60 |
| 1 | C | 170 | TYR | CB-CG-CD2 | -8.60 | 115.84 | 121.00 |
| 1 | A | 170 | TYR | CB-CG-CD2 | -8.52 | 115.89 | 121.00 |
| 1 | B | 66 | HIS | N-CA-CB | 8.52 | 125.93 | 110.60 |
| 1 | B | 170 | TYR | CB-CG-CD2 | -8.51 | 115.90 | 121.00 |
| 1 | C | 66 | HIS | N-CA-CB | 8.50 | 125.90 | 110.60 |
| 1 | A | 66 | HIS | N-CA-CB | 8.49 | 125.89 | 110.60 |
| 1 | A | 670 | ILE | CA-CB-CG1 | 8.39 | 126.94 | 111.00 |
| 1 | C | 670 | ILE | CA-CB-CG1 | 8.38 | 126.93 | 111.00 |
| 1 | B | 901 | GLN | CG-CD-NE2 | -8.35 | 96.65 | 116.70 |
| 1 | B | 670 | ILE | CA-CB-CG1 | 8.35 | 126.87 | 111.00 |
| 1 | C | 901 | GLN | CG-CD-NE2 | -8.34 | 96.67 | 116.70 |
| 1 | A | 901 | GLN | CG-CD-NE2 | -8.34 | 96.69 | 116.70 |
| 1 | B | 207 | HIS | CB-CA-C | 8.28 | 126.97 | 110.40 |
| 1 | A | 241 | LEU | CB-CG-CD1 | 8.28 | 125.07 | 111.00 |
| 1 | A | 877 | LEU | CA-CB-CG | 8.28 | 134.33 | 115.30 |
| 1 | C | 207 | HIS | CB-CA-C | 8.28 | 126.95 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | C | 877 | LEU | CA-CB-CG | 8.27 | 134.33 | 115.30 |
| 1 | B | 877 | LEU | CA-CB-CG | 8.27 | 134.32 | 115.30 |
| 1 | A | 207 | HIS | CB-CA-C | 8.27 | 126.93 | 110.40 |
| 1 | C | 241 | LEU | CB-CG-CD1 | 8.25 | 125.03 | 111.00 |
| 1 | B | 241 | LEU | CB-CG-CD1 | 8.24 | 125.01 | 111.00 |
| 1 | A | 942 | PRO | CA-N-CD | -8.23 | 99.97 | 111.50 |
| 1 | C | 942 | PRO | CA-N-CD | -8.23 | 99.98 | 111.50 |
| 1 | B | 942 | PRO | CA-N-CD | -8.19 | 100.03 | 111.50 |
| 1 | C | 811 | LYS | CB-CG-CD | 8.12 | 132.71 | 111.60 |
| 1 | A | 811 | LYS | CB-CG-CD | 8.11 | 132.69 | 111.60 |
| 1 | B | 811 | LYS | CB-CG-CD | 8.11 | 132.68 | 111.60 |
| 1 | A | 959 | LEU | CD1-CG-CD2 | -8.09 | 86.22 | 110.50 |
| 1 | B | 959 | LEU | CD1-CG-CD2 | -8.08 | 86.26 | 110.50 |
| 1 | C | 959 | LEU | CD1-CG-CD2 | -8.07 | 86.28 | 110.50 |
| 1 | A | 869 | MET | CA-CB-CG | 8.06 | 127.00 | 113.30 |
| 1 | C | 962 | LEU | CA-CB-CG | 8.06 | 133.83 | 115.30 |
| 1 | A | 962 | LEU | CA-CB-CG | 8.05 | 133.82 | 115.30 |
| 1 | B | 962 | LEU | CA-CB-CG | 8.04 | 133.79 | 115.30 |
| 1 | B | 869 | MET | CA-CB-CG | 8.03 | 126.96 | 113.30 |
| 1 | C | 869 | MET | CA-CB-CG | 8.03 | 126.95 | 113.30 |
| 1 | B | 767 | LEU | CB-CG-CD2 | -8.02 | 97.38 | 111.00 |
| 1 | A | 1088 | HIS | C-N-CA | 8.01 | 141.74 | 121.70 |
| 1 | A | 767 | LEU | CB-CG-CD2 | -8.01 | 97.38 | 111.00 |
| 1 | B | 1088 | HIS | C-N-CA | 8.01 | 141.72 | 121.70 |
| 1 | C | 767 | LEU | CB-CG-CD2 | -8.01 | 97.39 | 111.00 |
| 1 | C | 1088 | HIS | C-N-CA | 8.00 | 141.69 | 121.70 |
| 1 | B | 729 | VAL | CA-CB-CG1 | 7.98 | 122.87 | 110.90 |
| 1 | A | 729 | VAL | CA-CB-CG1 | 7.96 | 122.84 | 110.90 |
| 1 | C | 729 | VAL | CA-CB-CG1 | 7.96 | 122.84 | 110.90 |
| 1 | C | 1038 | LYS | CB-CG-CD | 7.95 | 132.27 | 111.60 |
| 1 | B | 1038 | LYS | CB-CG-CD | 7.94 | 132.25 | 111.60 |
| 1 | A | 1038 | LYS | CB-CG-CD | 7.92 | 132.21 | 111.60 |
| 1 | B | 1008 | VAL | CG1-CB-CG2 | 7.91 | 123.56 | 110.90 |
| 1 | C | 1040 | VAL | CG1-CB-CG2 | 7.91 | 123.56 | 110.90 |
| 1 | C | 1008 | VAL | CG1-CB-CG2 | 7.91 | 123.55 | 110.90 |
| 1 | A | 1040 | VAL | CG1-CB-CG2 | 7.89 | 123.53 | 110.90 |
| 1 | B | 1040 | VAL | CG1-CB-CG2 | 7.89 | 123.53 | 110.90 |
| 1 | A | 1008 | VAL | CG1-CB-CG2 | 7.89 | 123.52 | 110.90 |
| 1 | C | 752 | LEU | CB-CG-CD1 | 7.88 | 124.40 | 111.00 |
| 1 | A | 595 | VAL | CA-CB-CG1 | 7.88 | 122.71 | 110.90 |
| 1 | A | 752 | LEU | CB-CG-CD1 | 7.88 | 124.39 | 111.00 |
| 1 | B | 595 | VAL | CA-CB-CG1 | 7.87 | 122.71 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 752 | LEU | CB-CG-CD1 | 7.86 | 124.36 | 111.00 |
| 1 | C | 595 | VAL | CA-CB-CG1 | 7.85 | 122.68 | 110.90 |
| 1 | A | 699 | LEU | N-CA-CB | -7.84 | 94.72 | 110.40 |
| 1 | A | 269 | TYR | CB-CG-CD2 | -7.84 | 116.30 | 121.00 |
| 1 | B | 269 | TYR | CB-CG-CD2 | -7.83 | 116.30 | 121.00 |
| 1 | B | 699 | LEU | N-CA-CB | -7.83 | 94.75 | 110.40 |
| 1 | B | 792 | PRO | CA-N-CD | -7.83 | 100.54 | 111.50 |
| 1 | C | 699 | LEU | N-CA-CB | -7.82 | 94.77 | 110.40 |
| 1 | A | 792 | PRO | CA-N-CD | -7.79 | 100.59 | 111.50 |
| 1 | C | 792 | PRO | CA-N-CD | -7.79 | 100.60 | 111.50 |
| 1 | B | 781 | VAL | CG1-CB-CG2 | 7.79 | 123.36 | 110.90 |
| 1 | C | 269 | TYR | CB-CG-CD2 | -7.76 | 116.34 | 121.00 |
| 1 | C | 802 | PHE | CG-CD1-CE1 | 7.75 | 129.32 | 120.80 |
| 1 | B | 141 | LEU | CB-CA-C | -7.74 | 95.50 | 110.20 |
| 1 | A | 781 | VAL | CG1-CB-CG2 | 7.74 | 123.28 | 110.90 |
| 1 | C | 781 | VAL | CG1-CB-CG2 | 7.74 | 123.28 | 110.90 |
| 1 | A | 802 | PHE | CG-CD1-CE1 | 7.72 | 129.29 | 120.80 |
| 1 | A | 909 | ILE | CB-CA-C | -7.72 | 96.16 | 111.60 |
| 1 | B | 909 | ILE | CB-CA-C | -7.72 | 96.16 | 111.60 |
| 1 | C | 141 | LEU | CB-CG-CD2 | 7.72 | 124.12 | 111.00 |
| 1 | A | 141 | LEU | CB-CA-C | -7.72 | 95.54 | 110.20 |
| 1 | B | 802 | PHE | CG-CD1-CE1 | 7.71 | 129.28 | 120.80 |
| 1 | C | 909 | ILE | CB-CA-C | -7.71 | 96.17 | 111.60 |
| 1 | C | 141 | LEU | CB-CA-C | -7.71 | 95.56 | 110.20 |
| 1 | A | 141 | LEU | CB-CG-CD2 | 7.70 | 124.09 | 111.00 |
| 1 | B | 141 | LEU | CB-CG-CD2 | 7.70 | 124.09 | 111.00 |
| 1 | C | 216 | LEU | CB-CG-CD1 | 7.68 | 124.05 | 111.00 |
| 1 | B | 216 | LEU | CB-CG-CD1 | 7.67 | 124.05 | 111.00 |
| 1 | A | 216 | LEU | CB-CG-CD1 | 7.65 | 124.01 | 111.00 |
| 1 | B | 242 | LEU | CA-CB-CG | 7.60 | 132.78 | 115.30 |
| 1 | C | 242 | LEU | CA-CB-CG | 7.60 | 132.78 | 115.30 |
| 1 | A | 242 | LEU | CA-CB-CG | 7.59 | 132.76 | 115.30 |
| 1 | B | 230 | PRO | CA-CB-CG | -7.51 | 89.73 | 104.00 |
| 1 | C | 230 | PRO | CA-CB-CG | -7.50 | 89.74 | 104.00 |
| 1 | A | 997 | ILE | CB-CG1-CD1 | 7.48 | 134.85 | 113.90 |
| 1 | C | 997 | ILE | CB-CG1-CD1 | 7.48 | 134.85 | 113.90 |
| 1 | B | 699 | LEU | CA-CB-CG | 7.47 | 132.49 | 115.30 |
| 1 | A | 699 | LEU | CA-CB-CG | 7.47 | 132.48 | 115.30 |
| 1 | A | 230 | PRO | CA-CB-CG | -7.47 | 89.81 | 104.00 |
| 1 | B | 192 | PHE | CG-CD2-CE2 | 7.47 | 129.01 | 120.80 |
| 1 | B | 997 | ILE | CB-CG1-CD1 | 7.46 | 134.80 | 113.90 |
| 1 | C | 699 | LEU | CA-CB-CG | 7.46 | 132.47 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | C | 192 | PHE | CG-CD2-CE2 | 7.46 | 129.01 | 120.80 |
| 1 | A | 192 | PHE | CG-CD2-CE2 | 7.46 | 129.00 | 120.80 |
| 1 | C | 18 | LEU | CB-CG-CD1 | 7.44 | 123.65 | 111.00 |
| 1 | B | 18 | LEU | CB-CG-CD1 | 7.43 | 123.64 | 111.00 |
| 1 | A | 18 | LEU | CB-CG-CD1 | 7.42 | 123.62 | 111.00 |
| 1 | A | 1065 | VAL | CA-CB-CG2 | -7.40 | 99.80 | 110.90 |
| 1 | B | 1065 | VAL | CA-CB-CG2 | -7.37 | 99.85 | 110.90 |
| 1 | C | 754 | LEU | CA-CB-CG | 7.37 | 132.24 | 115.30 |
| 1 | B | 269 | TYR | CD1-CG-CD2 | -7.36 | 109.81 | 117.90 |
| 1 | C | 1065 | VAL | CA-CB-CG2 | -7.36 | 99.86 | 110.90 |
| 1 | B | 754 | LEU | CA-CB-CG | 7.35 | 132.21 | 115.30 |
| 1 | A | 754 | LEU | CA-CB-CG | 7.35 | 132.20 | 115.30 |
| 1 | C | 269 | TYR | CD1-CG-CD2 | -7.34 | 109.83 | 117.90 |
| 1 | C | 65 | PHE | C-N-CA | -7.32 | 103.40 | 121.70 |
| 1 | A | 65 | PHE | C-N-CA | -7.31 | 103.42 | 121.70 |
| 1 | B | 65 | PHE | C-N-CA | -7.31 | 103.43 | 121.70 |
| 1 | A | 269 | TYR | CD1-CG-CD2 | -7.30 | 109.87 | 117.90 |
| 1 | C | 767 | LEU | CD1-CG-CD2 | -7.27 | 88.68 | 110.50 |
| 1 | B | 767 | LEU | CD1-CG-CD2 | -7.27 | 88.70 | 110.50 |
| 1 | A | 767 | LEU | CD1-CG-CD2 | -7.26 | 88.71 | 110.50 |
| 1 | B | 791 | THR | OG1-CB-CG2 | -7.21 | 93.42 | 110.00 |
| 1 | C | 726 | ILE | CA-CB-CG1 | 7.20 | 124.69 | 111.00 |
| 1 | A | 726 | ILE | CA-CB-CG1 | 7.20 | 124.67 | 111.00 |
| 1 | B | 726 | ILE | CA-CB-CG1 | 7.20 | 124.67 | 111.00 |
| 1 | A | 791 | THR | OG1-CB-CG2 | -7.19 | 93.47 | 110.00 |
| 1 | C | 791 | THR | OG1-CB-CG2 | -7.18 | 93.50 | 110.00 |
| 1 | C | 666 | ILE | CA-CB-CG1 | 7.16 | 124.60 | 111.00 |
| 1 | C | 1141 | LEU | CB-CA-C | -7.16 | 96.60 | 110.20 |
| 1 | A | 666 | ILE | CA-CB-CG1 | 7.16 | 124.59 | 111.00 |
| 1 | A | 1141 | LEU | CB-CA-C | -7.15 | 96.61 | 110.20 |
| 1 | B | 1141 | LEU | CB-CA-C | -7.14 | 96.63 | 110.20 |
| 1 | C | 814 | LYS | CA-CB-CG | 7.13 | 129.09 | 113.40 |
| 1 | A | 814 | LYS | CA-CB-CG | 7.13 | 129.09 | 113.40 |
| 1 | B | 666 | ILE | CA-CB-CG1 | 7.13 | 124.55 | 111.00 |
| 1 | B | 814 | LYS | CA-CB-CG | 7.12 | 129.06 | 113.40 |
| 1 | C | 878 | LEU | CB-CG-CD2 | 7.03 | 122.94 | 111.00 |
| 1 | B | 878 | LEU | CB-CG-CD2 | 7.02 | 122.94 | 111.00 |
| 1 | B | 765 | ARG | NE-CZ-NH1 | -7.01 | 116.80 | 120.30 |
| 1 | A | 878 | LEU | CB-CG-CD2 | 7.01 | 122.91 | 111.00 |
| 1 | A | 308 | VAL | CA-CB-CG2 | -7.00 | 100.40 | 110.90 |
| 1 | C | 308 | VAL | CA-CB-CG2 | -7.00 | 100.41 | 110.90 |
| 1 | A | 765 | ARG | NE-CZ-NH1 | -6.98 | 116.81 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1005 | GLN | CB-CG-CD | 6.98 | 129.74 | 111.60 |
| 1 | B | 308 | VAL | CA-CB-CG2 | -6.97 | 100.44 | 110.90 |
| 1 | C | 1005 | GLN | CB-CG-CD | 6.97 | 129.74 | 111.60 |
| 1 | C | 741 | TYR | CB-CA-C | -6.97 | 96.46 | 110.40 |
| 1 | B | 1005 | GLN | CB-CG-CD | 6.96 | 129.71 | 111.60 |
| 1 | C | 765 | ARG | NE-CZ-NH1 | -6.96 | 116.82 | 120.30 |
| 1 | A | 741 | TYR | CB-CA-C | -6.96 | 96.48 | 110.40 |
| 1 | B | 741 | TYR | CB-CA-C | -6.95 | 96.49 | 110.40 |
| 1 | C | 1014 | ARG | CG-CD-NE | -6.94 | 97.23 | 111.80 |
| 1 | C | 772 | VAL | CA-CB-CG2 | 6.93 | 121.30 | 110.90 |
| 1 | A | 1014 | ARG | CG-CD-NE | -6.93 | 97.25 | 111.80 |
| 1 | A | 772 | VAL | CA-CB-CG2 | 6.92 | 121.28 | 110.90 |
| 1 | B | 772 | VAL | CA-CB-CG2 | 6.92 | 121.28 | 110.90 |
| 1 | B | 770 | ILE | CA-CB-CG1 | 6.91 | 124.13 | 111.00 |
| 1 | B | 1014 | ARG | CG-CD-NE | -6.91 | 97.29 | 111.80 |
| 1 | C | 770 | ILE | CA-CB-CG1 | 6.91 | 124.13 | 111.00 |
| 1 | C | 1089 | PHE | CB-CG-CD2 | -6.89 | 115.97 | 120.80 |
| 1 | B | 1089 | PHE | CB-CG-CD2 | -6.88 | 115.98 | 120.80 |
| 1 | A | 770 | ILE | CA-CB-CG1 | 6.88 | 124.07 | 111.00 |
| 1 | C | 229 | LEU | C-N-CD | -6.87 | 105.48 | 120.60 |
| 1 | B | 229 | LEU | C-N-CD | -6.87 | 105.48 | 120.60 |
| 1 | C | 860 | VAL | CG1-CB-CG2 | -6.87 | 99.91 | 110.90 |
| 1 | A | 229 | LEU | C-N-CD | -6.86 | 105.50 | 120.60 |
| 1 | A | 860 | VAL | CG1-CB-CG2 | -6.85 | 99.94 | 110.90 |
| 1 | B | 860 | VAL | CG1-CB-CG2 | -6.85 | 99.94 | 110.90 |
| 1 | A | 1089 | PHE | CB-CG-CD2 | -6.83 | 116.02 | 120.80 |
| 1 | C | 43 | PHE | CB-CA-C | -6.83 | 96.73 | 110.40 |
| 1 | A | 43 | PHE | CB-CA-C | -6.83 | 96.73 | 110.40 |
| 1 | B | 43 | PHE | CB-CA-C | -6.82 | 96.76 | 110.40 |
| 1 | A | 752 | LEU | CB-CG-CD2 | -6.81 | 99.42 | 111.00 |
| 1 | C | 752 | LEU | CB-CG-CD2 | -6.79 | 99.46 | 111.00 |
| 1 | B | 752 | LEU | CB-CG-CD2 | -6.78 | 99.48 | 111.00 |
| 1 | C | 729 | VAL | CA-CB-CG2 | -6.74 | 100.80 | 110.90 |
| 1 | A | 729 | VAL | CA-CB-CG2 | -6.74 | 100.80 | 110.90 |
| 1 | B | 729 | VAL | CA-CB-CG2 | -6.73 | 100.81 | 110.90 |
| 1 | C | 66 | HIS | CB-CA-C | -6.72 | 96.96 | 110.40 |
| 1 | C | 66 | HIS | N-CA-C | -6.71 | 92.89 | 111.00 |
| 1 | B | 66 | HIS | CB-CA-C | -6.70 | 97.00 | 110.40 |
| 1 | A | 66 | HIS | N-CA-C | -6.70 | 92.92 | 111.00 |
| 1 | B | 66 | HIS | N-CA-C | -6.70 | 92.91 | 111.00 |
| 1 | A | 66 | HIS | CB-CA-C | -6.69 | 97.02 | 110.40 |
| 1 | B | 869 | MET | N-CA-CB | 6.69 | 122.64 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 869 | MET | N-CA-CB | 6.69 | 122.64 | 110.60 |
| 1 | C | 869 | MET | N-CA-CB | 6.68 | 122.63 | 110.60 |
| 1 | C | 1038 | LYS | CG-CD-CE | 6.65 | 131.85 | 111.90 |
| 1 | B | 1038 | LYS | CG-CD-CE | 6.65 | 131.84 | 111.90 |
| 1 | A | 767 | LEU | CA-CB-CG | 6.64 | 130.58 | 115.30 |
| 1 | A | 1038 | LYS | CG-CD-CE | 6.64 | 131.82 | 111.90 |
| 1 | C | 767 | LEU | CA-CB-CG | 6.64 | 130.57 | 115.30 |
| 1 | B | 767 | LEU | CA-CB-CG | 6.62 | 130.53 | 115.30 |
| 1 | C | 1018 | ILE | CG1-CB-CG2 | -6.59 | 96.89 | 111.40 |
| 1 | A | 1018 | ILE | CG1-CB-CG2 | -6.59 | 96.90 | 111.40 |
| 1 | B | 269 | TYR | N-CA-CB | -6.59 | 98.74 | 110.60 |
| 1 | C | 269 | TYR | N-CA-CB | -6.59 | 98.74 | 110.60 |
| 1 | B | 1018 | ILE | CG1-CB-CG2 | -6.57 | 96.94 | 111.40 |
| 1 | A | 269 | TYR | N-CA-CB | -6.56 | 98.80 | 110.60 |
| 1 | C | 18 | LEU | CA-CB-CG | 6.53 | 130.32 | 115.30 |
| 1 | B | 18 | LEU | CA-CB-CG | 6.53 | 130.32 | 115.30 |
| 1 | A | 18 | LEU | CA-CB-CG | 6.52 | 130.30 | 115.30 |
| 1 | A | 1009 | THR | CA-CB-OG1 | 6.50 | 122.64 | 109.00 |
| 1 | C | 1009 | THR | CA-CB-OG1 | 6.50 | 122.64 | 109.00 |
| 1 | B | 1009 | THR | CA-CB-OG1 | 6.48 | 122.61 | 109.00 |
| 1 | A | 954 | GLN | CA-CB-CG | 6.48 | 127.65 | 113.40 |
| 1 | C | 954 | GLN | CA-CB-CG | 6.46 | 127.61 | 113.40 |
| 1 | B | 905 | ARG | CB-CG-CD | -6.45 | 94.82 | 111.60 |
| 1 | A | 905 | ARG | CB-CG-CD | -6.45 | 94.83 | 111.60 |
| 1 | C | 905 | ARG | CB-CG-CD | -6.45 | 94.83 | 111.60 |
| 1 | B | 954 | GLN | CA-CB-CG | 6.44 | 127.58 | 113.40 |
| 1 | A | 817 | PHE | CB-CG-CD2 | -6.39 | 116.33 | 120.80 |
| 1 | C | 141 | LEU | N-CA-C | -6.37 | 93.79 | 111.00 |
| 1 | B | 1106 | GLN | CB-CA-C | -6.37 | 97.66 | 110.40 |
| 1 | B | 141 | LEU | N-CA-C | -6.37 | 93.80 | 111.00 |
| 1 | A | 141 | LEU | N-CA-C | -6.37 | 93.80 | 111.00 |
| 1 | B | 1079 | PRO | N-CD-CG | -6.37 | 93.65 | 103.20 |
| 1 | A | 1079 | PRO | N-CD-CG | -6.36 | 93.66 | 103.20 |
| 1 | A | 1106 | GLN | CB-CA-C | -6.36 | 97.68 | 110.40 |
| 1 | C | 1106 | GLN | CB-CA-C | -6.36 | 97.69 | 110.40 |
| 1 | B | 762 | GLN | OE1-CD-NE2 | -6.35 | 107.28 | 121.90 |
| 1 | C | 811 | LYS | CG-CD-CE | 6.35 | 130.96 | 111.90 |
| 1 | A | 811 | LYS | CG-CD-CE | 6.35 | 130.94 | 111.90 |
| 1 | B | 811 | LYS | CG-CD-CE | 6.35 | 130.94 | 111.90 |
| 1 | C | 762 | GLN | OE1-CD-NE2 | -6.34 | 107.31 | 121.90 |
| 1 | C | 1079 | PRO | N-CD-CG | -6.33 | 93.70 | 103.20 |
| 1 | C | 817 | PHE | CB-CG-CD2 | -6.33 | 116.37 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 762 | GLN | OE1-CD-NE2 | -6.32 | 107.36 | 121.90 |
| 1 | B | 817 | PHE | CB-CG-CD2 | -6.31 | 116.38 | 120.80 |
| 1 | A | 1089 | PHE | CD1-CG-CD2 | -6.30 | 110.10 | 118.30 |
| 1 | B | 811 | LYS | CD-CE-NZ | -6.28 | 97.26 | 111.70 |
| 1 | C | 811 | LYS | CD-CE-NZ | -6.28 | 97.26 | 111.70 |
| 1 | C | 1089 | PHE | CD1-CG-CD2 | -6.28 | 110.14 | 118.30 |
| 1 | B | 57 | PRO | CA-N-CD | -6.27 | 102.72 | 111.50 |
| 1 | A | 57 | PRO | CA-N-CD | -6.27 | 102.72 | 111.50 |
| 1 | A | 811 | LYS | CD-CE-NZ | -6.27 | 97.28 | 111.70 |
| 1 | C | 57 | PRO | CA-N-CD | -6.26 | 102.74 | 111.50 |
| 1 | B | 1089 | PHE | CD1-CG-CD2 | -6.26 | 110.17 | 118.30 |
| 1 | C | 610 | VAL | CA-CB-CG2 | -6.24 | 101.54 | 110.90 |
| 1 | B | 610 | VAL | CA-CB-CG2 | -6.23 | 101.55 | 110.90 |
| 1 | A | 610 | VAL | CA-CB-CG2 | -6.23 | 101.56 | 110.90 |
| 1 | C | 1028 | LYS | CD-CE-NZ | 6.21 | 125.99 | 111.70 |
| 1 | B | 1028 | LYS | CD-CE-NZ | 6.21 | 125.97 | 111.70 |
| 1 | A | 1028 | LYS | CD-CE-NZ | 6.19 | 125.94 | 111.70 |
| 1 | B | 207 | HIS | CA-CB-CG | 6.18 | 124.11 | 113.60 |
| 1 | C | 781 | VAL | CA-CB-CG2 | 6.18 | 120.17 | 110.90 |
| 1 | A | 781 | VAL | CA-CB-CG2 | 6.17 | 120.16 | 110.90 |
| 1 | C | 991 | VAL | CA-CB-CG2 | -6.17 | 101.64 | 110.90 |
| 1 | A | 991 | VAL | CA-CB-CG2 | -6.17 | 101.65 | 110.90 |
| 1 | B | 991 | VAL | CA-CB-CG2 | -6.17 | 101.65 | 110.90 |
| 1 | A | 207 | HIS | CA-CB-CG | 6.17 | 124.08 | 113.60 |
| 1 | C | 207 | HIS | CA-CB-CG | 6.16 | 124.06 | 113.60 |
| 1 | B | 781 | VAL | CA-CB-CG2 | 6.13 | 120.09 | 110.90 |
| 1 | A | 477[A] | SER | C-N-CA | 6.00 | 136.71 | 121.70 |
| 1 | A | 477[B] | SER | C-N-CA | 6.00 | 136.71 | 121.70 |
| 1 | B | 191 | GLU | C-N-CA | -5.97 | 106.78 | 121.70 |
| 1 | C | 191 | GLU | C-N-CA | -5.96 | 106.79 | 121.70 |
| 1 | A | 997 | ILE | CB-CA-C | 5.96 | 123.52 | 111.60 |
| 1 | A | 191 | GLU | C-N-CA | -5.96 | 106.81 | 121.70 |
| 1 | B | 997 | ILE | CB-CA-C | 5.95 | 123.51 | 111.60 |
| 1 | C | 997 | ILE | CB-CA-C | 5.95 | 123.50 | 111.60 |
| 1 | C | 218 | GLN | CB-CG-CD | 5.94 | 127.05 | 111.60 |
| 1 | C | 216 | LEU | N-CA-C | -5.93 | 94.97 | 111.00 |
| 1 | A | 218 | GLN | CB-CG-CD | 5.92 | 127.00 | 111.60 |
| 1 | A | 216 | LEU | N-CA-C | -5.92 | 95.01 | 111.00 |
| 1 | B | 216 | LEU | N-CA-C | -5.91 | 95.03 | 111.00 |
| 1 | B | 218 | GLN | CB-CG-CD | 5.91 | 126.97 | 111.60 |
| 1 | B | 741 | TYR | CE1-CZ-CE2 | -5.90 | 110.36 | 119.80 |
| 1 | C | 741 | TYR | CE1-CZ-CE2 | -5.89 | 110.38 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 741 | TYR | CE1-CZ-CE2 | -5.89 | 110.38 | 119.80 |
| 1 | B | 817 | PHE | CB-CA-C | 5.85 | 122.10 | 110.40 |
| 1 | A | 308 | VAL | CA-CB-CG1 | 5.84 | 119.66 | 110.90 |
| 1 | B | 318 | PHE | CD1-CG-CD2 | -5.84 | 110.71 | 118.30 |
| 1 | A | 817 | PHE | CB-CA-C | 5.84 | 122.08 | 110.40 |
| 1 | C | 726 | ILE | CG1-CB-CG2 | -5.84 | 98.55 | 111.40 |
| 1 | B | 308 | VAL | CA-CB-CG1 | 5.84 | 119.66 | 110.90 |
| 1 | B | 726 | ILE | CG1-CB-CG2 | -5.84 | 98.56 | 111.40 |
| 1 | C | 308 | VAL | CA-CB-CG1 | 5.84 | 119.65 | 110.90 |
| 1 | A | 726 | ILE | CG1-CB-CG2 | -5.83 | 98.57 | 111.40 |
| 1 | A | 318 | PHE | CD1-CG-CD2 | -5.83 | 110.72 | 118.30 |
| 1 | C | 817 | PHE | CB-CA-C | 5.83 | 122.05 | 110.40 |
| 1 | B | 768 | THR | OG1-CB-CG2 | 5.82 | 123.38 | 110.00 |
| 1 | C | 318 | PHE | CD1-CG-CD2 | -5.82 | 110.74 | 118.30 |
| 1 | C | 768 | THR | OG1-CB-CG2 | 5.82 | 123.38 | 110.00 |
| 1 | A | 768 | THR | OG1-CB-CG2 | 5.82 | 123.38 | 110.00 |
| 1 | B | 770 | ILE | CA-CB-CG2 | -5.81 | 99.28 | 110.90 |
| 1 | A | 770 | ILE | CA-CB-CG2 | -5.80 | 99.30 | 110.90 |
| 1 | C | 770 | ILE | CA-CB-CG2 | -5.79 | 99.31 | 110.90 |
| 1 | C | 735 | SER | CA-CB-OG | 5.77 | 126.78 | 111.20 |
| 1 | A | 735 | SER | CA-CB-OG | 5.77 | 126.77 | 111.20 |
| 1 | B | 735 | SER | CA-CB-OG | 5.76 | 126.76 | 111.20 |
| 1 | B | 274 | THR | CA-CB-CG2 | 5.76 | 120.46 | 112.40 |
| 1 | C | 274 | THR | CA-CB-CG2 | 5.75 | 120.45 | 112.40 |
| 1 | A | 274 | THR | CA-CB-CG2 | 5.72 | 120.40 | 112.40 |
| 1 | A | 229 | LEU | CA-CB-CG | 5.67 | 128.33 | 115.30 |
| 1 | B | 229 | LEU | CA-CB-CG | 5.66 | 128.32 | 115.30 |
| 1 | B | 1091 | ARG | CB-CG-CD | 5.66 | 126.33 | 111.60 |
| 1 | A | 1091 | ARG | CB-CG-CD | 5.66 | 126.32 | 111.60 |
| 1 | C | 1091 | ARG | CB-CG-CD | 5.66 | 126.32 | 111.60 |
| 1 | C | 229 | LEU | CA-CB-CG | 5.65 | 128.29 | 115.30 |
| 1 | C | 655 | HIS | ND1-CG-CD2 | -5.61 | 98.14 | 106.00 |
| 1 | A | 655 | HIS | ND1-CG-CD2 | -5.61 | 98.14 | 106.00 |
| 1 | B | 655 | HIS | ND1-CG-CD2 | -5.61 | 98.15 | 106.00 |
| 1 | B | 869 | MET | CB-CG-SD | 5.60 | 129.21 | 112.40 |
| 1 | A | 869 | MET | CB-CG-SD | 5.60 | 129.19 | 112.40 |
| 1 | C | 883 | THR | OG1-CB-CG2 | 5.60 | 122.87 | 110.00 |
| 1 | C | 869 | MET | CB-CG-SD | 5.59 | 129.18 | 112.40 |
| 1 | A | 883 | THR | OG1-CB-CG2 | 5.59 | 122.86 | 110.00 |
| 1 | B | 883 | THR | OG1-CB-CG2 | 5.59 | 122.85 | 110.00 |
| 1 | C | 141 | LEU | CB-CG-CD1 | -5.57 | 101.54 | 111.00 |
| 1 | A | 141 | LEU | CB-CG-CD1 | -5.55 | 101.56 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | C | 140 | PHE | C-N-CA | -5.55 | 107.84 | 121.70 |
| 1 | A | 140 | PHE | C-N-CA | -5.54 | 107.86 | 121.70 |
| 1 | B | 141 | LEU | CB-CG-CD1 | -5.54 | 101.59 | 111.00 |
| 1 | B | 140 | PHE | C-N-CA | -5.53 | 107.88 | 121.70 |
| 1 | C | 859 | THR | N-CA-C | -5.52 | 96.09 | 111.00 |
| 1 | A | 859 | THR | N-CA-C | -5.52 | 96.10 | 111.00 |
| 1 | B | 859 | THR | N-CA-C | -5.52 | 96.10 | 111.00 |
| 1 | B | 980 | ILE | CG1-CB-CG2 | 5.51 | 123.53 | 111.40 |
| 1 | A | 980 | ILE | CG1-CB-CG2 | 5.49 | 123.48 | 111.40 |
| 1 | C | 478 | THR | CA-CB-CG2 | 5.49 | 120.08 | 112.40 |
| 1 | B | 821 | LEU | N-CA-CB | -5.48 | 99.44 | 110.40 |
| 1 | C | 821 | LEU | N-CA-CB | -5.48 | 99.44 | 110.40 |
| 1 | C | 980 | ILE | CG1-CB-CG2 | 5.48 | 123.45 | 111.40 |
| 1 | A | 821 | LEU | N-CA-CB | -5.46 | 99.48 | 110.40 |
| 1 | B | 818 | ILE | CG1-CB-CG2 | -5.46 | 99.39 | 111.40 |
| 1 | A | 818 | ILE | CG1-CB-CG2 | -5.45 | 99.41 | 111.40 |
| 1 | C | 818 | ILE | CG1-CB-CG2 | -5.45 | 99.41 | 111.40 |
| 1 | B | 794 | ILE | CG1-CB-CG2 | 5.43 | 123.36 | 111.40 |
| 1 | C | 756 | TYR | CZ-CE2-CD2 | -5.43 | 114.91 | 119.80 |
| 1 | C | 794 | ILE | CG1-CB-CG2 | 5.43 | 123.35 | 111.40 |
| 1 | B | 1039 | ARG | CG-CD-NE | 5.43 | 123.20 | 111.80 |
| 1 | C | 1039 | ARG | CG-CD-NE | 5.43 | 123.20 | 111.80 |
| 1 | C | 1008 | VAL | CA-CB-CG1 | 5.42 | 119.03 | 110.90 |
| 1 | A | 794 | ILE | CG1-CB-CG2 | 5.41 | 123.30 | 111.40 |
| 1 | A | 1039 | ARG | CG-CD-NE | 5.41 | 123.15 | 111.80 |
| 1 | C | 276 | LEU | CB-CG-CD2 | 5.41 | 120.19 | 111.00 |
| 1 | B | 1008 | VAL | CA-CB-CG1 | 5.40 | 119.00 | 110.90 |
| 1 | A | 1008 | VAL | CA-CB-CG1 | 5.40 | 118.99 | 110.90 |
| 1 | B | 756 | TYR | CZ-CE2-CD2 | -5.40 | 114.94 | 119.80 |
| 1 | A | 756 | TYR | CZ-CE2-CD2 | -5.39 | 114.95 | 119.80 |
| 1 | A | 276 | LEU | CB-CG-CD2 | 5.38 | 120.15 | 111.00 |
| 1 | A | 699 | LEU | CB-CG-CD2 | -5.38 | 101.85 | 111.00 |
| 1 | B | 1113 | GLN | CA-CB-CG | 5.38 | 125.23 | 113.40 |
| 1 | B | 276 | LEU | CB-CG-CD2 | 5.37 | 120.13 | 111.00 |
| 1 | B | 699 | LEU | CB-CG-CD2 | -5.37 | 101.87 | 111.00 |
| 1 | C | 1113 | GLN | CA-CB-CG | 5.37 | 125.21 | 113.40 |
| 1 | C | 699 | LEU | CB-CG-CD2 | -5.37 | 101.88 | 111.00 |
| 1 | A | 1113 | GLN | CA-CB-CG | 5.36 | 125.19 | 113.40 |
| 1 | B | 192 | PHE | CA-CB-CG | -5.36 | 101.05 | 113.90 |
| 1 | C | 192 | PHE | CA-CB-CG | -5.35 | 101.07 | 113.90 |
| 1 | A | 192 | PHE | CA-CB-CG | -5.34 | 101.07 | 113.90 |
| 1 | C | 269 | TYR | CB-CA-C | 5.34 | 121.08 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 269 | TYR | CB-CA-C | 5.33 | 121.05 | 110.40 |
| 1 | B | 286 | THR | CA-CB-CG2 | 5.32 | 119.85 | 112.40 |
| 1 | B | 269 | TYR | CB-CA-C | 5.31 | 121.03 | 110.40 |
| 1 | A | 286 | THR | CA-CB-CG2 | 5.30 | 119.82 | 112.40 |
| 1 | C | 286 | THR | CA-CB-CG2 | 5.30 | 119.81 | 112.40 |
| 1 | A | 1091 | ARG | CD-NE-CZ | 5.29 | 131.01 | 123.60 |
| 1 | B | 1091 | ARG | CD-NE-CZ | 5.28 | 130.99 | 123.60 |
| 1 | B | 1006 | THR | OG1-CB-CG2 | 5.27 | 122.13 | 110.00 |
| 1 | C | 1091 | ARG | CD-NE-CZ | 5.26 | 130.97 | 123.60 |
| 1 | C | 1006 | THR | OG1-CB-CG2 | 5.26 | 122.10 | 110.00 |
| 1 | A | 655 | HIS | CB-CG-CD2 | -5.26 | 114.50 | 130.80 |
| 1 | C | 655 | HIS | CB-CG-CD2 | -5.26 | 114.50 | 130.80 |
| 1 | A | 170 | TYR | CG-CD1-CE1 | 5.25 | 125.50 | 121.30 |
| 1 | A | 1006 | THR | OG1-CB-CG2 | 5.25 | 122.08 | 110.00 |
| 1 | B | 655 | HIS | CB-CG-CD2 | -5.25 | 114.54 | 130.80 |
| 1 | A | 699 | LEU | N-CA-C | 5.24 | 125.14 | 111.00 |
| 1 | A | 1058 | HIS | N-CA-CB | 5.24 | 120.03 | 110.60 |
| 1 | C | 170 | TYR | CG-CD1-CE1 | 5.23 | 125.48 | 121.30 |
| 1 | B | 170 | TYR | CG-CD1-CE1 | 5.23 | 125.48 | 121.30 |
| 1 | B | 1058 | HIS | N-CA-CB | 5.23 | 120.01 | 110.60 |
| 1 | B | 699 | LEU | N-CA-C | 5.23 | 125.11 | 111.00 |
| 1 | C | 1001 | LEU | CB-CG-CD2 | 5.23 | 119.89 | 111.00 |
| 1 | B | 1122 | VAL | CG1-CB-CG2 | 5.22 | 119.26 | 110.90 |
| 1 | A | 1018 | ILE | CB-CG1-CD1 | 5.22 | 128.52 | 113.90 |
| 1 | C | 699 | LEU | N-CA-C | 5.22 | 125.10 | 111.00 |
| 1 | C | 1018 | ILE | CB-CG1-CD1 | 5.22 | 128.52 | 113.90 |
| 1 | A | 1001 | LEU | CB-CG-CD2 | 5.22 | 119.87 | 111.00 |
| 1 | C | 1058 | HIS | N-CA-CB | 5.21 | 119.99 | 110.60 |
| 1 | B | 1018 | ILE | CB-CG1-CD1 | 5.21 | 128.50 | 113.90 |
| 1 | B | 1001 | LEU | CB-CG-CD2 | 5.20 | 119.83 | 111.00 |
| 1 | C | 1122 | VAL | CG1-CB-CG2 | 5.19 | 119.21 | 110.90 |
| 1 | A | 1122 | VAL | CG1-CB-CG2 | 5.18 | 119.19 | 110.90 |
| 1 | C | 741 | TYR | OH-CZ-CE2 | 5.17 | 134.06 | 120.10 |
| 1 | A | 977 | LEU | CB-CG-CD2 | 5.17 | 119.79 | 111.00 |
| 1 | B | 741 | TYR | OH-CZ-CE2 | 5.17 | 134.05 | 120.10 |
| 1 | A | 802 | PHE | N-CA-CB | 5.17 | 119.90 | 110.60 |
| 1 | A | 1006 | THR | CA-CB-OG1 | 5.16 | 119.84 | 109.00 |
| 1 | C | 1006 | THR | CA-CB-OG1 | 5.16 | 119.84 | 109.00 |
| 1 | A | 741 | TYR | OH-CZ-CE2 | 5.16 | 134.03 | 120.10 |
| 1 | B | 1006 | THR | CA-CB-OG1 | 5.16 | 119.84 | 109.00 |
| 1 | C | 802 | PHE | N-CA-CB | 5.16 | 119.88 | 110.60 |
| 1 | C | 977 | LEU | CB-CG-CD2 | 5.16 | 119.77 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 977 | LEU | CB-CG-CD2 | 5.15 | 119.76 | 111.00 |
| 1 | B | 764 | ASN | C-N-CA | -5.14 | 108.84 | 121.70 |
| 1 | B | 802 | PHE | N-CA-CB | 5.13 | 119.83 | 110.60 |
| 1 | C | 764 | ASN | C-N-CA | -5.12 | 108.90 | 121.70 |
| 1 | B | 160 | TYR | N-CA-CB | -5.12 | 101.39 | 110.60 |
| 1 | A | 764 | ASN | C-N-CA | -5.11 | 108.92 | 121.70 |
| 1 | A | 17 | ASN | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | A | 160 | TYR | N-CA-CB | -5.11 | 101.41 | 110.60 |
| 1 | C | 160 | TYR | N-CA-CB | -5.10 | 101.42 | 110.60 |
| 1 | B | 17 | ASN | CB-CA-C | -5.09 | 100.21 | 110.40 |
| 1 | C | 909 | ILE | N-CA-CB | 5.09 | 122.50 | 110.80 |
| 1 | C | 17 | ASN | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | C | 909 | ILE | CB-CG1-CD1 | 5.08 | 128.12 | 113.90 |
| 1 | A | 909 | ILE | CB-CG1-CD1 | 5.07 | 128.11 | 113.90 |
| 1 | B | 964 | LYS | CA-CB-CG | 5.07 | 124.56 | 113.40 |
| 1 | A | 964 | LYS | CA-CB-CG | 5.07 | 124.55 | 113.40 |
| 1 | B | 909 | ILE | N-CA-CB | 5.07 | 122.45 | 110.80 |
| 1 | A | 909 | ILE | N-CA-CB | 5.06 | 122.45 | 110.80 |
| 1 | C | 964 | LYS | CA-CB-CG | 5.06 | 124.54 | 113.40 |
| 1 | B | 909 | ILE | CB-CG1-CD1 | 5.06 | 128.06 | 113.90 |
| 1 | C | 726 | ILE | CB-CG1-CD1 | 5.06 | 128.06 | 113.90 |
| 1 | B | 726 | ILE | CB-CG1-CD1 | 5.05 | 128.05 | 113.90 |
| 1 | A | 43 | PHE | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 1 | A | 726 | ILE | CB-CG1-CD1 | 5.04 | 128.02 | 113.90 |
| 1 | B | 43 | PHE | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 1 | C | 43 | PHE | N-CA-CB | 5.02 | 119.64 | 110.60 |

All (33) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | A | 274 | THR | CB |
| 1 | A | 286 | THR | CB |
| 1 | A | 299 | THR | CB |
| 1 | A | 719 | THR | CB |
| 1 | A | 761 | THR | CB |
| 1 | A | 980 | ILE | CB |
| 1 | A | 997 | ILE | CB |
| 1 | A | 1006 | THR | CB |
| 1 | A | 1009 | THR | CB |
| 1 | A | 1013 | ILE | CB |
| 1 | A | 1116 | THR | CB |
| 1 | B | 274 | THR | CB |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | B | 286 | THR | CB |
| 1 | B | 299 | THR | CB |
| 1 | B | 719 | THR | CB |
| 1 | B | 761 | THR | CB |
| 1 | B | 980 | ILE | CB |
| 1 | B | 997 | ILE | CB |
| 1 | B | 1006 | THR | CB |
| 1 | B | 1009 | THR | CB |
| 1 | B | 1013 | ILE | CB |
| 1 | B | 1116 | THR | CB |
| 1 | C | 274 | THR | CB |
| 1 | C | 286 | THR | CB |
| 1 | C | 299 | THR | CB |
| 1 | C | 719 | THR | CB |
| 1 | C | 761 | THR | CB |
| 1 | C | 980 | ILE | CB |
| 1 | C | 997 | ILE | CB |
| 1 | C | 1006 | THR | CB |
| 1 | C | 1009 | THR | CB |
| 1 | C | 1013 | ILE | CB |
| 1 | C | 1116 | THR | CB |

All (116) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-------------------|
| 1 | A | 1014 | ARG | Sidechain |
| 1 | A | 1039 | ARG | Peptide,Sidechain |
| 1 | A | 1058 | HIS | Sidechain |
| 1 | A | 1064 | HIS | Peptide,Sidechain |
| 1 | A | 1089 | PHE | Sidechain |
| 1 | A | 1091 | ARG | Sidechain |
| 1 | A | 158 | ARG | Sidechain |
| 1 | A | 159 | VAL | Peptide |
| 1 | A | 160 | TYR | Sidechain |
| 1 | A | 170 | TYR | Sidechain |
| 1 | A | 192 | PHE | Sidechain |
| 1 | A | 206 | LYS | Peptide |
| 1 | A | 207 | HIS | Peptide,Sidechain |
| 1 | A | 25 | PRO | Peptide |
| 1 | A | 266 | TYR | Sidechain |
| 1 | A | 269 | TYR | Sidechain |
| 1 | A | 318 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|--------|------|-------------------|
| 1 | A | 43 | PHE | Sidechain |
| 1 | A | 476 | GLY | Peptide |
| 1 | A | 477[A] | SER | Peptide |
| 1 | A | 477[B] | SER | Peptide |
| 1 | A | 655 | HIS | Sidechain |
| 1 | A | 66 | HIS | Sidechain |
| 1 | A | 741 | TYR | Sidechain |
| 1 | A | 762 | GLN | Sidechain |
| 1 | A | 764 | ASN | Peptide |
| 1 | A | 765 | ARG | Sidechain |
| 1 | A | 802 | PHE | Sidechain |
| 1 | A | 817 | PHE | Sidechain |
| 1 | A | 872 | GLN | Sidechain |
| 1 | A | 901 | GLN | Sidechain |
| 1 | A | 905 | ARG | Sidechain |
| 1 | A | 926 | GLN | Sidechain |
| 1 | A | 927 | PHE | Sidechain |
| 1 | A | 961 | THR | Peptide |
| 1 | A | 969 | ASN | Sidechain |
| 1 | B | 1014 | ARG | Sidechain |
| 1 | B | 1039 | ARG | Peptide,Sidechain |
| 1 | B | 1058 | HIS | Sidechain |
| 1 | B | 1064 | HIS | Peptide,Sidechain |
| 1 | B | 1089 | PHE | Sidechain |
| 1 | B | 1091 | ARG | Sidechain |
| 1 | B | 158 | ARG | Sidechain |
| 1 | B | 159 | VAL | Peptide |
| 1 | B | 160 | TYR | Sidechain |
| 1 | B | 170 | TYR | Sidechain |
| 1 | B | 192 | PHE | Sidechain |
| 1 | B | 206 | LYS | Peptide |
| 1 | B | 207 | HIS | Peptide,Sidechain |
| 1 | B | 25 | PRO | Peptide |
| 1 | B | 266 | TYR | Sidechain |
| 1 | B | 269 | TYR | Sidechain |
| 1 | B | 318 | PHE | Sidechain |
| 1 | B | 43 | PHE | Sidechain |
| 1 | B | 488 | CYS | Peptide |
| 1 | B | 489 | TYR | Peptide |
| 1 | B | 655 | HIS | Sidechain |
| 1 | B | 66 | HIS | Sidechain |
| 1 | B | 741 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-------------------|
| 1 | B | 762 | GLN | Sidechain |
| 1 | B | 764 | ASN | Peptide |
| 1 | B | 765 | ARG | Sidechain |
| 1 | B | 802 | PHE | Sidechain |
| 1 | B | 817 | PHE | Sidechain |
| 1 | B | 872 | GLN | Sidechain |
| 1 | B | 901 | GLN | Sidechain |
| 1 | B | 905 | ARG | Sidechain |
| 1 | B | 926 | GLN | Sidechain |
| 1 | B | 927 | PHE | Sidechain |
| 1 | B | 961 | THR | Peptide |
| 1 | B | 969 | ASN | Sidechain |
| 1 | C | 1014 | ARG | Sidechain |
| 1 | C | 1039 | ARG | Peptide,Sidechain |
| 1 | C | 1058 | HIS | Sidechain |
| 1 | C | 1064 | HIS | Peptide,Sidechain |
| 1 | C | 1089 | PHE | Sidechain |
| 1 | C | 1091 | ARG | Sidechain |
| 1 | C | 158 | ARG | Sidechain |
| 1 | C | 159 | VAL | Peptide |
| 1 | C | 160 | TYR | Sidechain |
| 1 | C | 170 | TYR | Sidechain |
| 1 | C | 192 | PHE | Sidechain |
| 1 | C | 206 | LYS | Peptide |
| 1 | C | 207 | HIS | Peptide,Sidechain |
| 1 | C | 25 | PRO | Peptide |
| 1 | C | 266 | TYR | Sidechain |
| 1 | C | 269 | TYR | Sidechain |
| 1 | C | 318 | PHE | Sidechain |
| 1 | C | 43 | PHE | Sidechain |
| 1 | C | 459 | SER | Peptide |
| 1 | C | 476 | GLY | Peptide |
| 1 | C | 655 | HIS | Sidechain |
| 1 | C | 66 | HIS | Sidechain |
| 1 | C | 741 | TYR | Sidechain |
| 1 | C | 762 | GLN | Sidechain |
| 1 | C | 764 | ASN | Peptide |
| 1 | C | 765 | ARG | Sidechain |
| 1 | C | 802 | PHE | Sidechain |
| 1 | C | 817 | PHE | Sidechain |
| 1 | C | 872 | GLN | Sidechain |
| 1 | C | 901 | GLN | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | C | 905 | ARG | Sidechain |
| 1 | C | 926 | GLN | Sidechain |
| 1 | C | 927 | PHE | Sidechain |
| 1 | C | 961 | THR | Peptide |
| 1 | C | 969 | ASN | 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 | 8301 | 8079 | 8081 | 468 | 0 |
| 1 | B | 8253 | 8034 | 8043 | 502 | 0 |
| 1 | C | 8292 | 8069 | 8072 | 473 | 0 |
| 2 | D | 895 | 0 | 839 | 124 | 0 |
| 2 | E | 895 | 0 | 839 | 146 | 0 |
| 3 | F | 28 | 25 | 25 | 2 | 0 |
| 3 | G | 28 | 25 | 25 | 0 | 0 |
| 3 | H | 28 | 25 | 25 | 0 | 0 |
| 3 | I | 28 | 25 | 25 | 1 | 0 |
| 3 | J | 28 | 25 | 25 | 2 | 0 |
| 4 | A | 196 | 181 | 182 | 15 | 0 |
| 4 | B | 182 | 167 | 169 | 26 | 0 |
| 4 | C | 84 | 64 | 78 | 8 | 0 |
| All | All | 27238 | 24719 | 26428 | 1551 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (1551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:770:ILE:CB | 1:A:770:ILE:CG2 | 1.76 | 1.63 |
| 1:C:699:LEU:CD2 | 1:C:699:LEU:CG | 1.76 | 1.63 |
| 1:C:959:LEU:CG | 1:C:959:LEU:CD2 | 1.77 | 1.62 |
| 1:B:911:VAL:CG2 | 1:B:911:VAL:HG13 | 1.28 | 1.61 |
| 1:C:911:VAL:CG1 | 1:C:911:VAL:CG2 | 1.78 | 1.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:911:VAL:CG2 | 1:A:911:VAL:CB | 1.78 | 1.60 |
| 1:B:770:ILE:CG2 | 1:B:770:ILE:CB | 1.76 | 1.59 |
| 1:C:911:VAL:CG2 | 1:C:911:VAL:HG13 | 1.28 | 1.58 |
| 1:C:770:ILE:CG1 | 1:C:770:ILE:CG2 | 1.82 | 1.58 |
| 1:A:911:VAL:CG2 | 1:A:911:VAL:HG13 | 1.28 | 1.57 |
| 1:B:911:VAL:CG2 | 1:B:911:VAL:CB | 1.78 | 1.57 |
| 1:C:770:ILE:CG2 | 1:C:770:ILE:CB | 1.76 | 1.57 |
| 1:A:699:LEU:CD1 | 1:A:699:LEU:CD2 | 1.82 | 1.57 |
| 1:A:959:LEU:CG | 1:A:959:LEU:CD2 | 1.77 | 1.55 |
| 1:B:959:LEU:CD2 | 1:B:959:LEU:CG | 1.77 | 1.55 |
| 1:B:699:LEU:CD1 | 1:B:699:LEU:CD2 | 1.82 | 1.55 |
| 1:C:911:VAL:CG2 | 1:C:911:VAL:CB | 1.78 | 1.55 |
| 1:A:911:VAL:CG2 | 1:A:911:VAL:CG1 | 1.78 | 1.54 |
| 1:B:911:VAL:CG2 | 1:B:911:VAL:CG1 | 1.78 | 1.54 |
| 1:B:699:LEU:CD2 | 1:B:699:LEU:CG | 1.76 | 1.53 |
| 1:A:699:LEU:CD2 | 1:A:699:LEU:CG | 1.76 | 1.53 |
| 1:B:770:ILE:CG2 | 1:B:770:ILE:CG1 | 1.82 | 1.53 |
| 1:A:770:ILE:CG2 | 1:A:770:ILE:CG1 | 1.82 | 1.52 |
| 1:C:699:LEU:CD2 | 1:C:699:LEU:CD1 | 1.82 | 1.51 |
| 1:A:770:ILE:CG2 | 1:A:770:ILE:HG12 | 1.38 | 1.44 |
| 1:B:770:ILE:CG2 | 1:B:770:ILE:HG12 | 1.38 | 1.43 |
| 1:A:699:LEU:CD2 | 1:A:699:LEU:HD13 | 1.45 | 1.38 |
| 1:B:699:LEU:CD2 | 1:B:699:LEU:HD13 | 1.45 | 1.36 |
| 1:C:770:ILE:CG2 | 1:C:770:ILE:HG12 | 1.38 | 1.35 |
| 1:A:959:LEU:CD2 | 1:A:959:LEU:CB | 2.06 | 1.33 |
| 1:C:959:LEU:CD2 | 1:C:959:LEU:CB | 2.06 | 1.31 |
| 1:C:699:LEU:CD2 | 1:C:699:LEU:HD13 | 1.45 | 1.31 |
| 1:B:959:LEU:CD2 | 1:B:959:LEU:CB | 2.06 | 1.31 |
| 1:A:192:PHE:CE1 | 1:A:192:PHE:CE2 | 1.96 | 1.22 |
| 1:C:192:PHE:CZ | 1:C:192:PHE:CD1 | 1.95 | 1.21 |
| 1:B:959:LEU:CD2 | 1:B:959:LEU:CD1 | 2.25 | 1.15 |
| 1:A:192:PHE:CZ | 1:A:192:PHE:CD1 | 1.95 | 1.14 |
| 1:B:959:LEU:CD2 | 1:B:959:LEU:HB3 | 1.78 | 1.14 |
| 1:C:192:PHE:CE1 | 1:C:192:PHE:CE2 | 1.96 | 1.14 |
| 1:A:959:LEU:CD2 | 1:A:959:LEU:CD1 | 2.25 | 1.13 |
| 1:C:699:LEU:HD13 | 1:C:699:LEU:HD22 | 1.29 | 1.13 |
| 1:C:959:LEU:CD2 | 1:C:959:LEU:CD1 | 2.25 | 1.13 |
| 1:A:770:ILE:HG12 | 1:A:770:ILE:HG23 | 1.22 | 1.12 |
| 1:C:911:VAL:HG13 | 1:C:911:VAL:HG22 | 1.28 | 1.12 |
| 1:C:959:LEU:CD2 | 1:C:959:LEU:HB3 | 1.78 | 1.12 |
| 1:B:192:PHE:CZ | 1:B:192:PHE:CD1 | 1.96 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:699:LEU:HG | 1:C:872:GLN:OE1 | 1.46 | 1.11 |
| 1:B:192:PHE:CE1 | 1:B:192:PHE:CE2 | 1.96 | 1.10 |
| 1:B:911:VAL:HG13 | 1:B:911:VAL:HG22 | 1.28 | 1.10 |
| 1:A:699:LEU:HD13 | 1:A:699:LEU:HD22 | 1.29 | 1.09 |
| 1:C:770:ILE:HG12 | 1:C:770:ILE:HG23 | 1.22 | 1.09 |
| 1:A:911:VAL:HG13 | 1:A:911:VAL:HG22 | 1.28 | 1.08 |
| 1:B:770:ILE:HG12 | 1:B:770:ILE:HG23 | 1.22 | 1.08 |
| 1:B:699:LEU:HD13 | 1:B:699:LEU:HD22 | 1.29 | 1.08 |
| 1:B:480:CYS:O | 1:B:482:GLY:N | 1.87 | 1.07 |
| 1:A:1005:GLN:HE22 | 1:C:1006:THR:CG2 | 1.67 | 1.06 |
| 1:A:959:LEU:CD2 | 1:A:959:LEU:HB3 | 1.78 | 1.05 |
| 1:A:911:VAL:HG13 | 1:A:911:VAL:HG21 | 1.34 | 1.05 |
| 1:B:911:VAL:HG13 | 1:B:911:VAL:HG21 | 1.34 | 1.05 |
| 2:D:31:THR:HG21 | 2:D:98:SER:HB3 | 1.07 | 1.05 |
| 1:C:911:VAL:HG13 | 1:C:911:VAL:HG21 | 1.34 | 1.05 |
| 2:E:69:THR:HG22 | 2:E:82:GLN:HB3 | 1.40 | 1.04 |
| 2:E:31:THR:HG21 | 2:E:98:SER:HB3 | 1.06 | 1.04 |
| 1:B:378:LYS:HD2 | 2:E:106:TYR:HD2 | 1.22 | 1.04 |
| 1:A:282:ASN:ND2 | 4:A:1303:NAG:O5 | 1.89 | 1.04 |
| 2:D:69:THR:HG22 | 2:D:82:GLN:HB3 | 1.40 | 1.02 |
| 1:B:378:LYS:HD2 | 2:E:106:TYR:CD2 | 1.95 | 1.01 |
| 1:B:376:THR:HG23 | 2:E:106:TYR:HB2 | 1.43 | 1.00 |
| 1:B:770:ILE:CG1 | 1:B:770:ILE:HG21 | 1.91 | 1.00 |
| 1:A:911:VAL:CG1 | 1:A:911:VAL:HG21 | 1.88 | 1.00 |
| 1:C:959:LEU:HD13 | 1:C:959:LEU:HD21 | 1.44 | 0.99 |
| 2:D:22:CYS:HB3 | 2:D:79:VAL:HG12 | 1.45 | 0.99 |
| 1:A:759:PHE:HA | 1:A:762:GLN:OE1 | 1.64 | 0.98 |
| 1:B:759:PHE:HA | 1:B:762:GLN:OE1 | 1.64 | 0.98 |
| 1:B:357:ARG:NH2 | 1:B:396:TYR:OH | 1.97 | 0.98 |
| 1:C:759:PHE:HA | 1:C:762:GLN:OE1 | 1.63 | 0.98 |
| 1:A:959:LEU:HD13 | 1:A:959:LEU:HD21 | 1.44 | 0.97 |
| 1:B:959:LEU:HD21 | 1:B:959:LEU:HD13 | 1.44 | 0.97 |
| 1:C:770:ILE:CG1 | 1:C:770:ILE:HG21 | 1.91 | 0.97 |
| 1:B:911:VAL:CG1 | 1:B:911:VAL:HG21 | 1.88 | 0.97 |
| 1:A:1005:GLN:HE22 | 1:C:1006:THR:HG23 | 1.30 | 0.96 |
| 1:B:699:LEU:CD1 | 1:B:699:LEU:HD21 | 1.96 | 0.96 |
| 1:B:770:ILE:HG12 | 1:B:770:ILE:HG21 | 1.46 | 0.95 |
| 2:E:64:VAL:HA | 2:E:67:ARG:HE | 1.30 | 0.95 |
| 1:A:699:LEU:CD1 | 1:A:699:LEU:HD21 | 1.96 | 0.95 |
| 1:A:770:ILE:CG1 | 1:A:770:ILE:HG21 | 1.91 | 0.94 |
| 2:D:64:VAL:HA | 2:D:67:ARG:HE | 1.30 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:911:VAL:CG2 | 1:B:911:VAL:CA | 2.46 | 0.94 |
| 1:C:699:LEU:CD1 | 1:C:699:LEU:HD21 | 1.96 | 0.94 |
| 2:E:22:CYS:HB3 | 2:E:79:VAL:HG12 | 1.45 | 0.94 |
| 1:A:911:VAL:CG2 | 1:A:911:VAL:CA | 2.46 | 0.94 |
| 1:C:911:VAL:CG2 | 1:C:911:VAL:CA | 2.46 | 0.94 |
| 2:D:101:TYR:HE1 | 2:D:103:ALA:HB3 | 1.33 | 0.93 |
| 1:B:376:THR:OG1 | 2:E:106:TYR:CD1 | 2.18 | 0.93 |
| 1:B:669:GLY:CA | 1:C:869:MET:CE | 2.47 | 0.93 |
| 2:E:101:TYR:HE1 | 2:E:103:ALA:HB3 | 1.33 | 0.93 |
| 1:A:149:ASN:HD21 | 4:A:1301:NAG:C1 | 1.82 | 0.92 |
| 1:B:669:GLY:HA2 | 1:C:869:MET:CE | 1.99 | 0.92 |
| 2:E:31:THR:CG2 | 2:E:98:SER:HB3 | 1.98 | 0.92 |
| 1:A:959:LEU:HB3 | 1:A:959:LEU:HD23 | 1.52 | 0.91 |
| 1:C:911:VAL:CG1 | 1:C:911:VAL:HG21 | 1.88 | 0.91 |
| 1:B:192:PHE:CZ | 1:B:192:PHE:CE1 | 0.91 | 0.91 |
| 1:C:192:PHE:CZ | 1:C:192:PHE:CE1 | 0.91 | 0.91 |
| 2:D:31:THR:CG2 | 2:D:98:SER:HB3 | 1.99 | 0.91 |
| 1:A:192:PHE:CE1 | 1:A:192:PHE:CZ | 0.91 | 0.91 |
| 1:B:596:SER:OG | 1:B:613:GLN:OE1 | 1.89 | 0.91 |
| 1:C:130:VAL:HG21 | 1:C:231:ILE:HG21 | 1.53 | 0.90 |
| 1:C:959:LEU:HB3 | 1:C:959:LEU:HD23 | 1.52 | 0.90 |
| 1:A:596:SER:OG | 1:A:613:GLN:OE1 | 1.89 | 0.90 |
| 1:A:282:ASN:ND2 | 4:A:1303:NAG:C1 | 2.34 | 0.89 |
| 1:A:959:LEU:CD2 | 1:A:959:LEU:HD13 | 1.98 | 0.89 |
| 1:C:596:SER:OG | 1:C:613:GLN:OE1 | 1.89 | 0.89 |
| 1:B:959:LEU:HB3 | 1:B:959:LEU:HD23 | 1.52 | 0.89 |
| 1:A:192:PHE:CZ | 1:A:192:PHE:HE1 | 1.60 | 0.89 |
| 1:B:192:PHE:CE1 | 1:B:192:PHE:HZ | 1.63 | 0.89 |
| 1:B:130:VAL:HG21 | 1:B:231:ILE:HG21 | 1.53 | 0.89 |
| 1:B:708:SER:HB3 | 1:B:711:SER:HB3 | 1.52 | 0.89 |
| 1:B:770:ILE:CG2 | 1:B:770:ILE:CA | 2.51 | 0.89 |
| 1:C:192:PHE:CE1 | 1:C:192:PHE:HZ | 1.63 | 0.88 |
| 1:A:770:ILE:CG2 | 1:A:770:ILE:CA | 2.51 | 0.88 |
| 1:B:959:LEU:CD2 | 1:B:959:LEU:HD13 | 1.98 | 0.88 |
| 1:C:280:ASN:OD1 | 1:C:281:GLU:N | 2.07 | 0.88 |
| 1:B:376:THR:OG1 | 2:E:106:TYR:HD1 | 1.56 | 0.88 |
| 1:B:699:LEU:CG | 1:C:872:GLN:OE1 | 2.21 | 0.88 |
| 1:B:34:ARG:NH1 | 1:B:191:GLU:OE2 | 2.07 | 0.88 |
| 1:B:280:ASN:OD1 | 1:B:281:GLU:N | 2.07 | 0.88 |
| 1:C:280:ASN:OD1 | 1:C:282:ASN:N | 2.07 | 0.88 |
| 1:A:130:VAL:HG21 | 1:A:231:ILE:HG21 | 1.54 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:192:PHE:CE1 | 1:A:192:PHE:HZ | 1.63 | 0.88 |
| 1:B:699:LEU:CD2 | 1:B:699:LEU:CB | 2.52 | 0.87 |
| 1:A:280:ASN:OD1 | 1:A:282:ASN:N | 2.07 | 0.87 |
| 1:C:699:LEU:CD2 | 1:C:699:LEU:CB | 2.52 | 0.87 |
| 1:C:770:ILE:CG2 | 1:C:770:ILE:CA | 2.51 | 0.87 |
| 4:B:1304:NAG:H83 | 4:B:1304:NAG:H3 | 1.54 | 0.87 |
| 1:B:901:GLN:O | 1:B:905:ARG:HG2 | 1.75 | 0.87 |
| 1:C:192:PHE:CZ | 1:C:192:PHE:HE1 | 1.60 | 0.87 |
| 1:A:34:ARG:NH1 | 1:A:191:GLU:OE2 | 2.07 | 0.87 |
| 1:A:699:LEU:CD2 | 1:A:699:LEU:CB | 2.52 | 0.87 |
| 1:A:280:ASN:OD1 | 1:A:281:GLU:N | 2.07 | 0.86 |
| 1:A:901:GLN:O | 1:A:905:ARG:HG2 | 1.75 | 0.86 |
| 1:B:192:PHE:CZ | 1:B:192:PHE:HE1 | 1.60 | 0.86 |
| 1:B:376:THR:HG1 | 2:E:106:TYR:HD1 | 0.93 | 0.86 |
| 1:C:770:ILE:HG12 | 1:C:770:ILE:HG21 | 1.46 | 0.86 |
| 1:B:280:ASN:OD1 | 1:B:282:ASN:N | 2.07 | 0.86 |
| 1:B:669:GLY:CA | 1:C:869:MET:HE1 | 2.05 | 0.86 |
| 1:C:901:GLN:O | 1:C:905:ARG:HG2 | 1.75 | 0.86 |
| 2:E:105:GLY:HA2 | 2:E:108:PHE:CE1 | 2.11 | 0.86 |
| 1:C:34:ARG:NH1 | 1:C:191:GLU:OE2 | 2.07 | 0.86 |
| 2:D:105:GLY:HA2 | 2:D:108:PHE:CE1 | 2.11 | 0.85 |
| 2:D:83:MET:HB3 | 2:D:86:LEU:HD21 | 1.59 | 0.85 |
| 1:B:699:LEU:HB3 | 1:C:788:ILE:HG13 | 1.58 | 0.85 |
| 1:B:349:SER:OG | 1:B:452:LEU:O | 1.93 | 0.85 |
| 1:A:282:ASN:HD21 | 4:A:1303:NAG:C1 | 1.88 | 0.84 |
| 1:B:770:ILE:CG2 | 1:B:770:ILE:C | 2.46 | 0.84 |
| 2:D:101:TYR:CE1 | 2:D:103:ALA:HB3 | 2.13 | 0.84 |
| 1:C:770:ILE:CG2 | 1:C:770:ILE:C | 2.46 | 0.84 |
| 2:E:83:MET:HB3 | 2:E:86:LEU:HD21 | 1.59 | 0.84 |
| 1:C:905:ARG:NH1 | 1:C:1050:MET:HB3 | 1.93 | 0.83 |
| 2:E:101:TYR:CE1 | 2:E:103:ALA:HB3 | 2.13 | 0.83 |
| 1:A:770:ILE:CG2 | 1:A:770:ILE:C | 2.46 | 0.83 |
| 1:A:17:ASN:OD1 | 3:F:1:NAG:C1 | 2.27 | 0.83 |
| 1:A:1005:GLN:NE2 | 1:C:1006:THR:HG23 | 1.93 | 0.83 |
| 1:A:1028:LYS:NZ | 1:A:1042:PHE:O | 2.11 | 0.83 |
| 1:B:14:GLN:NE2 | 1:B:15:CYS:O | 2.11 | 0.83 |
| 1:C:1028:LYS:NZ | 1:C:1042:PHE:O | 2.11 | 0.83 |
| 1:A:14:GLN:NE2 | 1:A:15:CYS:O | 2.11 | 0.83 |
| 1:B:376:THR:HG23 | 2:E:106:TYR:CB | 2.08 | 0.83 |
| 1:A:770:ILE:HG12 | 1:A:770:ILE:HG21 | 1.46 | 0.83 |
| 1:C:14:GLN:NE2 | 1:C:15:CYS:O | 2.11 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:905:ARG:NH1 | 1:B:1050:MET:HB3 | 1.94 | 0.82 |
| 1:A:905:ARG:NH1 | 1:A:1050:MET:HB3 | 1.93 | 0.82 |
| 1:B:1028:LYS:NZ | 1:B:1042:PHE:O | 2.11 | 0.82 |
| 2:D:12:VAL:HG21 | 2:D:86:LEU:HD12 | 1.62 | 0.82 |
| 1:B:705:VAL:HG12 | 1:C:895:GLN:HB3 | 1.62 | 0.81 |
| 2:E:109:ASN:HA | 2:E:111:TRP:CZ3 | 2.14 | 0.81 |
| 1:A:894:LEU:HB3 | 1:C:713:ALA:HB3 | 1.63 | 0.81 |
| 2:E:12:VAL:HG21 | 2:E:86:LEU:HD12 | 1.62 | 0.81 |
| 2:E:67:ARG:HG3 | 2:E:68:PHE:HD1 | 1.45 | 0.81 |
| 1:C:959:LEU:CD2 | 1:C:959:LEU:HD13 | 1.98 | 0.81 |
| 2:D:109:ASN:HA | 2:D:111:TRP:CZ3 | 2.14 | 0.81 |
| 1:B:949:GLN:O | 1:B:953:ASN:OD1 | 2.00 | 0.80 |
| 1:B:669:GLY:CA | 1:C:869:MET:HE3 | 2.09 | 0.80 |
| 1:A:894:LEU:HD13 | 1:C:713:ALA:O | 1.80 | 0.80 |
| 1:A:1080:ALA:HB2 | 1:A:1089:PHE:CE2 | 2.17 | 0.80 |
| 1:A:949:GLN:O | 1:A:953:ASN:OD1 | 1.99 | 0.80 |
| 1:B:1080:ALA:HB2 | 1:B:1089:PHE:CE2 | 2.17 | 0.80 |
| 1:B:669:GLY:HA2 | 1:C:869:MET:HE3 | 1.64 | 0.80 |
| 1:A:886:TRP:HZ3 | 1:A:905:ARG:HD3 | 1.47 | 0.79 |
| 2:D:67:ARG:HG3 | 2:D:68:PHE:HD1 | 1.45 | 0.79 |
| 1:B:378:LYS:CD | 2:E:106:TYR:HD2 | 1.95 | 0.79 |
| 1:B:820:ASP:O | 1:B:824:ASN:OD1 | 2.01 | 0.79 |
| 1:C:1080:ALA:HB2 | 1:C:1089:PHE:CE2 | 2.17 | 0.79 |
| 1:C:820:ASP:O | 1:C:824:ASN:OD1 | 2.01 | 0.79 |
| 1:C:886:TRP:HZ3 | 1:C:905:ARG:HD3 | 1.47 | 0.79 |
| 1:A:917:TYR:CZ | 1:C:1079:PRO:HB3 | 2.17 | 0.79 |
| 1:B:669:GLY:HA3 | 1:C:869:MET:CE | 2.12 | 0.79 |
| 1:B:376:THR:CG2 | 2:E:106:TYR:HB2 | 2.12 | 0.79 |
| 1:A:589:PRO:HG2 | 1:B:855:PHE:HD1 | 1.48 | 0.79 |
| 1:C:919:ASN:OD1 | 1:C:923:ILE:HG13 | 1.84 | 0.78 |
| 1:C:949:GLN:O | 1:C:953:ASN:OD1 | 2.00 | 0.78 |
| 1:B:886:TRP:HZ3 | 1:B:905:ARG:HD3 | 1.47 | 0.78 |
| 1:A:762:GLN:HE21 | 1:C:961:THR:HG21 | 1.48 | 0.78 |
| 2:E:81:LEU:HG | 2:E:83:MET:SD | 2.23 | 0.78 |
| 1:A:892:ALA:CB | 1:C:1072:GLU:OE2 | 2.32 | 0.78 |
| 1:B:378:LYS:CD | 2:E:106:TYR:CD2 | 2.67 | 0.78 |
| 1:A:820:ASP:O | 1:A:824:ASN:OD1 | 2.01 | 0.78 |
| 2:D:81:LEU:HG | 2:D:83:MET:SD | 2.23 | 0.78 |
| 1:B:393:THR:O | 1:B:523:THR:OG1 | 2.01 | 0.77 |
| 1:C:130:VAL:HG21 | 1:C:231:ILE:CG2 | 2.14 | 0.77 |
| 2:D:38:ARG:CG | 2:D:92:ALA:HB3 | 2.14 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:38:ARG:CG | 2:E:92:ALA:HB3 | 2.14 | 0.77 |
| 1:B:919:ASN:OD1 | 1:B:923:ILE:HG13 | 1.84 | 0.77 |
| 1:A:802:PHE:O | 1:A:806:LEU:HB2 | 1.85 | 0.77 |
| 1:B:658:ASN:OD1 | 1:B:660:TYR:CE1 | 2.38 | 0.77 |
| 2:E:67:ARG:HG3 | 2:E:68:PHE:CD1 | 2.20 | 0.77 |
| 1:C:973:ILE:HD11 | 1:C:980:ILE:HG23 | 1.67 | 0.77 |
| 1:A:658:ASN:OD1 | 1:A:660:TYR:CE1 | 2.38 | 0.77 |
| 1:A:130:VAL:HG21 | 1:A:231:ILE:CG2 | 2.14 | 0.76 |
| 1:A:802:PHE:N | 1:A:802:PHE:CD2 | 2.53 | 0.76 |
| 1:C:658:ASN:OD1 | 1:C:660:TYR:CE1 | 2.38 | 0.76 |
| 1:C:802:PHE:O | 1:C:806:LEU:HB2 | 1.85 | 0.76 |
| 1:B:802:PHE:N | 1:B:802:PHE:CD2 | 2.53 | 0.76 |
| 1:A:332:ILE:CD1 | 1:A:527:PRO:HA | 2.15 | 0.76 |
| 1:A:919:ASN:OD1 | 1:A:923:ILE:HG13 | 1.83 | 0.76 |
| 1:B:802:PHE:O | 1:B:806:LEU:HB2 | 1.85 | 0.76 |
| 1:A:897:PRO:HB3 | 1:C:709:ASN:O | 1.86 | 0.76 |
| 1:B:130:VAL:HG21 | 1:B:231:ILE:CG2 | 2.14 | 0.76 |
| 1:B:707:TYR:OH | 1:C:897:PRO:O | 2.03 | 0.75 |
| 1:C:802:PHE:N | 1:C:802:PHE:CD2 | 2.53 | 0.75 |
| 2:D:67:ARG:HG3 | 2:D:68:PHE:CD1 | 2.20 | 0.75 |
| 1:A:1005:GLN:HE22 | 1:C:1006:THR:HG21 | 1.49 | 0.75 |
| 1:B:922:LEU:HD11 | 4:B:1310:NAG:C6 | 2.15 | 0.75 |
| 1:C:661:GLU:O | 1:C:695:TYR:OH | 2.05 | 0.75 |
| 1:B:667:GLY:HA2 | 1:C:864:LEU:HA | 1.68 | 0.75 |
| 1:B:661:GLU:O | 1:B:695:TYR:OH | 2.04 | 0.75 |
| 1:B:774:GLN:HA | 1:B:777:ASN:OD1 | 1.87 | 0.75 |
| 1:B:973:ILE:HD11 | 1:B:980:ILE:HG23 | 1.67 | 0.74 |
| 1:A:973:ILE:HD11 | 1:A:980:ILE:HG23 | 1.67 | 0.74 |
| 2:E:105:GLY:HA2 | 2:E:108:PHE:HE1 | 1.51 | 0.74 |
| 1:A:1030:SER:O | 1:C:1040:VAL:HG11 | 1.87 | 0.74 |
| 1:A:661:GLU:O | 1:A:695:TYR:OH | 2.05 | 0.74 |
| 1:A:918:GLU:HA | 1:C:1128:VAL:HG22 | 1.69 | 0.73 |
| 1:B:407:VAL:O | 2:E:106:TYR:OH | 2.06 | 0.73 |
| 1:C:774:GLN:HA | 1:C:777:ASN:OD1 | 1.87 | 0.73 |
| 1:A:774:GLN:HA | 1:A:777:ASN:OD1 | 1.87 | 0.73 |
| 1:C:117:LEU:HD13 | 1:C:130:VAL:HG22 | 1.71 | 0.73 |
| 1:A:1005:GLN:NE2 | 1:C:1006:THR:CG2 | 2.47 | 0.73 |
| 2:D:105:GLY:HA2 | 2:D:108:PHE:HE1 | 1.51 | 0.73 |
| 1:A:914:ASN:HB3 | 1:C:1089:PHE:HE1 | 1.53 | 0.73 |
| 1:B:454:ARG:NH1 | 1:B:467:ASP:OD2 | 2.21 | 0.73 |
| 1:B:669:GLY:HA3 | 1:C:869:MET:HE1 | 1.68 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:933:LYS:O | 1:C:936:ASP:OD2 | 2.07 | 0.73 |
| 1:C:762:GLN:HA | 1:C:765:ARG:NH1 | 2.04 | 0.73 |
| 1:B:959:LEU:CB | 1:B:959:LEU:HD22 | 2.18 | 0.73 |
| 1:A:748:GLU:O | 1:A:752:LEU:HG | 1.89 | 0.73 |
| 1:B:933:LYS:O | 1:B:936:ASP:OD2 | 2.07 | 0.73 |
| 1:B:748:GLU:O | 1:B:752:LEU:HG | 1.89 | 0.72 |
| 2:E:98:SER:O | 2:E:108:PHE:HA | 1.89 | 0.72 |
| 1:C:318:PHE:HD2 | 1:C:319:ARG:N | 1.87 | 0.72 |
| 1:A:762:GLN:HA | 1:A:765:ARG:NH1 | 2.04 | 0.72 |
| 2:D:98:SER:O | 2:D:108:PHE:HA | 1.89 | 0.72 |
| 1:B:117:LEU:HD13 | 1:B:130:VAL:HG22 | 1.71 | 0.72 |
| 1:C:748:GLU:O | 1:C:752:LEU:HG | 1.89 | 0.72 |
| 1:C:959:LEU:CB | 1:C:959:LEU:HD22 | 2.18 | 0.72 |
| 1:B:372:ALA:HA | 2:E:47:ARG:HH12 | 1.54 | 0.72 |
| 1:B:762:GLN:HA | 1:B:765:ARG:NH1 | 2.04 | 0.72 |
| 2:D:20:LEU:HD12 | 2:D:21:SER:N | 2.05 | 0.72 |
| 1:B:318:PHE:HD2 | 1:B:319:ARG:N | 1.87 | 0.72 |
| 4:B:1302:NAG:O7 | 4:B:1302:NAG:O3 | 2.07 | 0.72 |
| 1:C:476:GLY:O | 1:C:487:ASN:ND2 | 2.23 | 0.72 |
| 2:E:20:LEU:HD12 | 2:E:21:SER:N | 2.05 | 0.72 |
| 1:A:117:LEU:HD13 | 1:A:130:VAL:HG22 | 1.71 | 0.71 |
| 1:A:933:LYS:O | 1:A:936:ASP:OD2 | 2.07 | 0.71 |
| 1:A:318:PHE:HD2 | 1:A:319:ARG:N | 1.88 | 0.71 |
| 1:A:1126:CYS:HB2 | 1:A:1132:ILE:HD13 | 1.71 | 0.71 |
| 1:A:762:GLN:NE2 | 1:C:961:THR:HG21 | 2.05 | 0.71 |
| 2:D:60:TYR:HD2 | 2:D:64:VAL:HG23 | 1.55 | 0.71 |
| 2:E:95:TYR:HD2 | 2:E:114:GLY:HA3 | 1.55 | 0.71 |
| 1:C:1126:CYS:HB2 | 1:C:1132:ILE:HD13 | 1.71 | 0.71 |
| 1:B:707:TYR:CE2 | 1:C:897:PRO:HA | 2.26 | 0.71 |
| 1:B:1126:CYS:HB2 | 1:B:1132:ILE:HD13 | 1.71 | 0.71 |
| 1:C:802:PHE:N | 1:C:802:PHE:HD2 | 1.88 | 0.71 |
| 1:C:974:SER:OG | 1:C:979:ASP:OD2 | 2.09 | 0.71 |
| 2:E:60:TYR:HD2 | 2:E:64:VAL:HG23 | 1.55 | 0.71 |
| 1:A:43:PHE:HD1 | 1:A:44:ARG:N | 1.89 | 0.71 |
| 1:B:43:PHE:HD1 | 1:B:44:ARG:N | 1.89 | 0.71 |
| 1:B:708:SER:HB3 | 1:B:711:SER:CB | 2.21 | 0.71 |
| 1:C:962:LEU:C | 1:C:962:LEU:HD12 | 2.11 | 0.70 |
| 1:A:703:ASN:OD1 | 1:B:787:GLN:OE1 | 2.09 | 0.70 |
| 1:A:962:LEU:C | 1:A:962:LEU:HD12 | 2.11 | 0.70 |
| 1:C:1062:PHE:HB2 | 1:C:1064:HIS:HE2 | 1.56 | 0.70 |
| 1:C:43:PHE:HD1 | 1:C:44:ARG:N | 1.89 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:589:PRO:HG2 | 1:B:855:PHE:CD1 | 2.26 | 0.70 |
| 1:B:922:LEU:HD11 | 4:B:1310:NAG:H62 | 1.72 | 0.70 |
| 1:A:974:SER:OG | 1:A:979:ASP:OD2 | 2.09 | 0.70 |
| 1:B:407:VAL:C | 2:E:106:TYR:OH | 2.30 | 0.70 |
| 1:B:802:PHE:N | 1:B:802:PHE:HD2 | 1.88 | 0.70 |
| 2:E:19:ARG:CD | 2:E:80:TYR:CE1 | 2.75 | 0.70 |
| 1:A:1062:PHE:HB2 | 1:A:1064:HIS:HE2 | 1.56 | 0.70 |
| 1:B:974:SER:OG | 1:B:979:ASP:OD2 | 2.09 | 0.70 |
| 2:D:95:TYR:HD2 | 2:D:114:GLY:HA3 | 1.55 | 0.70 |
| 1:A:149:ASN:ND2 | 4:A:1301:NAG:C1 | 2.53 | 0.69 |
| 1:B:962:LEU:HD12 | 1:B:962:LEU:C | 2.11 | 0.69 |
| 1:C:806:LEU:HD23 | 1:C:878:LEU:HD22 | 1.75 | 0.69 |
| 1:A:802:PHE:N | 1:A:802:PHE:HD2 | 1.88 | 0.69 |
| 1:A:914:ASN:HB3 | 1:C:1089:PHE:CE1 | 2.27 | 0.69 |
| 1:B:1062:PHE:HB2 | 1:B:1064:HIS:HE2 | 1.56 | 0.69 |
| 1:B:911:VAL:CG2 | 1:B:911:VAL:N | 2.56 | 0.69 |
| 2:D:19:ARG:HD3 | 2:D:80:TYR:CD1 | 2.28 | 0.69 |
| 1:A:806:LEU:HD23 | 1:A:878:LEU:HD22 | 1.75 | 0.69 |
| 1:C:699:LEU:CD2 | 1:C:699:LEU:HD11 | 2.16 | 0.69 |
| 1:A:911:VAL:CG2 | 1:A:911:VAL:N | 2.56 | 0.69 |
| 1:A:959:LEU:CB | 1:A:959:LEU:HD22 | 2.18 | 0.69 |
| 2:D:19:ARG:CD | 2:D:80:TYR:CE1 | 2.75 | 0.69 |
| 1:A:1094:VAL:N | 1:A:1105:THR:O | 2.25 | 0.69 |
| 1:C:911:VAL:CG2 | 1:C:911:VAL:N | 2.56 | 0.69 |
| 2:D:30:ASN:HB3 | 2:D:100:TYR:CE2 | 2.28 | 0.69 |
| 2:D:93:LEU:HB3 | 2:D:95:TYR:CZ | 2.28 | 0.68 |
| 1:A:699:LEU:CD2 | 1:A:699:LEU:HD11 | 2.16 | 0.68 |
| 1:B:376:THR:HB | 1:B:435:ALA:H | 1.58 | 0.68 |
| 1:C:17:ASN:OD1 | 3:I:1:NAG:C1 | 2.42 | 0.68 |
| 2:E:30:ASN:HB3 | 2:E:100:TYR:CE2 | 2.28 | 0.68 |
| 2:E:109:ASN:HA | 2:E:111:TRP:HZ3 | 1.58 | 0.68 |
| 2:E:67:ARG:NH1 | 2:E:87:LYS:HD3 | 2.09 | 0.68 |
| 1:B:404:GLY:O | 1:B:407:VAL:HG22 | 1.94 | 0.68 |
| 2:E:19:ARG:HD3 | 2:E:80:TYR:CD1 | 2.28 | 0.68 |
| 1:B:472:ILE:HG23 | 1:B:489:TYR:O | 1.94 | 0.67 |
| 2:D:20:LEU:HD12 | 2:D:21:SER:H | 1.59 | 0.67 |
| 2:E:38:ARG:HG3 | 2:E:92:ALA:HB3 | 1.76 | 0.67 |
| 1:B:806:LEU:HD23 | 1:B:878:LEU:HD22 | 1.75 | 0.67 |
| 1:B:669:GLY:HA2 | 1:C:869:MET:HE1 | 1.68 | 0.67 |
| 2:D:67:ARG:NH1 | 2:D:87:LYS:HD3 | 2.09 | 0.67 |
| 2:E:93:LEU:HB3 | 2:E:95:TYR:CZ | 2.28 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1072:GLU:HG2 | 1:C:894:LEU:CD2 | 2.24 | 0.67 |
| 1:A:707:TYR:CD1 | 1:B:883:THR:HG22 | 2.30 | 0.67 |
| 1:B:354:ASN:OD1 | 1:B:399:SER:OG | 2.13 | 0.67 |
| 2:E:65:LYS:HE2 | 2:E:65:LYS:HA | 1.76 | 0.67 |
| 2:E:68:PHE:CD2 | 2:E:81:LEU:HD11 | 2.30 | 0.67 |
| 1:A:703:ASN:CG | 1:B:787:GLN:OE1 | 2.34 | 0.66 |
| 1:C:1094:VAL:N | 1:C:1105:THR:O | 2.25 | 0.66 |
| 4:A:1301:NAG:O7 | 4:A:1301:NAG:O3 | 2.12 | 0.66 |
| 2:E:70:ILE:HD12 | 2:E:80:TYR:O | 1.96 | 0.66 |
| 1:A:869:MET:HB2 | 1:C:699:LEU:HD11 | 1.78 | 0.66 |
| 2:D:68:PHE:CD2 | 2:D:81:LEU:HD11 | 2.30 | 0.66 |
| 2:D:70:ILE:HD12 | 2:D:80:TYR:O | 1.96 | 0.66 |
| 2:D:67:ARG:HB2 | 2:D:84:ASN:O | 1.96 | 0.66 |
| 1:A:894:LEU:CB | 1:C:713:ALA:HB3 | 2.26 | 0.66 |
| 2:D:65:LYS:HA | 2:D:65:LYS:HE2 | 1.76 | 0.66 |
| 1:A:670:ILE:HG23 | 1:A:695:TYR:O | 1.96 | 0.66 |
| 2:D:38:ARG:HG3 | 2:D:92:ALA:HB3 | 1.76 | 0.66 |
| 2:E:20:LEU:HD12 | 2:E:21:SER:H | 1.59 | 0.66 |
| 1:B:670:ILE:HG23 | 1:B:695:TYR:O | 1.96 | 0.66 |
| 2:E:67:ARG:HB2 | 2:E:84:ASN:O | 1.96 | 0.66 |
| 1:A:765:ARG:NE | 1:C:957:GLN:NE2 | 2.44 | 0.65 |
| 2:D:109:ASN:HA | 2:D:111:TRP:HZ3 | 1.58 | 0.65 |
| 1:B:1094:VAL:N | 1:B:1105:THR:O | 2.25 | 0.65 |
| 1:A:897:PRO:HD2 | 1:A:900:MET:HG3 | 1.79 | 0.65 |
| 1:B:376:THR:HG23 | 2:E:106:TYR:CG | 2.32 | 0.65 |
| 1:B:309:GLU:O | 1:B:313:TYR:OH | 2.11 | 0.65 |
| 1:B:475:ALA:HB2 | 1:B:489:TYR:HE2 | 1.62 | 0.65 |
| 2:D:95:TYR:CD2 | 2:D:114:GLY:HA3 | 2.31 | 0.65 |
| 1:B:390:LEU:HD11 | 1:C:983:ARG:HG2 | 1.78 | 0.64 |
| 1:C:699:LEU:HD13 | 1:C:699:LEU:HD21 | 1.64 | 0.64 |
| 2:D:37:PHE:CZ | 2:D:95:TYR:HD1 | 2.15 | 0.64 |
| 2:E:37:PHE:CZ | 2:E:95:TYR:HD1 | 2.15 | 0.64 |
| 2:E:95:TYR:CD2 | 2:E:114:GLY:HA3 | 2.31 | 0.64 |
| 1:B:367:VAL:HG23 | 1:B:368:LEU:HD12 | 1.78 | 0.64 |
| 1:A:703:ASN:OD1 | 1:B:787:GLN:HB3 | 1.97 | 0.64 |
| 1:B:323:THR:OG1 | 1:B:324:GLU:OE1 | 2.08 | 0.64 |
| 1:C:670:ILE:HG23 | 1:C:695:TYR:O | 1.96 | 0.64 |
| 1:C:578:ASP:OD1 | 1:C:583:GLU:N | 2.31 | 0.64 |
| 1:A:377:PHE:CD1 | 1:A:434:ILE:HD12 | 2.32 | 0.64 |
| 1:B:61:ASN:HD21 | 4:B:1307:NAG:C1 | 2.11 | 0.64 |
| 1:B:699:LEU:CD2 | 1:B:699:LEU:HD11 | 2.16 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:177:MET:HG3 | 1:A:179:LEU:HD12 | 1.79 | 0.64 |
| 1:A:1119:ASN:OD1 | 1:A:1119:ASN:O | 2.16 | 0.64 |
| 1:B:177:MET:HG3 | 1:B:179:LEU:HD12 | 1.79 | 0.64 |
| 1:C:177:MET:HG3 | 1:C:179:LEU:HD12 | 1.78 | 0.64 |
| 1:C:1119:ASN:OD1 | 1:C:1119:ASN:O | 2.16 | 0.64 |
| 1:A:309:GLU:O | 1:A:313:TYR:OH | 2.11 | 0.64 |
| 1:A:578:ASP:OD1 | 1:A:583:GLU:N | 2.30 | 0.64 |
| 1:B:1010:GLN:OE1 | 1:C:1012:LEU:HD11 | 1.98 | 0.64 |
| 1:C:377:PHE:CD1 | 1:C:434:ILE:HD12 | 2.32 | 0.64 |
| 1:A:917:TYR:HB3 | 1:C:1129:VAL:HG13 | 1.80 | 0.64 |
| 1:B:61:ASN:HD22 | 4:B:1307:NAG:C7 | 2.10 | 0.63 |
| 2:D:101:TYR:HD1 | 2:D:103:ALA:H | 1.47 | 0.63 |
| 1:B:897:PRO:HD2 | 1:B:900:MET:HG3 | 1.79 | 0.63 |
| 1:C:478:THR:HG23 | 1:C:479:PRO:HD2 | 1.81 | 0.63 |
| 2:E:65:LYS:HD3 | 2:E:66:GLY:N | 2.13 | 0.63 |
| 2:D:22:CYS:HB2 | 2:D:36:TRP:CZ2 | 2.34 | 0.63 |
| 2:E:109:ASN:HA | 2:E:111:TRP:CE3 | 2.33 | 0.63 |
| 2:D:35:ALA:HB2 | 2:D:50:VAL:HG13 | 1.80 | 0.63 |
| 1:A:76:THR:OG1 | 1:A:77:LYS:N | 2.32 | 0.63 |
| 1:C:897:PRO:HD2 | 1:C:900:MET:HG3 | 1.79 | 0.63 |
| 2:D:109:ASN:HA | 2:D:111:TRP:CE3 | 2.33 | 0.63 |
| 1:B:22:THR:OG1 | 1:B:76:THR:HA | 1.99 | 0.63 |
| 1:C:46:SER:N | 1:C:280:ASN:O | 2.32 | 0.63 |
| 1:A:611:LEU:HD22 | 1:A:666:ILE:HG23 | 1.81 | 0.62 |
| 1:B:61:ASN:ND2 | 4:B:1307:NAG:C7 | 2.62 | 0.62 |
| 1:B:699:LEU:HB3 | 1:C:788:ILE:CG1 | 2.28 | 0.62 |
| 1:B:1119:ASN:OD1 | 1:B:1119:ASN:O | 2.16 | 0.62 |
| 2:D:65:LYS:HD3 | 2:D:66:GLY:N | 2.14 | 0.62 |
| 2:E:60:TYR:HE2 | 2:E:68:PHE:CB | 2.12 | 0.62 |
| 2:E:101:TYR:HD1 | 2:E:103:ALA:H | 1.47 | 0.62 |
| 2:D:60:TYR:HE2 | 2:D:68:PHE:CB | 2.12 | 0.62 |
| 2:E:35:ALA:HB2 | 2:E:50:VAL:HG13 | 1.80 | 0.62 |
| 1:A:22:THR:OG1 | 1:A:76:THR:HA | 1.99 | 0.62 |
| 1:B:46:SER:N | 1:B:280:ASN:O | 2.32 | 0.62 |
| 1:B:699:LEU:HD13 | 1:B:699:LEU:HD21 | 1.65 | 0.62 |
| 1:B:472:ILE:HG23 | 1:B:489:TYR:C | 2.21 | 0.61 |
| 1:B:886:TRP:HZ3 | 1:B:905:ARG:CD | 2.13 | 0.61 |
| 1:C:280:ASN:OD1 | 1:C:282:ASN:OD1 | 2.18 | 0.61 |
| 1:C:309:GLU:O | 1:C:313:TYR:OH | 2.11 | 0.61 |
| 2:E:83:MET:CB | 2:E:86:LEU:HD21 | 2.29 | 0.61 |
| 1:A:280:ASN:OD1 | 1:A:282:ASN:OD1 | 2.18 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:46:SER:N | 1:A:280:ASN:O | 2.32 | 0.61 |
| 1:A:917:TYR:CE1 | 1:C:1079:PRO:HB3 | 2.36 | 0.61 |
| 1:B:770:ILE:HG21 | 1:B:770:ILE:CD1 | 2.30 | 0.61 |
| 4:B:1304:NAG:H3 | 4:B:1304:NAG:C8 | 2.29 | 0.61 |
| 1:C:924:ALA:O | 1:C:928:ASN:OD1 | 2.18 | 0.61 |
| 2:E:22:CYS:HB2 | 2:E:36:TRP:CZ2 | 2.34 | 0.61 |
| 1:A:770:ILE:HG21 | 1:A:770:ILE:CD1 | 2.30 | 0.61 |
| 1:C:22:THR:OG1 | 1:C:76:THR:HA | 1.99 | 0.61 |
| 2:D:83:MET:CB | 2:D:86:LEU:HD21 | 2.29 | 0.61 |
| 2:D:40:ALA:HB1 | 2:D:41:PRO:HD2 | 1.83 | 0.61 |
| 1:B:611:LEU:HD22 | 1:B:666:ILE:HG23 | 1.81 | 0.61 |
| 1:C:611:LEU:HD22 | 1:C:666:ILE:HG23 | 1.81 | 0.61 |
| 1:C:886:TRP:HE3 | 1:C:905:ARG:HH21 | 1.49 | 0.61 |
| 2:E:40:ALA:HB1 | 2:E:41:PRO:HD2 | 1.83 | 0.60 |
| 1:A:886:TRP:HZ3 | 1:A:905:ARG:CD | 2.14 | 0.60 |
| 1:A:924:ALA:O | 1:A:928:ASN:OD1 | 2.18 | 0.60 |
| 1:A:1030:SER:O | 1:C:1040:VAL:CG1 | 2.49 | 0.60 |
| 1:B:280:ASN:OD1 | 1:B:282:ASN:OD1 | 2.18 | 0.60 |
| 1:B:1017:GLU:OE1 | 1:C:1019:ARG:NH2 | 2.34 | 0.60 |
| 2:E:93:LEU:HB3 | 2:E:95:TYR:OH | 2.02 | 0.60 |
| 1:B:76:THR:OG1 | 1:B:77:LYS:N | 2.32 | 0.60 |
| 1:B:924:ALA:O | 1:B:928:ASN:OD1 | 2.18 | 0.60 |
| 2:D:93:LEU:HB3 | 2:D:95:TYR:OH | 2.02 | 0.60 |
| 2:E:4:LEU:HD21 | 2:E:98:SER:OG | 2.02 | 0.60 |
| 1:A:42:VAL:HG22 | 1:C:565:PHE:CZ | 2.37 | 0.60 |
| 1:A:886:TRP:HE3 | 1:A:905:ARG:HH21 | 1.49 | 0.60 |
| 1:B:1126:CYS:CB | 1:B:1132:ILE:HD13 | 2.31 | 0.60 |
| 1:B:376:THR:CB | 2:E:106:TYR:HB2 | 2.32 | 0.60 |
| 1:B:740:MET:O | 1:B:744:GLY:N | 2.35 | 0.60 |
| 1:B:886:TRP:HE3 | 1:B:905:ARG:HH21 | 1.49 | 0.60 |
| 1:C:616:ASN:HD21 | 4:C:1304:NAG:H2 | 1.66 | 0.60 |
| 1:A:658:ASN:OD1 | 1:A:660:TYR:CD1 | 2.55 | 0.59 |
| 1:A:740:MET:O | 1:A:744:GLY:N | 2.35 | 0.59 |
| 1:C:770:ILE:HG21 | 1:C:770:ILE:CD1 | 2.30 | 0.59 |
| 2:D:4:LEU:HD21 | 2:D:98:SER:OG | 2.02 | 0.59 |
| 2:D:19:ARG:CD | 2:D:80:TYR:CD1 | 2.86 | 0.59 |
| 1:A:872:GLN:OE1 | 1:C:699:LEU:HG | 2.02 | 0.59 |
| 1:B:190:ARG:HH11 | 1:B:207:HIS:CE1 | 2.20 | 0.59 |
| 1:C:76:THR:OG1 | 1:C:77:LYS:N | 2.32 | 0.59 |
| 1:C:740:MET:O | 1:C:744:GLY:N | 2.35 | 0.59 |
| 1:A:914:ASN:ND2 | 1:C:1123:SER:OG | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:665:PRO:HB2 | 1:C:864:LEU:HD22 | 1.84 | 0.59 |
| 1:B:1089:PHE:CE1 | 1:C:914:ASN:HB3 | 2.37 | 0.59 |
| 1:C:86:PHE:N | 1:C:236:THR:O | 2.36 | 0.59 |
| 1:C:1126:CYS:CB | 1:C:1132:ILE:HD13 | 2.31 | 0.59 |
| 4:C:1306:NAG:C1 | 4:C:1306:NAG:O7 | 2.49 | 0.59 |
| 2:D:58:THR:HG21 | 2:D:70:ILE:HG22 | 1.84 | 0.59 |
| 2:E:21:SER:HB2 | 2:E:80:TYR:CE1 | 2.37 | 0.59 |
| 1:A:855:PHE:HD1 | 1:C:589:PRO:HG2 | 1.68 | 0.59 |
| 1:A:110:LEU:O | 1:A:135:PHE:HB2 | 2.02 | 0.59 |
| 1:A:895:GLN:O | 1:C:712:ILE:HA | 2.02 | 0.59 |
| 1:C:190:ARG:HH11 | 1:C:207:HIS:CE1 | 2.20 | 0.59 |
| 1:C:658:ASN:OD1 | 1:C:660:TYR:CD1 | 2.55 | 0.59 |
| 2:D:38:ARG:NH2 | 2:D:46:GLU:HB3 | 2.18 | 0.59 |
| 1:B:658:ASN:OD1 | 1:B:660:TYR:CD1 | 2.55 | 0.59 |
| 2:D:2:VAL:HG23 | 2:D:110:ASN:ND2 | 2.18 | 0.59 |
| 1:A:1126:CYS:CB | 1:A:1132:ILE:HD13 | 2.32 | 0.59 |
| 1:B:922:LEU:CD2 | 4:B:1310:NAG:H5 | 2.32 | 0.59 |
| 2:D:12:VAL:HG21 | 2:D:86:LEU:CD1 | 2.33 | 0.59 |
| 2:D:18:LEU:HB2 | 2:D:83:MET:HE2 | 1.84 | 0.59 |
| 2:D:21:SER:HB2 | 2:D:80:TYR:CE1 | 2.37 | 0.59 |
| 2:E:12:VAL:HG21 | 2:E:86:LEU:CD1 | 2.33 | 0.59 |
| 2:E:19:ARG:CD | 2:E:80:TYR:CD1 | 2.86 | 0.59 |
| 1:C:110:LEU:O | 1:C:135:PHE:HB2 | 2.02 | 0.59 |
| 1:C:868:GLU:N | 1:C:868:GLU:OE1 | 2.36 | 0.59 |
| 2:E:38:ARG:HG3 | 2:E:94:TYR:CE2 | 2.38 | 0.59 |
| 2:E:64:VAL:HA | 2:E:67:ARG:NE | 2.12 | 0.59 |
| 1:B:318:PHE:C | 1:B:318:PHE:CD2 | 2.77 | 0.58 |
| 1:C:709:ASN:ND2 | 4:C:1306:NAG:O7 | 2.35 | 0.58 |
| 2:D:20:LEU:O | 2:D:80:TYR:HD1 | 1.86 | 0.58 |
| 1:A:603:ASN:ND2 | 4:A:1306:NAG:C1 | 2.66 | 0.58 |
| 1:B:110:LEU:O | 1:B:135:PHE:HB2 | 2.02 | 0.58 |
| 1:B:1106:GLN:OE1 | 1:B:1109:PHE:HB3 | 2.04 | 0.58 |
| 2:E:58:THR:HG21 | 2:E:70:ILE:HG22 | 1.84 | 0.58 |
| 1:A:190:ARG:HH11 | 1:A:207:HIS:CE1 | 2.20 | 0.58 |
| 1:A:868:GLU:N | 1:A:868:GLU:OE1 | 2.36 | 0.58 |
| 1:C:318:PHE:C | 1:C:318:PHE:CD2 | 2.77 | 0.58 |
| 2:D:19:ARG:HD2 | 2:D:80:TYR:CE1 | 2.38 | 0.58 |
| 2:E:37:PHE:CZ | 2:E:95:TYR:CD1 | 2.91 | 0.58 |
| 1:A:64:TRP:CE2 | 1:A:66:HIS:CE1 | 2.92 | 0.58 |
| 1:A:817:PHE:C | 1:A:817:PHE:CD2 | 2.77 | 0.58 |
| 1:A:133:PHE:CD1 | 1:A:160:TYR:CD2 | 2.92 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:770:ILE:CG2 | 1:A:770:ILE:CD1 | 2.76 | 0.58 |
| 2:D:38:ARG:HG3 | 2:D:94:TYR:CE2 | 2.38 | 0.58 |
| 2:E:20:LEU:O | 2:E:80:TYR:HD1 | 1.86 | 0.58 |
| 1:A:269:TYR:O | 1:A:271:GLN:OE1 | 2.22 | 0.58 |
| 1:A:318:PHE:C | 1:A:318:PHE:CD2 | 2.77 | 0.58 |
| 1:B:376:THR:HB | 1:B:435:ALA:N | 2.17 | 0.58 |
| 1:C:43:PHE:HE1 | 1:C:283:GLY:HA2 | 1.69 | 0.58 |
| 1:B:43:PHE:HE1 | 1:B:283:GLY:HA2 | 1.68 | 0.58 |
| 1:B:589:PRO:HG2 | 1:C:855:PHE:HD1 | 1.69 | 0.58 |
| 1:C:817:PHE:HA | 1:C:820:ASP:OD2 | 2.04 | 0.58 |
| 1:A:589:PRO:CG | 1:B:855:PHE:HD1 | 2.16 | 0.58 |
| 1:A:997:ILE:O | 1:A:1001:LEU:HB2 | 2.04 | 0.58 |
| 1:B:64:TRP:CE2 | 1:B:66:HIS:CE1 | 2.92 | 0.58 |
| 1:B:868:GLU:N | 1:B:868:GLU:OE1 | 2.36 | 0.58 |
| 1:C:133:PHE:CD1 | 1:C:160:TYR:CD2 | 2.92 | 0.58 |
| 1:C:314:GLN:OE1 | 1:C:595:VAL:O | 2.22 | 0.58 |
| 2:D:65:LYS:HD3 | 2:D:66:GLY:H | 1.69 | 0.58 |
| 1:A:86:PHE:N | 1:A:236:THR:O | 2.36 | 0.58 |
| 1:B:269:TYR:O | 1:B:271:GLN:OE1 | 2.22 | 0.58 |
| 1:B:668:ALA:C | 1:C:866:THR:HG23 | 2.24 | 0.58 |
| 1:B:997:ILE:O | 1:B:1001:LEU:HB2 | 2.04 | 0.58 |
| 1:C:817:PHE:C | 1:C:817:PHE:CD2 | 2.77 | 0.58 |
| 1:C:886:TRP:HZ3 | 1:C:905:ARG:CD | 2.13 | 0.58 |
| 1:B:725:GLU:OE1 | 1:B:1028:LYS:HE3 | 2.04 | 0.58 |
| 1:B:817:PHE:C | 1:B:817:PHE:CD2 | 2.77 | 0.58 |
| 2:E:2:VAL:HG23 | 2:E:110:ASN:ND2 | 2.18 | 0.58 |
| 1:C:269:TYR:O | 1:C:271:GLN:OE1 | 2.22 | 0.57 |
| 1:C:997:ILE:O | 1:C:1001:LEU:HB2 | 2.04 | 0.57 |
| 2:D:20:LEU:HG | 2:D:36:TRP:CH2 | 2.39 | 0.57 |
| 2:E:38:ARG:NH2 | 2:E:46:GLU:HB3 | 2.18 | 0.57 |
| 1:A:314:GLN:OE1 | 1:A:595:VAL:O | 2.22 | 0.57 |
| 1:A:705:VAL:HG23 | 1:B:789:TYR:HD1 | 1.68 | 0.57 |
| 1:A:817:PHE:HA | 1:A:820:ASP:OD2 | 2.04 | 0.57 |
| 1:B:133:PHE:CD1 | 1:B:160:TYR:CD2 | 2.92 | 0.57 |
| 1:C:64:TRP:CE2 | 1:C:66:HIS:CE1 | 2.92 | 0.57 |
| 2:E:65:LYS:HD3 | 2:E:66:GLY:H | 1.69 | 0.57 |
| 1:A:748:GLU:HA | 1:A:751:ASN:OD1 | 2.04 | 0.57 |
| 1:C:568:ASP:OD1 | 1:C:569:ILE:N | 2.35 | 0.57 |
| 2:D:64:VAL:HA | 2:D:67:ARG:NE | 2.12 | 0.57 |
| 2:E:20:LEU:HG | 2:E:36:TRP:CH2 | 2.39 | 0.57 |
| 1:A:725:GLU:OE1 | 1:A:1028:LYS:HE3 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:86:PHE:N | 1:B:236:THR:O | 2.36 | 0.57 |
| 2:D:37:PHE:CZ | 2:D:95:TYR:CD1 | 2.91 | 0.57 |
| 1:A:568:ASP:OD1 | 1:A:569:ILE:N | 2.34 | 0.57 |
| 1:A:883:THR:HG22 | 1:C:707:TYR:HB2 | 1.86 | 0.57 |
| 1:B:206:LYS:HD2 | 1:B:223:LEU:HA | 1.87 | 0.57 |
| 1:A:43:PHE:HE1 | 1:A:283:GLY:CA | 2.18 | 0.57 |
| 1:B:817:PHE:HA | 1:B:820:ASP:OD2 | 2.04 | 0.57 |
| 1:B:915:VAL:O | 1:B:919:ASN:HB3 | 2.05 | 0.57 |
| 1:C:748:GLU:HA | 1:C:751:ASN:OD1 | 2.04 | 0.57 |
| 1:C:725:GLU:OE1 | 1:C:1028:LYS:HE3 | 2.04 | 0.57 |
| 1:A:43:PHE:HE1 | 1:A:283:GLY:HA2 | 1.68 | 0.57 |
| 1:B:748:GLU:HA | 1:B:751:ASN:OD1 | 2.04 | 0.57 |
| 1:B:1104:VAL:CG1 | 1:B:1119:ASN:HD21 | 2.18 | 0.57 |
| 1:C:1106:GLN:OE1 | 1:C:1109:PHE:HB3 | 2.03 | 0.57 |
| 1:B:43:PHE:HE1 | 1:B:283:GLY:CA | 2.18 | 0.57 |
| 1:B:314:GLN:OE1 | 1:B:595:VAL:O | 2.22 | 0.57 |
| 1:C:332:ILE:O | 1:C:332:ILE:HG23 | 2.05 | 0.57 |
| 1:C:1104:VAL:CG1 | 1:C:1119:ASN:HD21 | 2.18 | 0.57 |
| 2:E:19:ARG:HD2 | 2:E:80:TYR:CE1 | 2.38 | 0.57 |
| 1:A:406:GLU:N | 1:A:406:GLU:OE1 | 2.39 | 0.56 |
| 1:A:1104:VAL:CG1 | 1:A:1119:ASN:HD21 | 2.18 | 0.56 |
| 1:B:378:LYS:HE2 | 1:B:380:TYR:CE2 | 2.40 | 0.56 |
| 4:B:1307:NAG:O7 | 4:B:1307:NAG:H3 | 2.03 | 0.56 |
| 1:C:43:PHE:HE1 | 1:C:283:GLY:CA | 2.18 | 0.56 |
| 1:C:310:LYS:HG2 | 1:C:600:PRO:HA | 1.87 | 0.56 |
| 1:C:527:PRO:O | 1:C:528:LYS:HG3 | 2.05 | 0.56 |
| 1:A:206:LYS:HD2 | 1:A:223:LEU:HA | 1.87 | 0.56 |
| 1:A:597:VAL:HG13 | 1:A:608:VAL:CG1 | 2.36 | 0.56 |
| 1:A:915:VAL:O | 1:A:919:ASN:HB3 | 2.05 | 0.56 |
| 1:A:1106:GLN:OE1 | 1:A:1109:PHE:HB3 | 2.03 | 0.56 |
| 1:B:141:LEU:HD23 | 1:B:157:PHE:HA | 1.88 | 0.56 |
| 1:B:1094:VAL:HG11 | 1:C:904:TYR:OH | 2.05 | 0.56 |
| 1:C:736:VAL:HG22 | 1:C:858:LEU:HD23 | 1.88 | 0.56 |
| 2:E:38:ARG:HG2 | 2:E:39:GLN:N | 2.21 | 0.56 |
| 1:A:332:ILE:HD12 | 1:A:527:PRO:HA | 1.88 | 0.56 |
| 1:B:43:PHE:CD1 | 1:B:44:ARG:N | 2.73 | 0.56 |
| 1:C:802:PHE:HB3 | 1:C:805:ILE:CG1 | 2.36 | 0.56 |
| 2:E:58:THR:HG21 | 2:E:70:ILE:CG2 | 2.36 | 0.56 |
| 1:A:318:PHE:HD2 | 1:A:318:PHE:C | 2.09 | 0.56 |
| 1:A:736:VAL:HG22 | 1:A:858:LEU:HD23 | 1.87 | 0.56 |
| 2:D:58:THR:HG21 | 2:D:70:ILE:CG2 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:802:PHE:HB3 | 1:B:805:ILE:CG1 | 2.36 | 0.56 |
| 2:D:38:ARG:HG2 | 2:D:39:GLN:N | 2.21 | 0.56 |
| 2:E:18:LEU:HB2 | 2:E:83:MET:HE2 | 1.86 | 0.56 |
| 1:A:966:LEU:HD12 | 1:A:1000:ARG:NE | 2.21 | 0.56 |
| 1:B:87:ASN:OD1 | 1:B:269:TYR:CE2 | 2.59 | 0.56 |
| 1:B:200:TYR:CD2 | 1:B:228:ASP:OD2 | 2.59 | 0.56 |
| 1:C:206:LYS:HD2 | 1:C:223:LEU:HA | 1.87 | 0.56 |
| 1:B:210:ILE:HG21 | 1:B:212:LEU:HD23 | 1.88 | 0.56 |
| 1:C:87:ASN:OD1 | 1:C:269:TYR:CE2 | 2.59 | 0.56 |
| 1:C:802:PHE:HB3 | 1:C:805:ILE:HG12 | 1.88 | 0.56 |
| 1:A:457:ARG:NH1 | 1:A:459[A]:SER:O | 2.39 | 0.56 |
| 1:B:318:PHE:HD2 | 1:B:318:PHE:C | 2.09 | 0.56 |
| 1:B:331:ASN:HB2 | 4:B:1305:NAG:C1 | 2.36 | 0.56 |
| 1:B:372:ALA:CA | 2:E:47:ARG:HH12 | 2.18 | 0.56 |
| 1:B:391:CYS:HB2 | 1:B:525:CYS:HA | 1.87 | 0.56 |
| 1:B:524:VAL:O | 1:B:524:VAL:HG13 | 2.06 | 0.56 |
| 1:C:597:VAL:HG13 | 1:C:608:VAL:CG1 | 2.36 | 0.56 |
| 1:C:915:VAL:O | 1:C:919:ASN:HB3 | 2.05 | 0.56 |
| 2:D:83:MET:SD | 2:D:83:MET:N | 2.79 | 0.56 |
| 1:A:802:PHE:HB3 | 1:A:805:ILE:CG1 | 2.36 | 0.56 |
| 1:C:43:PHE:CD1 | 1:C:44:ARG:N | 2.73 | 0.56 |
| 1:C:318:PHE:HD2 | 1:C:318:PHE:C | 2.09 | 0.56 |
| 1:C:966:LEU:HD12 | 1:C:1000:ARG:NE | 2.21 | 0.56 |
| 1:A:87:ASN:OD1 | 1:A:269:TYR:CE2 | 2.59 | 0.55 |
| 1:B:597:VAL:HG13 | 1:B:608:VAL:CG1 | 2.36 | 0.55 |
| 1:C:141:LEU:HD23 | 1:C:157:PHE:HA | 1.87 | 0.55 |
| 1:C:200:TYR:CD2 | 1:C:228:ASP:OD2 | 2.59 | 0.55 |
| 1:C:406:GLU:OE1 | 1:C:406:GLU:N | 2.38 | 0.55 |
| 1:C:484:GLU:N | 1:C:484:GLU:OE1 | 2.38 | 0.55 |
| 1:A:200:TYR:CD2 | 1:A:228:ASP:OD2 | 2.59 | 0.55 |
| 1:A:699:LEU:HD13 | 1:A:699:LEU:HD21 | 1.65 | 0.55 |
| 1:A:802:PHE:HB3 | 1:A:805:ILE:HG12 | 1.88 | 0.55 |
| 1:A:865:LEU:HD22 | 1:A:869:MET:HG3 | 1.89 | 0.55 |
| 1:B:802:PHE:HB3 | 1:B:805:ILE:HG12 | 1.88 | 0.55 |
| 1:C:210:ILE:HG21 | 1:C:212:LEU:HD23 | 1.88 | 0.55 |
| 1:A:43:PHE:CD1 | 1:A:44:ARG:N | 2.73 | 0.55 |
| 1:A:457:ARG:NH1 | 1:A:459[B]:SER:O | 2.39 | 0.55 |
| 1:B:310:LYS:HG2 | 1:B:600:PRO:HA | 1.87 | 0.55 |
| 1:A:141:LEU:HD23 | 1:A:157:PHE:HA | 1.88 | 0.55 |
| 1:A:711:SER:OG | 1:B:895:GLN:NE2 | 2.31 | 0.55 |
| 1:B:966:LEU:HD12 | 1:B:1000:ARG:NE | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1080:ALA:HB2 | 1:B:1089:PHE:HE2 | 1.70 | 0.55 |
| 1:B:736:VAL:HG22 | 1:B:858:LEU:HD23 | 1.87 | 0.55 |
| 1:C:29:THR:HG21 | 1:C:216:LEU:HD12 | 1.88 | 0.55 |
| 2:E:83:MET:SD | 2:E:83:MET:N | 2.79 | 0.55 |
| 1:A:118:LEU:HD13 | 1:A:120:VAL:HG23 | 1.89 | 0.55 |
| 1:B:376:THR:CA | 2:E:106:TYR:HB2 | 2.37 | 0.55 |
| 1:B:665:PRO:HB3 | 1:C:864:LEU:HD21 | 1.89 | 0.55 |
| 1:C:327:VAL:HG12 | 1:C:542:ASN:HB3 | 1.88 | 0.55 |
| 1:A:1141:LEU:O | 1:A:1144:GLU:N | 2.39 | 0.55 |
| 1:B:357:ARG:CZ | 1:B:396:TYR:OH | 2.55 | 0.55 |
| 1:C:865:LEU:HD22 | 1:C:869:MET:HG3 | 1.89 | 0.55 |
| 1:C:1141:LEU:O | 1:C:1144:GLU:OE2 | 2.25 | 0.55 |
| 1:A:310:LYS:HG2 | 1:A:600:PRO:HA | 1.87 | 0.55 |
| 1:B:29:THR:HG21 | 1:B:216:LEU:HD12 | 1.88 | 0.55 |
| 1:B:378:LYS:HD2 | 2:E:106:TYR:CE2 | 2.40 | 0.55 |
| 1:C:190:ARG:HD3 | 1:C:207:HIS:CE1 | 2.42 | 0.55 |
| 1:A:193:VAL:HG23 | 1:A:223:LEU:HD12 | 1.89 | 0.55 |
| 1:A:894:LEU:HD22 | 1:C:713:ALA:CB | 2.37 | 0.55 |
| 1:B:61:ASN:ND2 | 4:B:1307:NAG:C1 | 2.69 | 0.55 |
| 1:B:865:LEU:HD22 | 1:B:869:MET:HG3 | 1.89 | 0.54 |
| 1:A:855:PHE:CD1 | 1:C:589:PRO:HG2 | 2.41 | 0.54 |
| 1:A:1141:LEU:C | 1:A:1144:GLU:OE2 | 2.46 | 0.54 |
| 1:C:925:ASN:HA | 1:C:928:ASN:OD1 | 2.08 | 0.54 |
| 1:A:280:ASN:HB2 | 1:A:286:THR:HG21 | 1.89 | 0.54 |
| 1:A:1141:LEU:O | 1:A:1144:GLU:OE2 | 2.25 | 0.54 |
| 1:B:1141:LEU:C | 1:B:1144:GLU:OE2 | 2.46 | 0.54 |
| 1:B:1141:LEU:O | 1:B:1144:GLU:OE2 | 2.25 | 0.54 |
| 1:C:117:LEU:CD1 | 1:C:130:VAL:HG22 | 2.36 | 0.54 |
| 1:C:193:VAL:HG23 | 1:C:223:LEU:HD12 | 1.90 | 0.54 |
| 1:C:1141:LEU:C | 1:C:1144:GLU:OE2 | 2.46 | 0.54 |
| 1:A:29:THR:HG21 | 1:A:216:LEU:HD12 | 1.88 | 0.54 |
| 1:C:1141:LEU:O | 1:C:1144:GLU:N | 2.39 | 0.54 |
| 1:B:922:LEU:CD1 | 4:B:1310:NAG:H5 | 2.38 | 0.54 |
| 1:C:118:LEU:HD13 | 1:C:120:VAL:HG23 | 1.89 | 0.54 |
| 1:A:190:ARG:HD3 | 1:A:207:HIS:CE1 | 2.42 | 0.54 |
| 1:A:274:THR:OG1 | 1:A:291:CYS:HB2 | 2.08 | 0.54 |
| 1:B:118:LEU:HD13 | 1:B:120:VAL:HG23 | 1.89 | 0.54 |
| 1:B:274:THR:OG1 | 1:B:291:CYS:HB2 | 2.08 | 0.54 |
| 1:B:770:ILE:CG1 | 1:B:770:ILE:HG23 | 1.97 | 0.54 |
| 1:A:958:ALA:O | 1:A:961:THR:OG1 | 2.22 | 0.54 |
| 1:B:756:TYR:O | 1:B:756:TYR:CD1 | 2.61 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:770:ILE:CG2 | 1:B:770:ILE:CD1 | 2.76 | 0.54 |
| 1:B:280:ASN:HB2 | 1:B:286:THR:HG21 | 1.89 | 0.54 |
| 1:B:925:ASN:HA | 1:B:928:ASN:OD1 | 2.08 | 0.54 |
| 1:C:756:TYR:O | 1:C:756:TYR:CD1 | 2.61 | 0.54 |
| 1:A:210:ILE:HG21 | 1:A:212:LEU:HD23 | 1.88 | 0.54 |
| 1:A:925:ASN:HA | 1:A:928:ASN:OD1 | 2.08 | 0.53 |
| 1:B:190:ARG:HD3 | 1:B:207:HIS:CE1 | 2.42 | 0.53 |
| 1:B:1111:GLU:O | 1:B:1111:GLU:HG2 | 2.08 | 0.53 |
| 1:C:280:ASN:HB2 | 1:C:286:THR:HG21 | 1.89 | 0.53 |
| 1:A:657:ASN:CB | 4:A:1309:NAG:O5 | 2.56 | 0.53 |
| 1:B:376:THR:CG2 | 2:E:106:TYR:CG | 2.91 | 0.53 |
| 1:B:748:GLU:OE2 | 1:B:748:GLU:N | 2.29 | 0.53 |
| 1:B:979:ASP:OD2 | 1:B:980:ILE:N | 2.42 | 0.53 |
| 1:A:705:VAL:CG2 | 1:B:789:TYR:CD1 | 2.91 | 0.53 |
| 1:A:979:ASP:OD2 | 1:A:980:ILE:N | 2.42 | 0.53 |
| 1:B:193:VAL:HG23 | 1:B:223:LEU:HD12 | 1.89 | 0.53 |
| 1:B:465:GLU:OE1 | 3:J:1:NAG:C8 | 2.56 | 0.53 |
| 1:C:616:ASN:HD21 | 4:C:1304:NAG:C1 | 2.22 | 0.53 |
| 2:E:60:TYR:OH | 2:E:70:ILE:N | 2.41 | 0.53 |
| 1:A:756:TYR:CD1 | 1:A:756:TYR:O | 2.61 | 0.53 |
| 1:C:979:ASP:OD2 | 1:C:980:ILE:N | 2.42 | 0.53 |
| 2:D:60:TYR:OH | 2:D:70:ILE:N | 2.42 | 0.53 |
| 1:A:153:MET:HA | 1:A:179:LEU:HD22 | 1.91 | 0.53 |
| 1:A:792:PRO:HG3 | 1:C:707:TYR:HB3 | 1.90 | 0.53 |
| 1:A:954:GLN:HG2 | 1:A:1014:ARG:CZ | 2.39 | 0.53 |
| 1:A:1111:GLU:O | 1:A:1111:GLU:HG2 | 2.08 | 0.53 |
| 1:C:274:THR:OG1 | 1:C:291:CYS:HB2 | 2.08 | 0.53 |
| 1:B:190:ARG:NH1 | 1:B:207:HIS:HE1 | 2.07 | 0.53 |
| 1:B:452:LEU:HD12 | 1:B:493:GLN:O | 2.08 | 0.53 |
| 1:B:922:LEU:HD21 | 4:B:1310:NAG:H5 | 1.91 | 0.53 |
| 1:C:331:ASN:ND2 | 1:C:580:GLN:O | 2.42 | 0.53 |
| 2:E:60:TYR:HE2 | 2:E:68:PHE:HB2 | 1.73 | 0.53 |
| 1:A:117:LEU:CD1 | 1:A:130:VAL:HG22 | 2.36 | 0.53 |
| 1:A:159:VAL:HG23 | 1:A:160:TYR:HB3 | 1.91 | 0.53 |
| 1:B:1062:PHE:CB | 1:B:1064:HIS:HE2 | 2.21 | 0.53 |
| 1:C:905:ARG:HH12 | 1:C:1050:MET:HB3 | 1.72 | 0.53 |
| 1:A:892:ALA:HB3 | 1:C:1072:GLU:OE2 | 2.06 | 0.53 |
| 1:C:1074:ASN:O | 1:C:1075:PHE:CG | 2.62 | 0.53 |
| 1:A:892:ALA:HB1 | 1:C:1072:GLU:OE2 | 2.08 | 0.53 |
| 1:C:159:VAL:HG23 | 1:C:160:TYR:HB3 | 1.91 | 0.53 |
| 1:C:1097:SER:HA | 1:C:1101:HIS:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:65:LYS:HA | 2:D:65:LYS:CE | 2.38 | 0.53 |
| 1:A:770:ILE:HG23 | 1:A:770:ILE:C | 2.29 | 0.53 |
| 1:A:1097:SER:HA | 1:A:1101:HIS:O | 2.09 | 0.53 |
| 1:B:954:GLN:HG2 | 1:B:1014:ARG:CZ | 2.39 | 0.53 |
| 2:D:36:TRP:O | 2:D:48:VAL:HG22 | 2.10 | 0.53 |
| 1:A:190:ARG:NH1 | 1:A:207:HIS:HE1 | 2.07 | 0.52 |
| 1:A:224:GLU:N | 1:A:224:GLU:OE1 | 2.42 | 0.52 |
| 1:A:765:ARG:CZ | 1:C:957:GLN:HE21 | 2.22 | 0.52 |
| 1:A:897:PRO:HD2 | 1:A:900:MET:SD | 2.50 | 0.52 |
| 1:B:1141:LEU:O | 1:B:1144:GLU:N | 2.39 | 0.52 |
| 1:A:708:SER:HB3 | 1:A:711:SER:HB3 | 1.91 | 0.52 |
| 1:A:817:PHE:O | 1:A:821:LEU:HB2 | 2.10 | 0.52 |
| 1:A:897:PRO:HD2 | 1:A:900:MET:CG | 2.38 | 0.52 |
| 1:B:117:LEU:CD1 | 1:B:130:VAL:HG22 | 2.36 | 0.52 |
| 1:B:117:LEU:HD12 | 1:B:129:LYS:O | 2.09 | 0.52 |
| 1:B:224:GLU:N | 1:B:224:GLU:OE1 | 2.42 | 0.52 |
| 1:B:391:CYS:CB | 1:B:525:CYS:HA | 2.39 | 0.52 |
| 1:B:817:PHE:O | 1:B:821:LEU:HB2 | 2.10 | 0.52 |
| 1:B:897:PRO:HD2 | 1:B:900:MET:CG | 2.38 | 0.52 |
| 1:B:969:ASN:OD1 | 1:B:972:ALA:O | 2.27 | 0.52 |
| 1:A:918:GLU:HA | 1:C:1128:VAL:CG2 | 2.40 | 0.52 |
| 1:B:294:ASP:OD2 | 1:B:294:ASP:C | 2.48 | 0.52 |
| 1:B:699:LEU:HD21 | 1:B:699:LEU:HD11 | 1.85 | 0.52 |
| 1:B:1097:SER:HA | 1:B:1101:HIS:O | 2.09 | 0.52 |
| 1:C:190:ARG:NH1 | 1:C:207:HIS:HE1 | 2.07 | 0.52 |
| 1:A:770:ILE:HG22 | 1:A:771:ALA:N | 2.24 | 0.52 |
| 1:A:787:GLN:HB3 | 1:C:703:ASN:OD1 | 2.10 | 0.52 |
| 1:A:869:MET:CB | 1:C:699:LEU:HD11 | 2.40 | 0.52 |
| 1:A:895:GLN:HE21 | 1:C:711:SER:HG | 1.58 | 0.52 |
| 1:B:490:PHE:CE2 | 1:B:492:LEU:HB2 | 2.44 | 0.52 |
| 1:C:897:PRO:HD2 | 1:C:900:MET:CG | 2.38 | 0.52 |
| 2:D:60:TYR:HE2 | 2:D:68:PHE:HB2 | 1.74 | 0.52 |
| 2:E:36:TRP:O | 2:E:48:VAL:HG22 | 2.10 | 0.52 |
| 1:A:117:LEU:HD12 | 1:A:129:LYS:O | 2.10 | 0.52 |
| 1:A:736:VAL:HG22 | 1:A:858:LEU:CD2 | 2.40 | 0.52 |
| 1:A:905:ARG:HH12 | 1:A:1050:MET:HB3 | 1.72 | 0.52 |
| 1:A:1074:ASN:O | 1:A:1075:PHE:CG | 2.62 | 0.52 |
| 1:B:159:VAL:HG23 | 1:B:160:TYR:HB3 | 1.91 | 0.52 |
| 1:B:470:THR:HG22 | 1:B:470:THR:O | 2.09 | 0.52 |
| 1:B:1074:ASN:O | 1:B:1075:PHE:CG | 2.62 | 0.52 |
| 1:C:117:LEU:HD12 | 1:C:129:LYS:O | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:770:ILE:HG22 | 1:C:771:ALA:N | 2.25 | 0.52 |
| 1:C:1111:GLU:O | 1:C:1111:GLU:HG2 | 2.08 | 0.52 |
| 1:B:736:VAL:HG22 | 1:B:858:LEU:CD2 | 2.40 | 0.52 |
| 1:C:224:GLU:N | 1:C:224:GLU:OE1 | 2.42 | 0.52 |
| 1:C:468:ILE:HG22 | 1:C:468:ILE:O | 2.10 | 0.52 |
| 1:C:616:ASN:ND2 | 4:C:1304:NAG:H2 | 2.24 | 0.52 |
| 1:C:736:VAL:HG22 | 1:C:858:LEU:CD2 | 2.40 | 0.52 |
| 1:A:165:ASN:HD21 | 4:A:1302:NAG:C7 | 2.23 | 0.52 |
| 1:B:314:GLN:OE1 | 1:B:314:GLN:HA | 2.09 | 0.52 |
| 1:C:954:GLN:HG2 | 1:C:1014:ARG:CZ | 2.39 | 0.52 |
| 2:E:83:MET:HB3 | 2:E:86:LEU:CD2 | 2.37 | 0.52 |
| 1:B:897:PRO:HD2 | 1:B:900:MET:SD | 2.50 | 0.52 |
| 1:C:817:PHE:O | 1:C:821:LEU:HB2 | 2.10 | 0.52 |
| 1:A:298:GLU:OE2 | 1:A:315:THR:OG1 | 2.26 | 0.52 |
| 1:A:314:GLN:OE1 | 1:A:314:GLN:HA | 2.10 | 0.52 |
| 1:A:327:VAL:HG12 | 1:A:542:ASN:HB3 | 1.92 | 0.52 |
| 1:A:897:PRO:CB | 1:C:709:ASN:O | 2.58 | 0.52 |
| 1:A:1062:PHE:CB | 1:A:1064:HIS:HE2 | 2.21 | 0.52 |
| 1:B:770:ILE:HG22 | 1:B:771:ALA:N | 2.24 | 0.52 |
| 1:C:619:GLU:N | 1:C:619:GLU:OE1 | 2.43 | 0.52 |
| 1:C:718:PHE:CZ | 1:C:919:ASN:ND2 | 2.78 | 0.52 |
| 1:C:897:PRO:HD2 | 1:C:900:MET:SD | 2.50 | 0.52 |
| 2:D:83:MET:HB3 | 2:D:86:LEU:CD2 | 2.37 | 0.52 |
| 1:C:153:MET:HA | 1:C:179:LEU:HD22 | 1.91 | 0.51 |
| 1:C:314:GLN:OE1 | 1:C:314:GLN:HA | 2.09 | 0.51 |
| 1:A:718:PHE:CZ | 1:A:919:ASN:ND2 | 2.78 | 0.51 |
| 1:B:378:LYS:CD | 2:E:106:TYR:CE2 | 2.93 | 0.51 |
| 1:B:392:PHE:CE1 | 1:B:517:LEU:HD11 | 2.45 | 0.51 |
| 1:C:1062:PHE:CB | 1:C:1064:HIS:HE2 | 2.21 | 0.51 |
| 1:A:294:ASP:C | 1:A:294:ASP:OD2 | 2.48 | 0.51 |
| 1:C:969:ASN:OD1 | 1:C:972:ALA:O | 2.27 | 0.51 |
| 1:C:1080:ALA:HB2 | 1:C:1089:PHE:HE2 | 1.70 | 0.51 |
| 1:B:619:GLU:N | 1:B:619:GLU:OE1 | 2.43 | 0.51 |
| 1:A:619:GLU:OE1 | 1:A:619:GLU:N | 2.43 | 0.51 |
| 1:A:817:PHE:C | 1:A:817:PHE:HD2 | 2.14 | 0.51 |
| 1:B:153:MET:HA | 1:B:179:LEU:HD22 | 1.91 | 0.51 |
| 1:B:1072:GLU:HG2 | 1:C:894:LEU:HD21 | 1.93 | 0.51 |
| 2:E:39:GLN:HG2 | 2:E:95:TYR:HE1 | 1.75 | 0.51 |
| 1:A:193:VAL:HG23 | 1:A:223:LEU:CD1 | 2.41 | 0.51 |
| 1:A:1013:ILE:CD1 | 1:C:1013:ILE:HD12 | 2.39 | 0.51 |
| 1:B:718:PHE:CZ | 1:B:919:ASN:ND2 | 2.78 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:817:PHE:C | 1:C:817:PHE:HD2 | 2.14 | 0.51 |
| 2:E:65:LYS:HA | 2:E:65:LYS:CE | 2.38 | 0.51 |
| 1:A:43:PHE:HB3 | 1:C:566:GLY:HA2 | 1.92 | 0.51 |
| 2:D:30:ASN:HB3 | 2:D:100:TYR:CD2 | 2.46 | 0.51 |
| 2:D:82:GLN:OE1 | 2:D:83:MET:N | 2.43 | 0.51 |
| 2:E:82:GLN:OE1 | 2:E:83:MET:N | 2.43 | 0.51 |
| 1:A:468:ILE:HG22 | 1:A:468:ILE:O | 2.10 | 0.51 |
| 1:B:557:LYS:NZ | 1:B:574:ASP:OD2 | 2.43 | 0.51 |
| 1:B:663:ASP:C | 1:B:663:ASP:OD1 | 2.49 | 0.51 |
| 1:C:294:ASP:OD2 | 1:C:294:ASP:C | 2.48 | 0.51 |
| 1:C:617:CYS:O | 1:C:620:VAL:HG22 | 2.11 | 0.51 |
| 2:D:39:GLN:HG2 | 2:D:95:TYR:HE1 | 1.75 | 0.51 |
| 1:A:762:GLN:NE2 | 1:C:961:THR:CG2 | 2.74 | 0.51 |
| 1:A:813:SER:O | 1:A:814:LYS:HB2 | 2.10 | 0.51 |
| 1:B:386:LYS:NZ | 1:C:982:SER:HA | 2.26 | 0.51 |
| 1:B:905:ARG:NH1 | 1:B:1050:MET:CB | 2.72 | 0.51 |
| 1:C:193:VAL:HG23 | 1:C:223:LEU:CD1 | 2.41 | 0.51 |
| 1:C:658:ASN:CG | 1:C:659:SER:N | 2.65 | 0.51 |
| 2:E:39:GLN:HG2 | 2:E:95:TYR:CE1 | 2.46 | 0.51 |
| 1:A:53:ASP:OD2 | 1:A:53:ASP:C | 2.48 | 0.51 |
| 1:B:53:ASP:OD2 | 1:B:53:ASP:C | 2.48 | 0.51 |
| 1:B:193:VAL:HG23 | 1:B:223:LEU:CD1 | 2.41 | 0.51 |
| 1:B:206:LYS:HD2 | 1:B:222:ALA:O | 2.11 | 0.51 |
| 1:A:206:LYS:HD2 | 1:A:222:ALA:O | 2.12 | 0.50 |
| 1:A:663:ASP:OD1 | 1:A:663:ASP:C | 2.49 | 0.50 |
| 1:A:969:ASN:OD1 | 1:A:972:ALA:O | 2.27 | 0.50 |
| 1:B:53:ASP:OD2 | 1:B:55:PHE:CE2 | 2.64 | 0.50 |
| 1:B:190:ARG:HH11 | 1:B:207:HIS:HE1 | 1.58 | 0.50 |
| 1:B:390:LEU:HD11 | 1:C:983:ARG:CG | 2.40 | 0.50 |
| 1:B:503:VAL:HG11 | 2:E:111:TRP:CD1 | 2.46 | 0.50 |
| 1:B:702:GLU:HA | 1:C:788:ILE:O | 2.10 | 0.50 |
| 1:C:53:ASP:OD2 | 1:C:53:ASP:C | 2.49 | 0.50 |
| 1:A:560:LEU:O | 1:A:577:ARG:NH2 | 2.44 | 0.50 |
| 1:A:658:ASN:CG | 1:A:659:SER:N | 2.65 | 0.50 |
| 1:A:707:TYR:CG | 1:B:883:THR:HG22 | 2.46 | 0.50 |
| 1:B:813:SER:O | 1:B:814:LYS:HB2 | 2.10 | 0.50 |
| 1:C:53:ASP:OD2 | 1:C:55:PHE:CE2 | 2.64 | 0.50 |
| 1:C:958:ALA:O | 1:C:961:THR:OG1 | 2.22 | 0.50 |
| 2:D:39:GLN:HG2 | 2:D:95:TYR:CE1 | 2.46 | 0.50 |
| 2:E:31:THR:HG23 | 2:E:99:GLY:N | 2.25 | 0.50 |
| 1:A:1080:ALA:HB2 | 1:A:1089:PHE:HE2 | 1.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:378:LYS:HE2 | 1:B:380:TYR:CZ | 2.46 | 0.50 |
| 2:D:60:TYR:HE2 | 2:D:68:PHE:HB3 | 1.77 | 0.50 |
| 1:B:1002:GLN:HE21 | 1:B:1002:GLN:C | 2.15 | 0.50 |
| 2:D:91:THR:HG23 | 2:D:118:THR:HA | 1.94 | 0.50 |
| 2:E:30:ASN:HB3 | 2:E:100:TYR:CD2 | 2.46 | 0.50 |
| 2:E:60:TYR:HE2 | 2:E:68:PHE:HB3 | 1.77 | 0.50 |
| 1:A:317:ASN:OD1 | 1:A:317:ASN:N | 2.43 | 0.50 |
| 1:A:1005:GLN:CD | 1:C:1006:THR:HG23 | 2.31 | 0.50 |
| 1:C:190:ARG:HH11 | 1:C:207:HIS:HE1 | 1.57 | 0.50 |
| 2:E:58:THR:HG23 | 2:E:70:ILE:HG21 | 1.94 | 0.50 |
| 1:A:190:ARG:HH11 | 1:A:207:HIS:HE1 | 1.58 | 0.50 |
| 1:A:332:ILE:HD11 | 1:A:527:PRO:HA | 1.94 | 0.50 |
| 1:A:372:ALA:HB1 | 2:D:63:SER:OG | 2.11 | 0.50 |
| 1:A:1002:GLN:HE21 | 1:A:1002:GLN:C | 2.15 | 0.50 |
| 1:B:192:PHE:HB2 | 1:B:194:PHE:CZ | 2.47 | 0.50 |
| 1:B:317:ASN:OD1 | 1:B:317:ASN:N | 2.43 | 0.50 |
| 1:B:357:ARG:NH2 | 1:C:200:TYR:CE1 | 2.79 | 0.50 |
| 1:B:617:CYS:O | 1:B:620:VAL:HG22 | 2.11 | 0.50 |
| 1:B:658:ASN:CG | 1:B:659:SER:N | 2.65 | 0.50 |
| 1:B:817:PHE:C | 1:B:817:PHE:HD2 | 2.14 | 0.50 |
| 1:C:97:LYS:HD2 | 1:C:182:LYS:HB2 | 1.93 | 0.50 |
| 1:C:658:ASN:OD1 | 1:C:660:TYR:CZ | 2.65 | 0.50 |
| 2:D:31:THR:HG23 | 2:D:99:GLY:N | 2.25 | 0.50 |
| 1:B:608:VAL:HG12 | 1:B:609:ALA:N | 2.27 | 0.50 |
| 1:C:524:VAL:O | 1:C:524:VAL:HG13 | 2.12 | 0.50 |
| 1:C:813:SER:O | 1:C:814:LYS:HB2 | 2.10 | 0.50 |
| 1:A:608:VAL:HG12 | 1:A:609:ALA:N | 2.27 | 0.50 |
| 1:B:97:LYS:HD2 | 1:B:182:LYS:HB2 | 1.93 | 0.50 |
| 1:B:767:LEU:HD21 | 1:B:1008:VAL:HG22 | 1.94 | 0.50 |
| 1:B:770:ILE:HG23 | 1:B:770:ILE:C | 2.29 | 0.50 |
| 1:C:560:LEU:O | 1:C:577:ARG:NH2 | 2.44 | 0.50 |
| 2:D:93:LEU:HD22 | 2:D:95:TYR:HE2 | 1.76 | 0.50 |
| 2:E:93:LEU:HD22 | 2:E:95:TYR:HE2 | 1.76 | 0.50 |
| 1:A:53:ASP:OD2 | 1:A:55:PHE:CE2 | 2.64 | 0.50 |
| 1:A:617:CYS:O | 1:A:620:VAL:HG22 | 2.11 | 0.50 |
| 1:A:1017:GLU:OE1 | 1:B:1019:ARG:NH2 | 2.45 | 0.50 |
| 1:B:647:ALA:HA | 1:C:862:PRO:HG3 | 1.94 | 0.50 |
| 1:C:317:ASN:N | 1:C:317:ASN:OD1 | 2.43 | 0.50 |
| 2:D:1:GLN:O | 2:D:26:GLY:HA3 | 2.12 | 0.50 |
| 2:E:95:TYR:HD2 | 2:E:114:GLY:CA | 2.22 | 0.50 |
| 1:A:768:THR:O | 1:A:769:GLY:C | 2.50 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:768:THR:O | 1:A:770:ILE:N | 2.45 | 0.49 |
| 1:C:768:THR:O | 1:C:770:ILE:N | 2.45 | 0.49 |
| 1:A:97:LYS:HD2 | 1:A:182:LYS:HB2 | 1.93 | 0.49 |
| 1:A:658:ASN:OD1 | 1:A:660:TYR:CZ | 2.65 | 0.49 |
| 1:B:905:ARG:HH12 | 1:B:1050:MET:HB3 | 1.72 | 0.49 |
| 1:C:884:SER:C | 1:C:901:GLN:OE1 | 2.51 | 0.49 |
| 2:E:1:GLN:O | 2:E:26:GLY:HA3 | 2.12 | 0.49 |
| 1:A:296:LEU:HB2 | 1:A:608:VAL:HG21 | 1.94 | 0.49 |
| 1:C:192:PHE:HB2 | 1:C:194:PHE:CZ | 2.47 | 0.49 |
| 1:B:214:ARG:HG2 | 1:B:214:ARG:O | 2.12 | 0.49 |
| 1:B:386:LYS:HZ1 | 1:C:982:SER:HA | 1.77 | 0.49 |
| 1:B:487:ASN:HA | 1:B:489:TYR:CZ | 2.47 | 0.49 |
| 1:C:608:VAL:HG12 | 1:C:609:ALA:N | 2.27 | 0.49 |
| 1:C:725:GLU:CD | 1:C:1028:LYS:HE3 | 2.33 | 0.49 |
| 2:D:4:LEU:HD23 | 2:D:22:CYS:SG | 2.53 | 0.49 |
| 2:E:4:LEU:HD23 | 2:E:22:CYS:SG | 2.53 | 0.49 |
| 1:A:192:PHE:HB2 | 1:A:194:PHE:CZ | 2.47 | 0.49 |
| 4:B:1302:NAG:HO3 | 4:B:1302:NAG:C7 | 2.18 | 0.49 |
| 2:E:68:PHE:HA | 2:E:82:GLN:O | 2.13 | 0.49 |
| 1:B:282:ASN:OD1 | 4:B:1304:NAG:N2 | 2.45 | 0.49 |
| 1:B:671:CYS:SG | 1:B:697:MET:SD | 3.11 | 0.49 |
| 1:B:768:THR:O | 1:B:769:GLY:C | 2.50 | 0.49 |
| 1:C:726:ILE:HG23 | 1:C:1061:VAL:HG22 | 1.95 | 0.49 |
| 1:A:131:CYS:HA | 1:A:166:CYS:HB3 | 1.95 | 0.49 |
| 1:B:658:ASN:OD1 | 1:B:660:TYR:CZ | 2.65 | 0.49 |
| 1:C:206:LYS:HD2 | 1:C:222:ALA:O | 2.12 | 0.49 |
| 1:C:768:THR:O | 1:C:769:GLY:C | 2.50 | 0.49 |
| 2:D:58:THR:CG2 | 2:D:70:ILE:CG2 | 2.91 | 0.49 |
| 2:D:68:PHE:HA | 2:D:82:GLN:O | 2.13 | 0.49 |
| 1:A:324:GLU:O | 1:A:539:VAL:HG13 | 2.12 | 0.49 |
| 1:A:767:LEU:HD21 | 1:A:1008:VAL:HG22 | 1.94 | 0.49 |
| 1:B:487:ASN:HA | 1:B:489:TYR:OH | 2.13 | 0.49 |
| 1:C:452:LEU:HD12 | 1:C:492:LEU:HD13 | 1.95 | 0.49 |
| 1:C:663:ASP:OD1 | 1:C:663:ASP:C | 2.49 | 0.49 |
| 2:E:91:THR:HG23 | 2:E:118:THR:HA | 1.94 | 0.49 |
| 1:A:273:ARG:NH2 | 1:A:290:ASP:OD2 | 2.45 | 0.49 |
| 1:A:726:ILE:HG23 | 1:A:1061:VAL:HG22 | 1.95 | 0.49 |
| 1:B:141:LEU:HD23 | 1:B:141:LEU:HA | 1.74 | 0.49 |
| 1:B:665:PRO:HB2 | 1:C:864:LEU:CD2 | 2.42 | 0.49 |
| 1:C:273:ARG:NH2 | 1:C:290:ASP:OD2 | 2.45 | 0.49 |
| 1:A:671:CYS:SG | 1:A:697:MET:SD | 3.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:296:LEU:HB2 | 1:B:608:VAL:HG21 | 1.94 | 0.49 |
| 1:B:377:PHE:C | 2:E:104:SER:OG | 2.51 | 0.49 |
| 1:B:725:GLU:CD | 1:B:1028:LYS:HE3 | 2.33 | 0.49 |
| 1:B:726:ILE:HG23 | 1:B:1061:VAL:HG22 | 1.95 | 0.49 |
| 1:C:296:LEU:HB2 | 1:C:608:VAL:HG21 | 1.94 | 0.49 |
| 1:C:671:CYS:SG | 1:C:697:MET:SD | 3.11 | 0.49 |
| 1:A:712:ILE:O | 1:A:1074:ASN:HA | 2.13 | 0.48 |
| 1:A:767:LEU:CD2 | 1:A:1008:VAL:HG22 | 2.43 | 0.48 |
| 1:A:894:LEU:HB3 | 1:C:713:ALA:O | 2.12 | 0.48 |
| 1:B:273:ARG:NH2 | 1:B:290:ASP:OD2 | 2.45 | 0.48 |
| 1:B:718:PHE:HZ | 1:B:919:ASN:CG | 2.17 | 0.48 |
| 1:C:30:ASN:OD1 | 4:C:1303:NAG:H81 | 2.12 | 0.48 |
| 1:C:767:LEU:HD21 | 1:C:1008:VAL:HG22 | 1.94 | 0.48 |
| 1:A:214:ARG:O | 1:A:214:ARG:HG2 | 2.12 | 0.48 |
| 1:A:537:LYS:N | 1:A:551:VAL:HG23 | 2.28 | 0.48 |
| 1:B:768:THR:O | 1:B:770:ILE:N | 2.45 | 0.48 |
| 1:C:214:ARG:O | 1:C:214:ARG:HG2 | 2.12 | 0.48 |
| 1:C:770:ILE:CG1 | 1:C:770:ILE:HG23 | 1.97 | 0.48 |
| 1:A:177:MET:CG | 1:A:179:LEU:HD12 | 2.44 | 0.48 |
| 1:A:884:SER:C | 1:A:901:GLN:OE1 | 2.51 | 0.48 |
| 1:B:331:ASN:CB | 4:B:1305:NAG:C1 | 2.91 | 0.48 |
| 1:C:712:ILE:O | 1:C:1074:ASN:HA | 2.14 | 0.48 |
| 1:C:770:ILE:HG23 | 1:C:770:ILE:C | 2.29 | 0.48 |
| 2:D:2:VAL:HG23 | 2:D:110:ASN:CG | 2.33 | 0.48 |
| 2:D:58:THR:CG2 | 2:D:70:ILE:HG21 | 2.43 | 0.48 |
| 1:A:524:VAL:O | 1:A:524:VAL:HG13 | 2.12 | 0.48 |
| 1:A:725:GLU:CD | 1:A:1028:LYS:HE3 | 2.33 | 0.48 |
| 1:B:767:LEU:CD2 | 1:B:1008:VAL:HG22 | 2.43 | 0.48 |
| 1:B:884:SER:C | 1:B:901:GLN:OE1 | 2.51 | 0.48 |
| 1:C:452:LEU:HD12 | 1:C:492:LEU:CD1 | 2.44 | 0.48 |
| 2:D:4:LEU:HD13 | 2:D:110:ASN:CB | 2.43 | 0.48 |
| 1:B:665:PRO:CB | 1:C:864:LEU:CD2 | 2.91 | 0.48 |
| 1:B:770:ILE:HG21 | 1:B:770:ILE:HD13 | 1.96 | 0.48 |
| 1:A:283:GLY:HA3 | 1:C:563:GLN:HE22 | 1.77 | 0.48 |
| 1:A:452:LEU:HD12 | 1:A:492:LEU:HD13 | 1.94 | 0.48 |
| 1:A:452:LEU:HD12 | 1:A:492:LEU:CD1 | 2.44 | 0.48 |
| 1:A:603:ASN:HD21 | 4:A:1306:NAG:C1 | 2.27 | 0.48 |
| 1:A:748:GLU:OE2 | 1:A:748:GLU:N | 2.29 | 0.48 |
| 1:C:767:LEU:CD2 | 1:C:1008:VAL:HG22 | 2.43 | 0.48 |
| 2:D:58:THR:HG23 | 2:D:70:ILE:HG21 | 1.94 | 0.48 |
| 1:A:770:ILE:HG21 | 1:A:770:ILE:HD13 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:376:THR:HB | 1:B:435:ALA:HB3 | 1.95 | 0.48 |
| 1:C:177:MET:CG | 1:C:179:LEU:HD12 | 2.44 | 0.48 |
| 1:C:770:ILE:C | 1:C:770:ILE:HG22 | 2.32 | 0.48 |
| 2:D:4:LEU:HB2 | 2:D:110:ASN:O | 2.14 | 0.48 |
| 2:E:6:GLU:HG2 | 2:E:95:TYR:HA | 1.96 | 0.48 |
| 1:A:280:ASN:CG | 1:A:281:GLU:N | 2.67 | 0.48 |
| 1:A:963:VAL:O | 1:A:966:LEU:HB3 | 2.14 | 0.48 |
| 1:B:280:ASN:CG | 1:B:281:GLU:N | 2.67 | 0.48 |
| 1:C:131:CYS:HA | 1:C:166:CYS:HB3 | 1.95 | 0.48 |
| 1:C:537:LYS:N | 1:C:551:VAL:HG23 | 2.29 | 0.48 |
| 2:E:4:LEU:HD13 | 2:E:110:ASN:CB | 2.43 | 0.48 |
| 2:E:12:VAL:HG11 | 2:E:18:LEU:HG | 1.96 | 0.48 |
| 2:E:58:THR:CG2 | 2:E:70:ILE:HG21 | 2.43 | 0.48 |
| 2:E:58:THR:CG2 | 2:E:70:ILE:CG2 | 2.91 | 0.48 |
| 1:A:765:ARG:NE | 1:C:957:GLN:HE21 | 2.11 | 0.48 |
| 1:B:712:ILE:O | 1:B:1074:ASN:HA | 2.13 | 0.48 |
| 1:B:977:LEU:HA | 1:B:980:ILE:HD11 | 1.96 | 0.48 |
| 2:E:2:VAL:HG23 | 2:E:110:ASN:CG | 2.33 | 0.48 |
| 1:B:433:VAL:HG22 | 1:B:512:VAL:HG22 | 1.95 | 0.47 |
| 1:C:616:ASN:HD21 | 4:C:1304:NAG:C2 | 2.27 | 0.47 |
| 1:C:963:VAL:O | 1:C:966:LEU:HB3 | 2.14 | 0.47 |
| 2:E:94:TYR:CE2 | 2:E:117:VAL:CG1 | 2.97 | 0.47 |
| 1:A:765:ARG:CD | 1:C:957:GLN:HE22 | 2.27 | 0.47 |
| 1:A:905:ARG:NH1 | 1:A:1050:MET:CB | 2.72 | 0.47 |
| 1:B:61:ASN:ND2 | 4:B:1307:NAG:N2 | 2.62 | 0.47 |
| 1:C:718:PHE:HZ | 1:C:919:ASN:CG | 2.17 | 0.47 |
| 1:C:905:ARG:NH1 | 1:C:1050:MET:CB | 2.72 | 0.47 |
| 2:D:6:GLU:HG2 | 2:D:95:TYR:HA | 1.96 | 0.47 |
| 2:D:39:GLN:C | 2:D:92:ALA:HB1 | 2.34 | 0.47 |
| 2:E:39:GLN:C | 2:E:92:ALA:HB1 | 2.34 | 0.47 |
| 1:A:565:PHE:CZ | 1:B:42:VAL:HG22 | 2.50 | 0.47 |
| 1:A:571:ASP:OD1 | 1:B:44:ARG:NH1 | 2.47 | 0.47 |
| 1:B:963:VAL:O | 1:B:966:LEU:HB3 | 2.14 | 0.47 |
| 1:C:974:SER:HG | 1:C:979:ASP:CG | 2.13 | 0.47 |
| 1:C:994:ASP:C | 1:C:994:ASP:OD2 | 2.53 | 0.47 |
| 2:D:73:ASP:CG | 2:D:76:LYS:HG2 | 2.35 | 0.47 |
| 2:D:95:TYR:HD2 | 2:D:114:GLY:CA | 2.22 | 0.47 |
| 2:E:4:LEU:HB2 | 2:E:110:ASN:O | 2.14 | 0.47 |
| 2:E:73:ASP:CG | 2:E:76:LYS:HG2 | 2.35 | 0.47 |
| 1:A:64:TRP:NE1 | 1:A:66:HIS:CE1 | 2.82 | 0.47 |
| 1:A:749:CYS:HA | 1:A:752:LEU:HD12 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:765:ARG:HD2 | 1:C:957:GLN:HE22 | 1.80 | 0.47 |
| 1:A:904:TYR:OH | 1:C:1094:VAL:HG12 | 2.13 | 0.47 |
| 1:B:475:ALA:CB | 1:B:489:TYR:HE2 | 2.27 | 0.47 |
| 1:C:334:ASN:O | 1:C:362:VAL:HG12 | 2.14 | 0.47 |
| 1:A:455:LEU:HD11 | 1:A:493:GLN:HB2 | 1.96 | 0.47 |
| 1:A:770:ILE:C | 1:A:770:ILE:HG22 | 2.32 | 0.47 |
| 1:B:618:THR:OG1 | 1:B:619:GLU:OE1 | 2.24 | 0.47 |
| 1:B:911:VAL:N | 1:B:911:VAL:HG23 | 2.30 | 0.47 |
| 1:B:994:ASP:OD2 | 1:B:994:ASP:C | 2.53 | 0.47 |
| 1:A:569:ILE:HD12 | 1:A:569:ILE:H | 1.79 | 0.47 |
| 1:A:1029:MET:HE2 | 1:A:1062:PHE:CE1 | 2.49 | 0.47 |
| 1:B:190:ARG:HB2 | 1:B:192:PHE:CE1 | 2.50 | 0.47 |
| 1:B:658:ASN:O | 1:B:659:SER:OG | 2.27 | 0.47 |
| 1:B:922:LEU:HD11 | 4:B:1310:NAG:C5 | 2.45 | 0.47 |
| 1:B:1080:ALA:HB2 | 1:B:1089:PHE:CD2 | 2.49 | 0.47 |
| 1:C:770:ILE:HG21 | 1:C:770:ILE:HD13 | 1.96 | 0.47 |
| 1:A:568:ASP:OD1 | 1:A:569:ILE:HD12 | 2.14 | 0.47 |
| 1:A:611:LEU:HD12 | 1:A:649:CYS:O | 2.15 | 0.47 |
| 1:A:718:PHE:HZ | 1:A:919:ASN:CG | 2.17 | 0.47 |
| 1:B:922:LEU:HD11 | 4:B:1310:NAG:H5 | 1.96 | 0.47 |
| 1:B:1039:ARG:NH2 | 1:B:1042:PHE:CD1 | 2.83 | 0.47 |
| 1:C:314:GLN:OE1 | 1:C:314:GLN:CA | 2.63 | 0.47 |
| 1:C:737:ASP:OD2 | 1:C:740:MET:HB3 | 2.15 | 0.47 |
| 1:C:749:CYS:HA | 1:C:752:LEU:HD12 | 1.97 | 0.47 |
| 2:D:94:TYR:CE2 | 2:D:117:VAL:CG1 | 2.97 | 0.47 |
| 1:A:190:ARG:HB2 | 1:A:192:PHE:CE1 | 2.50 | 0.47 |
| 1:A:618:THR:OG1 | 1:A:619:GLU:OE1 | 2.24 | 0.47 |
| 1:A:1002:GLN:O | 1:A:1002:GLN:NE2 | 2.40 | 0.47 |
| 1:B:131:CYS:HA | 1:B:166:CYS:HB3 | 1.95 | 0.47 |
| 1:B:1064:HIS:N | 1:B:1064:HIS:CD2 | 2.83 | 0.47 |
| 1:B:1107:ARG:NH2 | 1:C:913:GLN:NE2 | 2.63 | 0.47 |
| 2:E:20:LEU:O | 2:E:80:TYR:CD1 | 2.67 | 0.47 |
| 1:A:699:LEU:HD21 | 1:A:699:LEU:HD11 | 1.85 | 0.47 |
| 1:A:705:VAL:CG2 | 1:B:789:TYR:HD1 | 2.28 | 0.47 |
| 1:A:1030:SER:OG | 1:C:1041:ASP:HB2 | 2.14 | 0.47 |
| 1:B:472:ILE:CG2 | 1:B:489:TYR:O | 2.63 | 0.47 |
| 1:B:487:ASN:HA | 1:B:489:TYR:CE1 | 2.49 | 0.47 |
| 1:C:64:TRP:NE1 | 1:C:66:HIS:CE1 | 2.82 | 0.47 |
| 2:E:69:THR:CG2 | 2:E:82:GLN:HB3 | 2.29 | 0.47 |
| 1:A:146:HIS:O | 1:A:150:LYS:HA | 2.15 | 0.47 |
| 1:A:314:GLN:OE1 | 1:A:314:GLN:CA | 2.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:334:ASN:O | 1:A:362:VAL:HG12 | 2.15 | 0.47 |
| 1:A:408:ARG:HE | 2:D:103:ALA:HB1 | 1.79 | 0.47 |
| 1:A:551:VAL:HG12 | 1:A:588:THR:O | 2.15 | 0.47 |
| 1:A:737:ASP:OD2 | 1:A:740:MET:HB3 | 2.15 | 0.47 |
| 1:A:781:VAL:HG23 | 1:A:782:PHE:CD2 | 2.50 | 0.47 |
| 1:A:1050:MET:SD | 1:A:1052:PHE:CZ | 3.08 | 0.47 |
| 1:B:177:MET:CG | 1:B:179:LEU:HD12 | 2.44 | 0.47 |
| 1:A:1039:ARG:NH2 | 1:A:1042:PHE:CD1 | 2.83 | 0.46 |
| 1:A:1062:PHE:CB | 1:A:1064:HIS:NE2 | 2.79 | 0.46 |
| 1:A:1064:HIS:N | 1:A:1064:HIS:CD2 | 2.83 | 0.46 |
| 1:B:146:HIS:O | 1:B:150:LYS:HA | 2.15 | 0.46 |
| 1:C:190:ARG:HB2 | 1:C:192:PHE:CE1 | 2.50 | 0.46 |
| 1:C:611:LEU:HD12 | 1:C:649:CYS:O | 2.15 | 0.46 |
| 1:C:781:VAL:HG23 | 1:C:782:PHE:CD2 | 2.50 | 0.46 |
| 1:C:1142:GLN:N | 1:C:1143:PRO:HD2 | 2.30 | 0.46 |
| 1:A:403:ARG:NH1 | 1:A:406:GLU:OE2 | 2.48 | 0.46 |
| 1:A:1031:GLU:OE1 | 1:C:1039:ARG:HG2 | 2.14 | 0.46 |
| 1:A:1080:ALA:HB2 | 1:A:1089:PHE:CD2 | 2.49 | 0.46 |
| 1:B:64:TRP:NE1 | 1:B:66:HIS:CE1 | 2.82 | 0.46 |
| 1:B:737:ASP:OD2 | 1:B:740:MET:HB3 | 2.15 | 0.46 |
| 1:B:1050:MET:SD | 1:B:1052:PHE:CZ | 3.08 | 0.46 |
| 1:B:1062:PHE:CB | 1:B:1064:HIS:NE2 | 2.79 | 0.46 |
| 1:C:403:ARG:NH1 | 1:C:406:GLU:OE2 | 2.48 | 0.46 |
| 1:C:618:THR:OG1 | 1:C:619:GLU:OE1 | 2.24 | 0.46 |
| 2:D:12:VAL:HG11 | 2:D:18:LEU:HG | 1.96 | 0.46 |
| 2:D:36:TRP:HD1 | 2:D:70:ILE:HD13 | 1.80 | 0.46 |
| 1:A:894:LEU:HA | 1:C:713:ALA:HB3 | 1.96 | 0.46 |
| 1:A:1019:ARG:NH2 | 1:C:1017:GLU:OE1 | 2.48 | 0.46 |
| 1:B:364:ASP:OD1 | 1:B:367:VAL:HG22 | 2.15 | 0.46 |
| 4:B:1310:NAG:O7 | 4:B:1310:NAG:H3 | 2.14 | 0.46 |
| 1:C:404:GLY:O | 1:C:407:VAL:HG22 | 2.15 | 0.46 |
| 1:C:734:THR:HG21 | 1:C:959:LEU:CD1 | 2.45 | 0.46 |
| 1:A:314:GLN:OE1 | 1:A:595:VAL:C | 2.54 | 0.46 |
| 1:A:734:THR:HG21 | 1:A:959:LEU:CD1 | 2.45 | 0.46 |
| 1:A:965:GLN:OE1 | 1:A:1003:SER:HB3 | 2.16 | 0.46 |
| 1:B:314:GLN:OE1 | 1:B:595:VAL:C | 2.54 | 0.46 |
| 1:B:465:GLU:OE1 | 3:J:1:NAG:H81 | 2.16 | 0.46 |
| 1:C:146:HIS:O | 1:C:150:LYS:HA | 2.15 | 0.46 |
| 1:C:770:ILE:CG2 | 1:C:770:ILE:CD1 | 2.76 | 0.46 |
| 2:D:93:LEU:HB3 | 2:D:95:TYR:CE2 | 2.50 | 0.46 |
| 2:E:93:LEU:HB3 | 2:E:95:TYR:CE2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:994:ASP:OD2 | 1:A:994:ASP:C | 2.53 | 0.46 |
| 1:A:1005:GLN:OE1 | 1:C:1006:THR:HG23 | 2.16 | 0.46 |
| 1:B:423:TYR:HE2 | 1:B:512:VAL:HG21 | 1.79 | 0.46 |
| 1:B:452:LEU:HD12 | 1:B:493:GLN:C | 2.36 | 0.46 |
| 1:B:611:LEU:HD12 | 1:B:649:CYS:O | 2.15 | 0.46 |
| 1:B:734:THR:HG21 | 1:B:959:LEU:CD1 | 2.45 | 0.46 |
| 1:C:280:ASN:CG | 1:C:281:GLU:N | 2.67 | 0.46 |
| 1:C:569:ILE:H | 1:C:569:ILE:HD12 | 1.80 | 0.46 |
| 1:C:1039:ARG:NH2 | 1:C:1042:PHE:CD1 | 2.83 | 0.46 |
| 1:C:1050:MET:SD | 1:C:1052:PHE:CZ | 3.08 | 0.46 |
| 1:A:1005:GLN:NE2 | 1:C:1006:THR:HG21 | 2.23 | 0.46 |
| 1:B:357:ARG:HH21 | 1:C:200:TYR:HE1 | 1.63 | 0.46 |
| 1:B:749:CYS:HA | 1:B:752:LEU:HD12 | 1.97 | 0.46 |
| 1:B:1107:ARG:HH21 | 1:C:913:GLN:NE2 | 2.13 | 0.46 |
| 1:C:87:ASN:OD1 | 1:C:269:TYR:HE2 | 1.98 | 0.46 |
| 1:C:314:GLN:OE1 | 1:C:595:VAL:C | 2.54 | 0.46 |
| 1:C:1062:PHE:CB | 1:C:1064:HIS:NE2 | 2.79 | 0.46 |
| 1:C:1080:ALA:HB2 | 1:C:1089:PHE:CD2 | 2.49 | 0.46 |
| 1:C:1116:THR:OG1 | 1:C:1118:ASP:OD2 | 2.32 | 0.46 |
| 1:A:96:GLU:OE2 | 1:A:263:ALA:HB1 | 2.16 | 0.46 |
| 1:A:377:PHE:HD1 | 1:A:434:ILE:HD12 | 1.81 | 0.46 |
| 1:A:661:GLU:OE1 | 1:A:661:GLU:HA | 2.16 | 0.46 |
| 1:A:904:TYR:OH | 1:C:1094:VAL:CG1 | 2.64 | 0.46 |
| 1:B:139:PRO:HB3 | 1:B:159:VAL:HG12 | 1.98 | 0.46 |
| 1:B:457:ARG:NH1 | 1:B:459[A]:SER:O | 2.41 | 0.46 |
| 1:B:457:ARG:NH1 | 1:B:459[B]:SER:O | 2.41 | 0.46 |
| 1:B:473:TYR:HB3 | 1:B:489:TYR:HB2 | 1.97 | 0.46 |
| 1:B:781:VAL:HG23 | 1:B:782:PHE:CD2 | 2.50 | 0.46 |
| 1:C:139:PRO:HB3 | 1:C:159:VAL:HG12 | 1.97 | 0.46 |
| 1:C:568:ASP:OD1 | 1:C:569:ILE:HD12 | 2.16 | 0.46 |
| 1:C:977:LEU:HA | 1:C:980:ILE:HD11 | 1.96 | 0.46 |
| 1:A:977:LEU:HA | 1:A:980:ILE:HD11 | 1.96 | 0.46 |
| 1:B:958:ALA:O | 1:B:961:THR:OG1 | 2.22 | 0.46 |
| 1:C:661:GLU:OE1 | 1:C:661:GLU:HA | 2.16 | 0.46 |
| 1:B:87:ASN:OD1 | 1:B:269:TYR:HE2 | 1.98 | 0.46 |
| 1:B:96:GLU:OE2 | 1:B:96:GLU:HA | 2.16 | 0.46 |
| 1:C:658:ASN:O | 1:C:659:SER:OG | 2.27 | 0.46 |
| 1:B:707:TYR:HE2 | 1:C:896:ILE:O | 1.99 | 0.46 |
| 1:A:404:GLY:O | 1:A:407:VAL:HG22 | 2.15 | 0.45 |
| 1:B:1104:VAL:O | 1:B:1104:VAL:HG13 | 2.16 | 0.45 |
| 1:C:96:GLU:OE2 | 1:C:96:GLU:HA | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1064:HIS:N | 1:C:1064:HIS:CD2 | 2.83 | 0.45 |
| 1:C:1104:VAL:O | 1:C:1104:VAL:HG13 | 2.16 | 0.45 |
| 1:B:332:ILE:HG13 | 1:B:362:VAL:CG1 | 2.46 | 0.45 |
| 1:B:702:GLU:HG2 | 1:C:788:ILE:HB | 1.98 | 0.45 |
| 1:A:17:ASN:OD1 | 3:F:1:NAG:C2 | 2.64 | 0.45 |
| 1:A:405:ASP:N | 1:A:504:GLY:O | 2.48 | 0.45 |
| 1:B:661:GLU:HA | 1:B:661:GLU:OE1 | 2.16 | 0.45 |
| 1:C:911:VAL:N | 1:C:911:VAL:HG23 | 2.30 | 0.45 |
| 1:C:965:GLN:OE1 | 1:C:1003:SER:HB3 | 2.16 | 0.45 |
| 1:A:139:PRO:HB3 | 1:A:159:VAL:HG12 | 1.97 | 0.45 |
| 1:A:1030:SER:C | 1:C:1040:VAL:HG12 | 2.36 | 0.45 |
| 1:B:326:ILE:HD11 | 1:B:552:LEU:HD11 | 1.98 | 0.45 |
| 1:B:919:ASN:OD1 | 1:B:923:ILE:CG1 | 2.61 | 0.45 |
| 1:C:751:ASN:HA | 1:C:754:LEU:HG | 1.99 | 0.45 |
| 2:D:24:ALA:HB1 | 2:D:28:THR:HG21 | 1.97 | 0.45 |
| 1:A:894:LEU:HD22 | 1:C:713:ALA:HB1 | 1.97 | 0.45 |
| 1:B:699:LEU:HG | 1:C:872:GLN:CD | 2.27 | 0.45 |
| 1:C:718:PHE:HZ | 1:C:919:ASN:ND2 | 2.15 | 0.45 |
| 2:D:68:PHE:HD2 | 2:D:81:LEU:HD11 | 1.81 | 0.45 |
| 2:E:24:ALA:HB1 | 2:E:28:THR:HG21 | 1.97 | 0.45 |
| 2:E:87:LYS:HB3 | 2:E:88:PRO:HD2 | 1.98 | 0.45 |
| 1:A:165:ASN:OD1 | 4:A:1302:NAG:H83 | 2.16 | 0.45 |
| 1:A:894:LEU:CA | 1:C:713:ALA:HB3 | 2.47 | 0.45 |
| 1:A:1142:GLN:N | 1:A:1143:PRO:HD2 | 2.31 | 0.45 |
| 1:B:965:GLN:OE1 | 1:B:1003:SER:HB3 | 2.15 | 0.45 |
| 1:B:984:LEU:HD13 | 1:B:988:GLU:HG2 | 1.99 | 0.45 |
| 1:C:96:GLU:OE2 | 1:C:263:ALA:HB1 | 2.16 | 0.45 |
| 1:C:826:VAL:HG23 | 1:C:945:LEU:HD22 | 1.99 | 0.45 |
| 1:A:1116:THR:OG1 | 1:A:1118:ASP:OD2 | 2.32 | 0.45 |
| 1:B:96:GLU:OE2 | 1:B:263:ALA:HB1 | 2.16 | 0.45 |
| 1:B:314:GLN:OE1 | 1:B:314:GLN:CA | 2.63 | 0.45 |
| 1:B:1116:THR:OG1 | 1:B:1118:ASP:OD2 | 2.32 | 0.45 |
| 2:D:87:LYS:HB3 | 2:D:88:PRO:HD2 | 1.98 | 0.45 |
| 1:B:43:PHE:CE1 | 1:B:283:GLY:CA | 3.00 | 0.45 |
| 1:B:158:ARG:HG3 | 1:B:158:ARG:HH11 | 1.82 | 0.45 |
| 2:D:6:GLU:HB3 | 2:D:115:THR:HG23 | 1.99 | 0.45 |
| 1:A:645:THR:HB | 1:A:670:ILE:HD13 | 1.99 | 0.45 |
| 1:A:765:ARG:O | 1:A:768:THR:OG1 | 2.30 | 0.45 |
| 1:B:1029:MET:HE2 | 1:B:1062:PHE:CE1 | 2.52 | 0.45 |
| 1:C:158:ARG:HG3 | 1:C:158:ARG:HH11 | 1.82 | 0.45 |
| 1:C:377:PHE:HD1 | 1:C:434:ILE:HD12 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:455:LEU:HD11 | 1:C:493:GLN:HB2 | 1.98 | 0.45 |
| 1:C:748:GLU:OE2 | 1:C:748:GLU:N | 2.29 | 0.45 |
| 1:A:96:GLU:OE2 | 1:A:96:GLU:HA | 2.16 | 0.45 |
| 1:A:718:PHE:HZ | 1:A:919:ASN:ND2 | 2.15 | 0.45 |
| 1:A:984:LEU:HD13 | 1:A:988:GLU:HG2 | 1.99 | 0.45 |
| 1:A:1104:VAL:HG13 | 1:A:1104:VAL:O | 2.16 | 0.45 |
| 1:B:131:CYS:SG | 1:B:163:ALA:HB1 | 2.57 | 0.45 |
| 1:B:376:THR:HG22 | 1:B:434:ILE:HA | 1.98 | 0.45 |
| 1:B:751:ASN:HA | 1:B:754:LEU:HG | 1.99 | 0.45 |
| 1:B:921:LYS:O | 1:B:922:LEU:C | 2.55 | 0.45 |
| 1:B:1142:GLN:N | 1:B:1143:PRO:HD2 | 2.31 | 0.45 |
| 2:D:20:LEU:O | 2:D:80:TYR:CD1 | 2.67 | 0.45 |
| 2:D:45:ASP:OD1 | 2:D:46:GLU:N | 2.50 | 0.45 |
| 1:A:43:PHE:CD1 | 1:A:43:PHE:C | 2.91 | 0.44 |
| 1:B:376:THR:HA | 2:E:106:TYR:HB2 | 1.98 | 0.44 |
| 1:B:457:ARG:CZ | 1:B:461:LEU:HD23 | 2.47 | 0.44 |
| 1:C:131:CYS:SG | 1:C:163:ALA:HB1 | 2.58 | 0.44 |
| 1:C:1029:MET:HE2 | 1:C:1062:PHE:CE1 | 2.52 | 0.44 |
| 2:E:34:VAL:HG11 | 2:E:79:VAL:HG11 | 1.99 | 0.44 |
| 2:E:45:ASP:OD1 | 2:E:46:GLU:N | 2.50 | 0.44 |
| 1:A:21:ARG:HD3 | 1:A:79:PHE:HB3 | 2.00 | 0.44 |
| 1:A:131:CYS:SG | 1:A:163:ALA:HB1 | 2.57 | 0.44 |
| 1:B:705:VAL:CG1 | 1:C:895:GLN:HB3 | 2.40 | 0.44 |
| 1:B:933:LYS:HA | 1:B:936:ASP:OD2 | 2.18 | 0.44 |
| 4:B:1307:NAG:O7 | 4:B:1307:NAG:C3 | 2.65 | 0.44 |
| 1:C:699:LEU:HD21 | 1:C:699:LEU:HD11 | 1.85 | 0.44 |
| 1:C:1062:PHE:HB3 | 1:C:1064:HIS:CD2 | 2.53 | 0.44 |
| 2:E:36:TRP:HD1 | 2:E:70:ILE:HD13 | 1.80 | 0.44 |
| 1:B:665:PRO:CB | 1:C:864:LEU:HD22 | 2.47 | 0.44 |
| 1:B:1062:PHE:HB3 | 1:B:1064:HIS:CD2 | 2.53 | 0.44 |
| 1:C:858:LEU:CD2 | 1:C:962:LEU:HD21 | 2.48 | 0.44 |
| 1:C:984:LEU:HD13 | 1:C:988:GLU:HG2 | 1.99 | 0.44 |
| 1:A:826:VAL:HG23 | 1:A:945:LEU:HD22 | 1.99 | 0.44 |
| 1:A:1013:ILE:HD12 | 1:B:1013:ILE:HD12 | 1.98 | 0.44 |
| 1:B:709:ASN:HB3 | 1:C:796:ASP:OD2 | 2.17 | 0.44 |
| 1:C:645:THR:HB | 1:C:670:ILE:HD13 | 1.99 | 0.44 |
| 1:A:87:ASN:OD1 | 1:A:269:TYR:HE2 | 1.98 | 0.44 |
| 1:A:1019:ARG:NH2 | 1:C:1017:GLU:CD | 2.70 | 0.44 |
| 1:C:43:PHE:CD1 | 1:C:43:PHE:C | 2.91 | 0.44 |
| 1:C:997:ILE:HD12 | 1:C:997:ILE:HG21 | 1.82 | 0.44 |
| 1:A:610:VAL:O | 1:A:650:LEU:HD12 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1076:THR:O | 1:A:1102:TRP:CH2 | 2.71 | 0.44 |
| 1:B:668:ALA:HA | 1:C:866:THR:HG23 | 2.00 | 0.44 |
| 1:B:826:VAL:HG23 | 1:B:945:LEU:HD22 | 1.99 | 0.44 |
| 1:A:21:ARG:HD2 | 1:A:79:PHE:O | 2.18 | 0.44 |
| 1:A:962:LEU:HD12 | 1:A:962:LEU:O | 2.18 | 0.44 |
| 1:B:200:TYR:HD2 | 1:B:228:ASP:OD2 | 2.01 | 0.44 |
| 1:B:645:THR:HB | 1:B:670:ILE:HD13 | 1.99 | 0.44 |
| 1:B:921:LYS:O | 1:B:925:ASN:OD1 | 2.36 | 0.44 |
| 1:C:610:VAL:O | 1:C:650:LEU:HD12 | 2.17 | 0.44 |
| 2:D:19:ARG:HD3 | 2:D:80:TYR:CE1 | 2.48 | 0.44 |
| 2:D:81:LEU:HD12 | 2:D:82:GLN:N | 2.32 | 0.44 |
| 1:A:44:ARG:NH1 | 1:C:571:ASP:OD1 | 2.51 | 0.44 |
| 1:A:158:ARG:HG3 | 1:A:158:ARG:HH11 | 1.82 | 0.44 |
| 1:A:787:GLN:OE1 | 1:C:703:ASN:OD1 | 2.35 | 0.44 |
| 1:B:503:VAL:HG11 | 2:E:111:TRP:NE1 | 2.33 | 0.44 |
| 1:B:718:PHE:HZ | 1:B:919:ASN:ND2 | 2.15 | 0.44 |
| 1:B:1002:GLN:O | 1:B:1002:GLN:NE2 | 2.40 | 0.44 |
| 2:E:81:LEU:HD12 | 2:E:82:GLN:N | 2.32 | 0.44 |
| 1:A:141:LEU:HD23 | 1:A:141:LEU:HA | 1.75 | 0.44 |
| 1:A:474:GLN:HG2 | 1:A:476:GLY:H | 1.83 | 0.44 |
| 1:A:751:ASN:HA | 1:A:754:LEU:HG | 1.99 | 0.44 |
| 1:A:919:ASN:OD1 | 1:A:923:ILE:CG1 | 2.61 | 0.44 |
| 1:B:770:ILE:C | 1:B:770:ILE:HG22 | 2.32 | 0.44 |
| 1:B:858:LEU:CD2 | 1:B:962:LEU:HD21 | 2.48 | 0.44 |
| 1:B:962:LEU:HD12 | 1:B:962:LEU:O | 2.18 | 0.44 |
| 1:B:1076:THR:O | 1:B:1102:TRP:CH2 | 2.71 | 0.44 |
| 2:D:64:VAL:O | 2:D:67:ARG:HG2 | 2.18 | 0.44 |
| 2:E:6:GLU:HB3 | 2:E:115:THR:HG23 | 1.98 | 0.44 |
| 1:A:883:THR:CG2 | 1:C:707:TYR:HB2 | 2.47 | 0.43 |
| 1:A:905:ARG:NH1 | 1:A:1049:LEU:O | 2.45 | 0.43 |
| 1:A:911:VAL:N | 1:A:911:VAL:HG23 | 2.30 | 0.43 |
| 1:A:919:ASN:OD1 | 1:A:919:ASN:O | 2.36 | 0.43 |
| 1:B:21:ARG:HD2 | 1:B:79:PHE:O | 2.18 | 0.43 |
| 1:B:569:ILE:HD12 | 1:B:569:ILE:H | 1.83 | 0.43 |
| 1:B:610:VAL:O | 1:B:650:LEU:HD12 | 2.17 | 0.43 |
| 1:B:800:PHE:HB3 | 1:B:802:PHE:CZ | 2.53 | 0.43 |
| 1:C:569:ILE:O | 1:C:570:ALA:HB3 | 2.18 | 0.43 |
| 1:C:1076:THR:O | 1:C:1102:TRP:CH2 | 2.71 | 0.43 |
| 2:D:37:PHE:HB2 | 2:D:46:GLU:O | 2.19 | 0.43 |
| 2:E:68:PHE:CE2 | 2:E:83:MET:HG3 | 2.53 | 0.43 |
| 1:B:280:ASN:OD1 | 1:B:281:GLU:CA | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:298:GLU:OE2 | 1:B:315:THR:OG1 | 2.26 | 0.43 |
| 1:C:405:ASP:N | 1:C:504:GLY:O | 2.49 | 0.43 |
| 1:C:800:PHE:HB3 | 1:C:802:PHE:CZ | 2.53 | 0.43 |
| 1:C:905:ARG:NH1 | 1:C:1049:LEU:O | 2.45 | 0.43 |
| 1:A:280:ASN:OD1 | 1:A:281:GLU:CA | 2.66 | 0.43 |
| 1:A:294:ASP:OD2 | 1:A:296:LEU:N | 2.52 | 0.43 |
| 1:A:824:ASN:OD1 | 1:A:824:ASN:N | 2.43 | 0.43 |
| 1:B:376:THR:CB | 1:B:435:ALA:HB3 | 2.48 | 0.43 |
| 1:B:743:CYS:SG | 1:B:753:LEU:HD23 | 2.59 | 0.43 |
| 1:B:919:ASN:OD1 | 1:B:919:ASN:O | 2.36 | 0.43 |
| 1:C:21:ARG:HD2 | 1:C:79:PHE:O | 2.18 | 0.43 |
| 1:C:100:ILE:O | 1:C:243:ALA:N | 2.45 | 0.43 |
| 1:C:921:LYS:O | 1:C:925:ASN:OD1 | 2.36 | 0.43 |
| 1:A:921:LYS:O | 1:A:925:ASN:OD1 | 2.36 | 0.43 |
| 1:B:21:ARG:HD3 | 1:B:79:PHE:HB3 | 2.00 | 0.43 |
| 1:B:131:CYS:HA | 1:B:166:CYS:CB | 2.49 | 0.43 |
| 1:B:131:CYS:HB3 | 1:B:133:PHE:CE2 | 2.53 | 0.43 |
| 1:B:922:LEU:HA | 1:B:925:ASN:OD1 | 2.19 | 0.43 |
| 4:B:1304:NAG:H83 | 4:B:1304:NAG:C3 | 2.37 | 0.43 |
| 1:C:21:ARG:HD3 | 1:C:79:PHE:HB3 | 2.00 | 0.43 |
| 1:C:131:CYS:HA | 1:C:166:CYS:CB | 2.49 | 0.43 |
| 1:C:280:ASN:OD1 | 1:C:281:GLU:CA | 2.66 | 0.43 |
| 1:C:323:THR:O | 1:C:539:VAL:HG22 | 2.19 | 0.43 |
| 1:C:743:CYS:SG | 1:C:753:LEU:HD23 | 2.59 | 0.43 |
| 1:C:878:LEU:O | 1:C:882:ILE:HG13 | 2.19 | 0.43 |
| 2:E:37:PHE:HB2 | 2:E:46:GLU:O | 2.18 | 0.43 |
| 1:A:711:SER:O | 1:B:895:GLN:CG | 2.67 | 0.43 |
| 1:A:755:GLN:NE2 | 1:C:969:ASN:HB3 | 2.33 | 0.43 |
| 1:A:800:PHE:HB3 | 1:A:802:PHE:CZ | 2.53 | 0.43 |
| 1:A:921:LYS:O | 1:A:922:LEU:C | 2.55 | 0.43 |
| 1:A:974:SER:HG | 1:A:979:ASP:CG | 2.19 | 0.43 |
| 1:A:997:ILE:HD12 | 1:A:997:ILE:HG21 | 1.82 | 0.43 |
| 1:B:294:ASP:OD2 | 1:B:296:LEU:N | 2.52 | 0.43 |
| 1:B:936:ASP:OD2 | 1:B:936:ASP:N | 2.50 | 0.43 |
| 1:B:1027:THR:O | 1:B:1031:GLU:HG3 | 2.19 | 0.43 |
| 1:C:984:LEU:HD13 | 1:C:988:GLU:CG | 2.49 | 0.43 |
| 2:D:6:GLU:CB | 2:D:115:THR:HG23 | 2.49 | 0.43 |
| 2:E:4:LEU:HD13 | 2:E:110:ASN:HB3 | 2.01 | 0.43 |
| 2:E:19:ARG:HD3 | 2:E:80:TYR:CE1 | 2.49 | 0.43 |
| 1:A:858:LEU:CD2 | 1:A:962:LEU:HD21 | 2.48 | 0.43 |
| 1:A:933:LYS:HA | 1:A:936:ASP:OD2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:936:ASP:OD2 | 1:A:936:ASP:N | 2.50 | 0.43 |
| 1:C:919:ASN:OD1 | 1:C:919:ASN:O | 2.36 | 0.43 |
| 1:C:936:ASP:OD2 | 1:C:936:ASP:N | 2.50 | 0.43 |
| 2:D:34:VAL:HG11 | 2:D:79:VAL:HG11 | 1.99 | 0.43 |
| 1:A:131:CYS:HB3 | 1:A:133:PHE:CE2 | 2.54 | 0.43 |
| 1:B:43:PHE:CD1 | 1:B:43:PHE:C | 2.91 | 0.43 |
| 1:B:376:THR:HB | 1:B:435:ALA:O | 2.18 | 0.43 |
| 1:B:905:ARG:NH1 | 1:B:1049:LEU:O | 2.45 | 0.43 |
| 1:C:131:CYS:HB3 | 1:C:133:PHE:CE2 | 2.54 | 0.43 |
| 1:C:663:ASP:OD1 | 1:C:664:ILE:HG13 | 2.19 | 0.43 |
| 1:C:921:LYS:O | 1:C:922:LEU:C | 2.55 | 0.43 |
| 2:E:6:GLU:CB | 2:E:115:THR:HG23 | 2.49 | 0.43 |
| 1:A:743:CYS:SG | 1:A:753:LEU:HD23 | 2.59 | 0.43 |
| 1:A:984:LEU:HD13 | 1:A:988:GLU:CG | 2.49 | 0.43 |
| 1:A:1062:PHE:HB3 | 1:A:1064:HIS:CD2 | 2.53 | 0.43 |
| 1:B:239:GLN:HG2 | 1:B:240:THR:O | 2.19 | 0.43 |
| 1:B:1056:ALA:HB1 | 1:B:1057:PRO:HD2 | 2.01 | 0.43 |
| 1:C:96:GLU:OE1 | 1:C:264:ALA:O | 2.37 | 0.43 |
| 1:C:294:ASP:OD2 | 1:C:296:LEU:N | 2.52 | 0.43 |
| 1:C:1056:ALA:HB1 | 1:C:1057:PRO:HD2 | 2.01 | 0.43 |
| 2:D:4:LEU:HD23 | 2:D:96:CYS:SG | 2.59 | 0.43 |
| 2:D:68:PHE:CE2 | 2:D:83:MET:HG3 | 2.53 | 0.43 |
| 1:A:43:PHE:CE1 | 1:A:283:GLY:CA | 3.00 | 0.43 |
| 1:A:503:VAL:HG23 | 2:D:45:ASP:HB3 | 2.01 | 0.43 |
| 1:A:1027:THR:O | 1:A:1031:GLU:HG3 | 2.19 | 0.43 |
| 1:B:376:THR:HB | 1:B:435:ALA:CA | 2.48 | 0.43 |
| 2:E:4:LEU:HD23 | 2:E:96:CYS:SG | 2.59 | 0.43 |
| 2:E:60:TYR:HD2 | 2:E:64:VAL:CG2 | 2.29 | 0.43 |
| 1:A:216:LEU:O | 1:A:217:PRO:O | 2.37 | 0.43 |
| 1:A:372:ALA:CB | 2:D:63:SER:OG | 2.67 | 0.43 |
| 1:A:569:ILE:O | 1:A:570:ALA:HB3 | 2.18 | 0.43 |
| 1:A:878:LEU:O | 1:A:882:ILE:HG13 | 2.19 | 0.43 |
| 1:A:922:LEU:HA | 1:A:925:ASN:OD1 | 2.18 | 0.43 |
| 1:B:128:ILE:HG21 | 1:B:229:LEU:HD11 | 2.01 | 0.43 |
| 1:B:765:ARG:O | 1:B:768:THR:OG1 | 2.30 | 0.43 |
| 1:C:878:LEU:HD23 | 1:C:882:ILE:HD11 | 2.01 | 0.43 |
| 1:C:933:LYS:HA | 1:C:936:ASP:OD2 | 2.18 | 0.43 |
| 1:A:883:THR:HG22 | 1:C:707:TYR:CD1 | 2.54 | 0.42 |
| 1:A:1056:ALA:HB1 | 1:A:1057:PRO:HD2 | 2.01 | 0.42 |
| 1:B:96:GLU:OE1 | 1:B:264:ALA:O | 2.37 | 0.42 |
| 1:B:974:SER:HG | 1:B:979:ASP:CG | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:984:LEU:HD13 | 1:B:988:GLU:CG | 2.49 | 0.42 |
| 1:C:324:GLU:O | 1:C:539:VAL:HG13 | 2.19 | 0.42 |
| 1:A:1075:PHE:HB3 | 1:A:1096:VAL:HB | 2.01 | 0.42 |
| 1:B:171:VAL:HG21 | 4:B:1301:NAG:H62 | 2.01 | 0.42 |
| 1:C:239:GLN:HG2 | 1:C:240:THR:O | 2.19 | 0.42 |
| 2:D:7:SER:O | 2:D:20:LEU:HD12 | 2.19 | 0.42 |
| 1:A:96:GLU:OE1 | 1:A:264:ALA:O | 2.37 | 0.42 |
| 1:A:131:CYS:HA | 1:A:166:CYS:CB | 2.48 | 0.42 |
| 1:A:239:GLN:HG2 | 1:A:240:THR:O | 2.19 | 0.42 |
| 1:A:455:LEU:HD11 | 1:A:493:GLN:CB | 2.49 | 0.42 |
| 1:A:1101:HIS:ND1 | 4:A:1313:NAG:H5 | 2.34 | 0.42 |
| 1:B:228:ASP:O | 1:B:230:PRO:HD2 | 2.19 | 0.42 |
| 2:E:7:SER:O | 2:E:20:LEU:HD12 | 2.19 | 0.42 |
| 2:E:64:VAL:O | 2:E:67:ARG:HG2 | 2.18 | 0.42 |
| 1:A:103:GLY:HA3 | 1:A:119:ILE:O | 2.20 | 0.42 |
| 1:A:855:PHE:HD1 | 1:C:589:PRO:CG | 2.31 | 0.42 |
| 1:A:897:PRO:CG | 1:C:709:ASN:O | 2.67 | 0.42 |
| 1:A:964:LYS:HD3 | 1:A:964:LYS:O | 2.20 | 0.42 |
| 1:B:466:ARG:O | 1:B:466:ARG:CG | 2.68 | 0.42 |
| 1:C:922:LEU:HA | 1:C:925:ASN:OD1 | 2.18 | 0.42 |
| 2:E:98:SER:C | 2:E:108:PHE:HA | 2.40 | 0.42 |
| 1:A:592:PHE:HE2 | 1:B:857:GLY:HA2 | 1.84 | 0.42 |
| 1:A:878:LEU:HD23 | 1:A:882:ILE:HD11 | 2.01 | 0.42 |
| 1:A:885:GLY:HA3 | 1:A:901:GLN:OE1 | 2.20 | 0.42 |
| 1:A:979:ASP:O | 1:A:983:ARG:HG3 | 2.20 | 0.42 |
| 1:B:216:LEU:O | 1:B:217:PRO:O | 2.37 | 0.42 |
| 1:B:390:LEU:CD1 | 1:C:983:ARG:HG2 | 2.48 | 0.42 |
| 1:B:878:LEU:O | 1:B:882:ILE:HG13 | 2.19 | 0.42 |
| 1:B:898:PHE:HA | 1:B:901:GLN:HB3 | 2.01 | 0.42 |
| 1:C:43:PHE:CE1 | 1:C:283:GLY:CA | 3.00 | 0.42 |
| 1:C:898:PHE:HA | 1:C:901:GLN:HB3 | 2.01 | 0.42 |
| 1:C:1043:CYS:C | 1:C:1064:HIS:ND1 | 2.73 | 0.42 |
| 1:A:128:ILE:HG21 | 1:A:229:LEU:HD11 | 2.01 | 0.42 |
| 1:B:171:VAL:CG2 | 4:B:1301:NAG:H62 | 2.50 | 0.42 |
| 1:B:361:CYS:O | 1:B:524:VAL:HG23 | 2.19 | 0.42 |
| 1:B:465:GLU:OE2 | 1:B:466:ARG:O | 2.37 | 0.42 |
| 1:B:743:CYS:HA | 1:B:977:LEU:HD21 | 2.02 | 0.42 |
| 1:C:765:ARG:O | 1:C:768:THR:OG1 | 2.30 | 0.42 |
| 1:A:743:CYS:HA | 1:A:977:LEU:HD21 | 2.02 | 0.42 |
| 1:A:898:PHE:HA | 1:A:901:GLN:HB3 | 2.01 | 0.42 |
| 1:A:1103:PHE:HB3 | 1:A:1113:GLN:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:133:PHE:CE1 | 1:B:160:TYR:CE2 | 3.08 | 0.42 |
| 1:B:663:ASP:OD1 | 1:B:664:ILE:HG13 | 2.19 | 0.42 |
| 1:B:727:LEU:HD11 | 1:B:1028:LYS:HD2 | 2.02 | 0.42 |
| 1:B:985:ASP:O | 1:B:986:PRO:C | 2.58 | 0.42 |
| 1:C:985:ASP:O | 1:C:986:PRO:C | 2.58 | 0.42 |
| 1:C:1027:THR:O | 1:C:1031:GLU:HG3 | 2.19 | 0.42 |
| 2:D:60:TYR:HD2 | 2:D:64:VAL:CG2 | 2.29 | 0.42 |
| 1:A:133:PHE:CE1 | 1:A:160:TYR:CE2 | 3.08 | 0.42 |
| 1:A:711:SER:O | 1:B:895:GLN:HG2 | 2.19 | 0.42 |
| 1:A:869:MET:HB2 | 1:C:699:LEU:CD1 | 2.48 | 0.42 |
| 1:A:1141:LEU:O | 1:A:1144:GLU:HB2 | 2.20 | 0.42 |
| 1:B:193:VAL:CG2 | 1:B:223:LEU:HD12 | 2.50 | 0.42 |
| 1:B:280:ASN:HB2 | 1:B:286:THR:CG2 | 2.50 | 0.42 |
| 1:B:392:PHE:HE1 | 1:B:517:LEU:HD11 | 1.84 | 0.42 |
| 1:B:772:VAL:HA | 1:B:775:ASP:OD2 | 2.20 | 0.42 |
| 1:B:1103:PHE:HB3 | 1:B:1113:GLN:H | 1.84 | 0.42 |
| 1:C:200:TYR:HD2 | 1:C:228:ASP:OD2 | 2.01 | 0.42 |
| 1:C:964:LYS:O | 1:C:964:LYS:HD3 | 2.20 | 0.42 |
| 2:D:3:GLN:C | 2:D:4:LEU:HD12 | 2.40 | 0.42 |
| 2:D:20:LEU:HD21 | 2:D:36:TRP:CZ3 | 2.55 | 0.42 |
| 2:D:69:THR:CG2 | 2:D:82:GLN:HB3 | 2.29 | 0.42 |
| 2:E:3:GLN:C | 2:E:4:LEU:HD12 | 2.40 | 0.42 |
| 2:E:99:GLY:HA3 | 2:E:107:ASP:OD1 | 2.20 | 0.42 |
| 1:A:666:ILE:CD1 | 1:A:672:ALA:HB2 | 2.50 | 0.42 |
| 1:A:1043:CYS:C | 1:A:1064:HIS:ND1 | 2.73 | 0.42 |
| 4:A:1301:NAG:HO3 | 4:A:1301:NAG:C7 | 2.25 | 0.42 |
| 1:B:103:GLY:HA3 | 1:B:119:ILE:O | 2.20 | 0.42 |
| 1:B:473:TYR:HD2 | 1:B:489:TYR:CD2 | 2.38 | 0.42 |
| 1:B:885:GLY:HA3 | 1:B:901:GLN:OE1 | 2.20 | 0.42 |
| 1:B:964:LYS:O | 1:B:964:LYS:HD3 | 2.20 | 0.42 |
| 2:E:60:TYR:CE2 | 2:E:68:PHE:HB2 | 2.55 | 0.42 |
| 1:A:282:ASN:HD22 | 4:A:1303:NAG:C1 | 2.23 | 0.42 |
| 1:A:308:VAL:HB | 1:A:602:THR:HG23 | 2.02 | 0.42 |
| 1:A:592:PHE:CE2 | 1:B:857:GLY:HA2 | 2.55 | 0.42 |
| 1:A:663:ASP:OD1 | 1:A:664:ILE:HG13 | 2.19 | 0.42 |
| 1:A:985:ASP:O | 1:A:986:PRO:C | 2.58 | 0.42 |
| 1:B:555:SER:OG | 1:B:586:ASP:OD1 | 2.35 | 0.42 |
| 1:B:878:LEU:HD23 | 1:B:882:ILE:HD11 | 2.01 | 0.42 |
| 1:B:1043:CYS:C | 1:B:1064:HIS:ND1 | 2.73 | 0.42 |
| 1:C:103:GLY:HA3 | 1:C:119:ILE:O | 2.20 | 0.42 |
| 1:C:359:SER:OG | 1:C:394:ASN:OD1 | 2.25 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:962:LEU:HD12 | 1:C:962:LEU:O | 2.18 | 0.42 |
| 1:C:1075:PHE:HB3 | 1:C:1096:VAL:HB | 2.01 | 0.42 |
| 1:A:139:PRO:HD2 | 1:A:239:GLN:OE1 | 2.20 | 0.41 |
| 1:A:752:LEU:HG | 1:A:752:LEU:H | 1.75 | 0.41 |
| 1:C:228:ASP:O | 1:C:230:PRO:HD2 | 2.19 | 0.41 |
| 2:D:99:GLY:HA3 | 2:D:107:ASP:OD1 | 2.20 | 0.41 |
| 1:A:597:VAL:HG13 | 1:A:608:VAL:HG11 | 2.02 | 0.41 |
| 1:A:770:ILE:CG1 | 1:A:770:ILE:HG23 | 1.97 | 0.41 |
| 1:B:378:LYS:HD3 | 2:E:106:TYR:CE2 | 2.56 | 0.41 |
| 1:B:907:ASN:HA | 1:B:911:VAL:O | 2.21 | 0.41 |
| 1:C:411:ALA:HB3 | 1:C:414:GLN:NE2 | 2.35 | 0.41 |
| 1:C:885:GLY:HA3 | 1:C:901:GLN:OE1 | 2.20 | 0.41 |
| 1:C:905:ARG:HG2 | 1:C:905:ARG:H | 1.52 | 0.41 |
| 1:C:1103:PHE:HB3 | 1:C:1113:GLN:H | 1.84 | 0.41 |
| 1:A:228:ASP:O | 1:A:230:PRO:HD2 | 2.19 | 0.41 |
| 1:A:713:ALA:O | 1:B:894:LEU:HD13 | 2.20 | 0.41 |
| 1:B:385:THR:O | 1:B:385:THR:HG23 | 2.20 | 0.41 |
| 1:B:979:ASP:O | 1:B:983:ARG:HG3 | 2.20 | 0.41 |
| 1:B:993:ILE:O | 1:B:997:ILE:HG12 | 2.21 | 0.41 |
| 1:B:997:ILE:HD12 | 1:B:997:ILE:HG21 | 1.82 | 0.41 |
| 1:C:216:LEU:O | 1:C:217:PRO:O | 2.37 | 0.41 |
| 2:E:93:LEU:HD22 | 2:E:95:TYR:CE2 | 2.54 | 0.41 |
| 1:A:61:ASN:OD1 | 1:A:61:ASN:N | 2.51 | 0.41 |
| 1:A:141:LEU:CD2 | 1:A:157:PHE:HD2 | 2.33 | 0.41 |
| 1:A:727:LEU:HD11 | 1:A:1028:LYS:HD2 | 2.02 | 0.41 |
| 1:B:391:CYS:HB2 | 1:B:524:VAL:O | 2.20 | 0.41 |
| 1:B:517:LEU:N | 1:B:517:LEU:HD12 | 2.35 | 0.41 |
| 1:B:558:LYS:NZ | 4:C:1301:NAG:H82 | 2.34 | 0.41 |
| 1:C:81:ASN:N | 1:C:82:PRO:HD3 | 2.36 | 0.41 |
| 1:C:128:ILE:HG21 | 1:C:229:LEU:HD11 | 2.01 | 0.41 |
| 1:C:979:ASP:O | 1:C:983:ARG:HG3 | 2.20 | 0.41 |
| 1:A:737:ASP:OD1 | 1:A:739:THR:OG1 | 2.32 | 0.41 |
| 1:B:707:TYR:CE2 | 1:C:896:ILE:O | 2.74 | 0.41 |
| 2:D:91:THR:O | 2:D:92:ALA:HB2 | 2.21 | 0.41 |
| 1:A:53:ASP:OD2 | 1:A:55:PHE:CD2 | 2.74 | 0.41 |
| 1:A:411:ALA:HB3 | 1:A:414:GLN:NE2 | 2.35 | 0.41 |
| 1:B:1028:LYS:O | 1:B:1029:MET:C | 2.59 | 0.41 |
| 1:B:1075:PHE:HB3 | 1:B:1096:VAL:HB | 2.01 | 0.41 |
| 1:C:149:ASN:OD1 | 1:C:149:ASN:O | 2.39 | 0.41 |
| 1:C:280:ASN:HB2 | 1:C:286:THR:CG2 | 2.50 | 0.41 |
| 1:C:410:ILE:O | 1:C:410:ILE:HG22 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:374:PHE:C | 1:B:376:THR:N | 2.73 | 0.41 |
| 1:C:133:PHE:CE1 | 1:C:160:TYR:CE2 | 3.08 | 0.41 |
| 1:C:139:PRO:HD2 | 1:C:239:GLN:OE1 | 2.20 | 0.41 |
| 1:C:410:ILE:HD13 | 1:C:510:VAL:HG11 | 2.03 | 0.41 |
| 1:C:666:ILE:CD1 | 1:C:672:ALA:HB2 | 2.50 | 0.41 |
| 1:C:727:LEU:HD11 | 1:C:1028:LYS:HD2 | 2.02 | 0.41 |
| 1:C:812:PRO:O | 1:C:813:SER:HB3 | 2.21 | 0.41 |
| 1:C:993:ILE:O | 1:C:997:ILE:HG12 | 2.21 | 0.41 |
| 2:D:4:LEU:HD13 | 2:D:110:ASN:HB3 | 2.01 | 0.41 |
| 2:E:68:PHE:HD2 | 2:E:81:LEU:HD11 | 1.81 | 0.41 |
| 1:A:96:GLU:OE2 | 1:A:263:ALA:CB | 2.69 | 0.41 |
| 1:A:280:ASN:HB2 | 1:A:286:THR:CG2 | 2.50 | 0.41 |
| 1:B:81:ASN:N | 1:B:82:PRO:HD3 | 2.36 | 0.41 |
| 1:B:139:PRO:HD2 | 1:B:239:GLN:OE1 | 2.20 | 0.41 |
| 1:B:812:PRO:O | 1:B:813:SER:HB3 | 2.21 | 0.41 |
| 1:C:43:PHE:CZ | 1:C:45:SER:HB2 | 2.56 | 0.41 |
| 1:C:658:ASN:CG | 1:C:659:SER:H | 2.24 | 0.41 |
| 1:C:743:CYS:HA | 1:C:977:LEU:HD21 | 2.02 | 0.41 |
| 1:C:1096:VAL:CA | 1:C:1102:TRP:HZ3 | 2.34 | 0.41 |
| 2:D:37:PHE:CE2 | 2:D:95:TYR:HD1 | 2.38 | 0.41 |
| 1:A:388:ASN:CB | 1:A:527:PRO:HD2 | 2.51 | 0.41 |
| 1:A:410:ILE:HD13 | 1:A:510:VAL:HG11 | 2.03 | 0.41 |
| 1:A:565:PHE:CE2 | 1:B:42:VAL:HG22 | 2.56 | 0.41 |
| 1:A:657:ASN:HB2 | 4:A:1309:NAG:H2 | 2.02 | 0.41 |
| 1:A:712:ILE:HG13 | 1:B:895:GLN:O | 2.21 | 0.41 |
| 1:A:746:SER:CB | 1:A:977:LEU:HD11 | 2.51 | 0.41 |
| 1:A:767:LEU:HD21 | 1:A:1008:VAL:CG2 | 2.51 | 0.41 |
| 1:A:781:VAL:CG2 | 1:A:782:PHE:CD2 | 3.04 | 0.41 |
| 1:A:812:PRO:O | 1:A:813:SER:HB3 | 2.21 | 0.41 |
| 1:A:986:PRO:O | 1:A:990:GLU:HG3 | 2.21 | 0.41 |
| 1:A:1040:VAL:CG1 | 1:B:1030:SER:O | 2.69 | 0.41 |
| 1:A:1088:HIS:CE1 | 1:A:1122:VAL:HG23 | 2.56 | 0.41 |
| 1:B:53:ASP:OD2 | 1:B:55:PHE:CD2 | 2.74 | 0.41 |
| 1:B:308:VAL:HB | 1:B:602:THR:HG23 | 2.02 | 0.41 |
| 1:B:378:LYS:CE | 1:B:380:TYR:OH | 2.69 | 0.41 |
| 1:B:666:ILE:CD1 | 1:B:672:ALA:HB2 | 2.50 | 0.41 |
| 1:B:747:THR:O | 1:B:751:ASN:OD1 | 2.39 | 0.41 |
| 1:B:1088:HIS:CE1 | 1:B:1122:VAL:HG23 | 2.56 | 0.41 |
| 1:C:53:ASP:OD2 | 1:C:55:PHE:CD2 | 2.74 | 0.41 |
| 1:C:97:LYS:O | 1:C:97:LYS:HD3 | 2.21 | 0.41 |
| 1:C:781:VAL:CG2 | 1:C:782:PHE:CD2 | 3.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1028:LYS:O | 1:C:1029:MET:C | 2.59 | 0.41 |
| 1:C:1088:HIS:CE1 | 1:C:1122:VAL:HG23 | 2.56 | 0.41 |
| 2:D:38:ARG:CD | 2:D:92:ALA:HB3 | 2.51 | 0.41 |
| 2:E:1:GLN:O | 2:E:1:GLN:HG2 | 2.20 | 0.41 |
| 2:E:20:LEU:HD21 | 2:E:36:TRP:CZ3 | 2.55 | 0.41 |
| 2:E:106:TYR:O | 2:E:108:PHE:O | 2.38 | 0.41 |
| 1:A:918:GLU:HG2 | 1:C:1128:VAL:HG11 | 2.03 | 0.41 |
| 1:A:993:ILE:O | 1:A:997:ILE:HG12 | 2.21 | 0.41 |
| 1:A:1074:ASN:O | 1:A:1075:PHE:CD1 | 2.74 | 0.41 |
| 1:B:531:THR:HG22 | 1:B:532:ASN:N | 2.35 | 0.41 |
| 1:B:569:ILE:O | 1:B:570:ALA:HB3 | 2.21 | 0.41 |
| 1:B:746:SER:CB | 1:B:977:LEU:HD11 | 2.51 | 0.41 |
| 1:B:781:VAL:CG2 | 1:B:782:PHE:CD2 | 3.04 | 0.41 |
| 1:B:824:ASN:OD1 | 1:B:824:ASN:N | 2.43 | 0.41 |
| 1:B:1141:LEU:O | 1:B:1144:GLU:HB2 | 2.20 | 0.41 |
| 1:C:986:PRO:O | 1:C:990:GLU:HG3 | 2.21 | 0.41 |
| 2:D:1:GLN:O | 2:D:1:GLN:HG2 | 2.20 | 0.41 |
| 2:E:91:THR:O | 2:E:92:ALA:HB2 | 2.21 | 0.41 |
| 1:A:410:ILE:O | 1:A:410:ILE:HG22 | 2.20 | 0.40 |
| 1:A:658:ASN:CG | 1:A:659:SER:H | 2.24 | 0.40 |
| 1:A:907:ASN:HA | 1:A:911:VAL:O | 2.20 | 0.40 |
| 1:A:911:VAL:HG12 | 1:A:1106:GLN:HE22 | 1.86 | 0.40 |
| 1:A:1094:VAL:HG12 | 1:B:904:TYR:OH | 2.21 | 0.40 |
| 1:B:376:THR:N | 1:B:435:ALA:O | 2.54 | 0.40 |
| 1:B:784:GLN:OE1 | 1:B:1034:LEU:HD11 | 2.21 | 0.40 |
| 1:B:922:LEU:CD1 | 4:B:1310:NAG:H62 | 2.44 | 0.40 |
| 1:B:954:GLN:OE1 | 1:B:1014:ARG:CD | 2.69 | 0.40 |
| 1:C:308:VAL:HB | 1:C:602:THR:HG23 | 2.02 | 0.40 |
| 1:C:455:LEU:HD11 | 1:C:493:GLN:CB | 2.51 | 0.40 |
| 1:C:907:ASN:HA | 1:C:911:VAL:O | 2.21 | 0.40 |
| 1:C:954:GLN:OE1 | 1:C:1014:ARG:CD | 2.69 | 0.40 |
| 2:E:93:LEU:HD23 | 2:E:115:THR:C | 2.41 | 0.40 |
| 1:A:43:PHE:CZ | 1:A:45:SER:HB2 | 2.56 | 0.40 |
| 1:A:97:LYS:O | 1:A:97:LYS:HD3 | 2.21 | 0.40 |
| 1:A:1074:ASN:C | 1:A:1075:PHE:CG | 2.95 | 0.40 |
| 1:A:1096:VAL:CA | 1:A:1102:TRP:HZ3 | 2.34 | 0.40 |
| 1:B:141:LEU:CD2 | 1:B:157:PHE:HD2 | 2.33 | 0.40 |
| 1:B:262:ALA:O | 1:B:263:ALA:HB2 | 2.22 | 0.40 |
| 1:B:986:PRO:O | 1:B:990:GLU:HG3 | 2.21 | 0.40 |
| 1:C:767:LEU:HD21 | 1:C:1008:VAL:CG2 | 2.51 | 0.40 |
| 1:C:772:VAL:HA | 1:C:775:ASP:OD2 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:484:GLU:HG2 | 1:A:485:GLY:N | 2.37 | 0.40 |
| 1:A:733:LYS:NZ | 1:A:775:ASP:OD1 | 2.48 | 0.40 |
| 1:A:772:VAL:HA | 1:A:775:ASP:OD2 | 2.20 | 0.40 |
| 1:B:407:VAL:CG2 | 2:E:106:TYR:HE1 | 2.34 | 0.40 |
| 1:C:746:SER:CB | 1:C:977:LEU:HD11 | 2.51 | 0.40 |
| 2:D:93:LEU:HD22 | 2:D:95:TYR:CE2 | 2.54 | 0.40 |
| 1:A:278:LYS:HB2 | 1:A:306:PHE:CE2 | 2.57 | 0.40 |
| 1:A:705:VAL:HG23 | 1:B:789:TYR:CD1 | 2.50 | 0.40 |
| 1:A:747:THR:O | 1:A:751:ASN:OD1 | 2.39 | 0.40 |
| 1:B:97:LYS:O | 1:B:97:LYS:HD3 | 2.21 | 0.40 |
| 1:B:149:ASN:O | 1:B:149:ASN:OD1 | 2.39 | 0.40 |
| 1:B:695:TYR:HE1 | 1:B:697:MET:HA | 1.87 | 0.40 |
| 1:B:777:ASN:HB3 | 1:B:1022:ALA:CB | 2.52 | 0.40 |
| 1:B:1040:VAL:O | 1:B:1041:ASP:HB2 | 2.22 | 0.40 |
| 1:B:1062:PHE:HB3 | 1:B:1064:HIS:NE2 | 2.37 | 0.40 |
| 1:C:141:LEU:CD2 | 1:C:157:PHE:HD2 | 2.33 | 0.40 |
| 1:C:330:PRO:HA | 1:C:579:PRO:HB2 | 2.03 | 0.40 |
| 1:C:747:THR:O | 1:C:751:ASN:OD1 | 2.39 | 0.40 |
| 1:C:1141:LEU:O | 1:C:1144:GLU:HB2 | 2.20 | 0.40 |
| 2:D:39:GLN:O | 2:D:92:ALA:HB1 | 2.21 | 0.40 |
| 2:D:60:TYR:OH | 2:D:69:THR:C | 2.60 | 0.40 |
| 2:D:106:TYR:O | 2:D:108:PHE:O | 2.38 | 0.40 |
| 2:E:39:GLN:O | 2:E:92:ALA:HB1 | 2.21 | 0.40 |
| 1:B:96:GLU:OE2 | 1:B:263:ALA:CB | 2.69 | 0.40 |
| 1:B:1089:PHE:CD1 | 1:C:914:ASN:HB3 | 2.56 | 0.40 |
| 1:C:310:LYS:C | 1:C:310:LYS:HD2 | 2.42 | 0.40 |
| 1:C:502:GLY:O | 1:C:506:GLN:N | 2.55 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 1044/1264 (83%) | 948 (91%) | 94 (9%) | 2 (0%) | 44 | 73 |
| 1 | B | 1039/1264 (82%) | 938 (90%) | 99 (10%) | 2 (0%) | 44 | 73 |
| 1 | C | 1042/1264 (82%) | 946 (91%) | 92 (9%) | 4 (0%) | 30 | 63 |
| 2 | D | 118/126 (94%) | 114 (97%) | 4 (3%) | 0 | 100 | 100 |
| 2 | E | 118/126 (94%) | 114 (97%) | 4 (3%) | 0 | 100 | 100 |
| All | All | 3361/4044 (83%) | 3060 (91%) | 293 (9%) | 8 (0%) | 45 | 73 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 459 | SER |
| 1 | A | 25 | PRO |
| 1 | A | 699 | LEU |
| 1 | B | 25 | PRO |
| 1 | B | 699 | LEU |
| 1 | C | 25 | PRO |
| 1 | C | 699 | LEU |
| 1 | C | 709 | ASN |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 931/1100 (85%) | 891 (96%) | 40 (4%) | 25 | 54 |
| 1 | B | 925/1100 (84%) | 887 (96%) | 38 (4%) | 26 | 55 |
| 1 | C | 929/1100 (84%) | 892 (96%) | 37 (4%) | 27 | 56 |
| 2 | D | 92/97 (95%) | 86 (94%) | 6 (6%) | 14 | 42 |
| 2 | E | 92/97 (95%) | 86 (94%) | 6 (6%) | 14 | 42 |
| All | All | 2969/3494 (85%) | 2842 (96%) | 127 (4%) | 27 | 54 |

All (127) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 43 | PHE |
| 1 | A | 53 | ASP |
| 1 | A | 160 | TYR |
| 1 | A | 192 | PHE |
| 1 | A | 206 | LYS |
| 1 | A | 216 | LEU |
| 1 | A | 241 | LEU |
| 1 | A | 269 | TYR |
| 1 | A | 286 | THR |
| 1 | A | 294 | ASP |
| 1 | A | 329 | PHE |
| 1 | A | 477[A] | SER |
| 1 | A | 477[B] | SER |
| 1 | A | 643 | PHE |
| 1 | A | 730 | SER |
| 1 | A | 741 | TYR |
| 1 | A | 751 | ASN |
| 1 | A | 761 | THR |
| 1 | A | 767 | LEU |
| 1 | A | 777 | ASN |
| 1 | A | 781 | VAL |
| 1 | A | 791 | THR |
| 1 | A | 802 | PHE |
| 1 | A | 817 | PHE |
| 1 | A | 869 | MET |
| 1 | A | 873 | TYR |
| 1 | A | 886 | TRP |
| 1 | A | 887 | THR |
| 1 | A | 926 | GLN |
| 1 | A | 928 | ASN |
| 1 | A | 961 | THR |
| 1 | A | 1002 | GLN |
| 1 | A | 1005 | GLN |
| 1 | A | 1014 | ARG |
| 1 | A | 1040 | VAL |
| 1 | A | 1091 | ARG |
| 1 | A | 1102 | TRP |
| 1 | A | 1106 | GLN |
| 1 | A | 1118 | ASP |
| 1 | A | 1122 | VAL |
| 1 | B | 43 | PHE |
| 1 | B | 53 | ASP |
| 1 | B | 160 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 192 | PHE |
| 1 | B | 206 | LYS |
| 1 | B | 216 | LEU |
| 1 | B | 241 | LEU |
| 1 | B | 269 | TYR |
| 1 | B | 286 | THR |
| 1 | B | 294 | ASP |
| 1 | B | 444 | LYS |
| 1 | B | 643 | PHE |
| 1 | B | 730 | SER |
| 1 | B | 741 | TYR |
| 1 | B | 751 | ASN |
| 1 | B | 761 | THR |
| 1 | B | 767 | LEU |
| 1 | B | 777 | ASN |
| 1 | B | 781 | VAL |
| 1 | B | 791 | THR |
| 1 | B | 802 | PHE |
| 1 | B | 817 | PHE |
| 1 | B | 869 | MET |
| 1 | B | 873 | TYR |
| 1 | B | 886 | TRP |
| 1 | B | 887 | THR |
| 1 | B | 926 | GLN |
| 1 | B | 928 | ASN |
| 1 | B | 961 | THR |
| 1 | B | 1002 | GLN |
| 1 | B | 1005 | GLN |
| 1 | B | 1014 | ARG |
| 1 | B | 1040 | VAL |
| 1 | B | 1091 | ARG |
| 1 | B | 1102 | TRP |
| 1 | B | 1106 | GLN |
| 1 | B | 1118 | ASP |
| 1 | B | 1122 | VAL |
| 1 | C | 43 | PHE |
| 1 | C | 53 | ASP |
| 1 | C | 160 | TYR |
| 1 | C | 192 | PHE |
| 1 | C | 206 | LYS |
| 1 | C | 216 | LEU |
| 1 | C | 241 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 269 | TYR |
| 1 | C | 286 | THR |
| 1 | C | 294 | ASP |
| 1 | C | 643 | PHE |
| 1 | C | 730 | SER |
| 1 | C | 741 | TYR |
| 1 | C | 751 | ASN |
| 1 | C | 761 | THR |
| 1 | C | 767 | LEU |
| 1 | C | 777 | ASN |
| 1 | C | 781 | VAL |
| 1 | C | 791 | THR |
| 1 | C | 802 | PHE |
| 1 | C | 817 | PHE |
| 1 | C | 869 | MET |
| 1 | C | 873 | TYR |
| 1 | C | 886 | TRP |
| 1 | C | 887 | THR |
| 1 | C | 926 | GLN |
| 1 | C | 928 | ASN |
| 1 | C | 961 | THR |
| 1 | C | 1002 | GLN |
| 1 | C | 1005 | GLN |
| 1 | C | 1014 | ARG |
| 1 | C | 1040 | VAL |
| 1 | C | 1091 | ARG |
| 1 | C | 1102 | TRP |
| 1 | C | 1106 | GLN |
| 1 | C | 1118 | ASP |
| 1 | C | 1122 | VAL |
| 2 | D | 37 | PHE |
| 2 | D | 52 | TYR |
| 2 | D | 59 | ASN |
| 2 | D | 80 | TYR |
| 2 | D | 95 | TYR |
| 2 | D | 108 | PHE |
| 2 | E | 37 | PHE |
| 2 | E | 52 | TYR |
| 2 | E | 59 | ASN |
| 2 | E | 80 | TYR |
| 2 | E | 95 | TYR |
| 2 | E | 108 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 66 | HIS |
| 1 | A | 99 | ASN |
| 1 | A | 165 | ASN |
| 1 | A | 207 | HIS |
| 1 | A | 603 | ASN |
| 1 | A | 1002 | GLN |
| 1 | A | 1005 | GLN |
| 1 | A | 1119 | ASN |
| 1 | B | 66 | HIS |
| 1 | B | 99 | ASN |
| 1 | B | 207 | HIS |
| 1 | B | 1002 | GLN |
| 1 | B | 1119 | ASN |
| 1 | C | 66 | HIS |
| 1 | C | 99 | ASN |
| 1 | C | 207 | HIS |
| 1 | C | 616 | ASN |
| 1 | C | 957 | GLN |
| 1 | C | 1119 | ASN |

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 ⓘ

10 monosaccharides 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 |
| 3 | NAG | F | 1 | 3 | 14,14,15 | 1.19 | 1 (7%) | 17,19,21 | 0.87 | 0 |
| 3 | NAG | F | 2 | 3 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.32 | 0 |
| 3 | NAG | G | 1 | 3 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | NAG | G | 2 | 3 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | NAG | H | 1 | 3 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | NAG | H | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | NAG | I | 1 | 3 | 14,14,15 | 0.70 | 1 (7%) | 17,19,21 | 0.52 | 0 |
| 3 | NAG | I | 2 | 3 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.38 | 0 |
| 3 | NAG | J | 1 | 3,1 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.70 | 1 (5%) |
| 3 | NAG | J | 2 | 3 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.46 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3 | NAG | F | 1 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | F | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | G | 1 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | G | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | H | 1 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | H | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | I | 1 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | I | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | J | 1 | 3,1 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | J | 2 | 3 | - | 0/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | F | 1 | NAG | C1-C2 | 4.21 | 1.58 | 1.52 |
| 3 | I | 1 | NAG | O5-C1 | -2.59 | 1.39 | 1.43 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3 | J | 1 | NAG | C1-O5-C5 | 2.21 | 115.19 | 112.19 |

There are no chirality outliers.

All (22) torsion outliers are listed below:

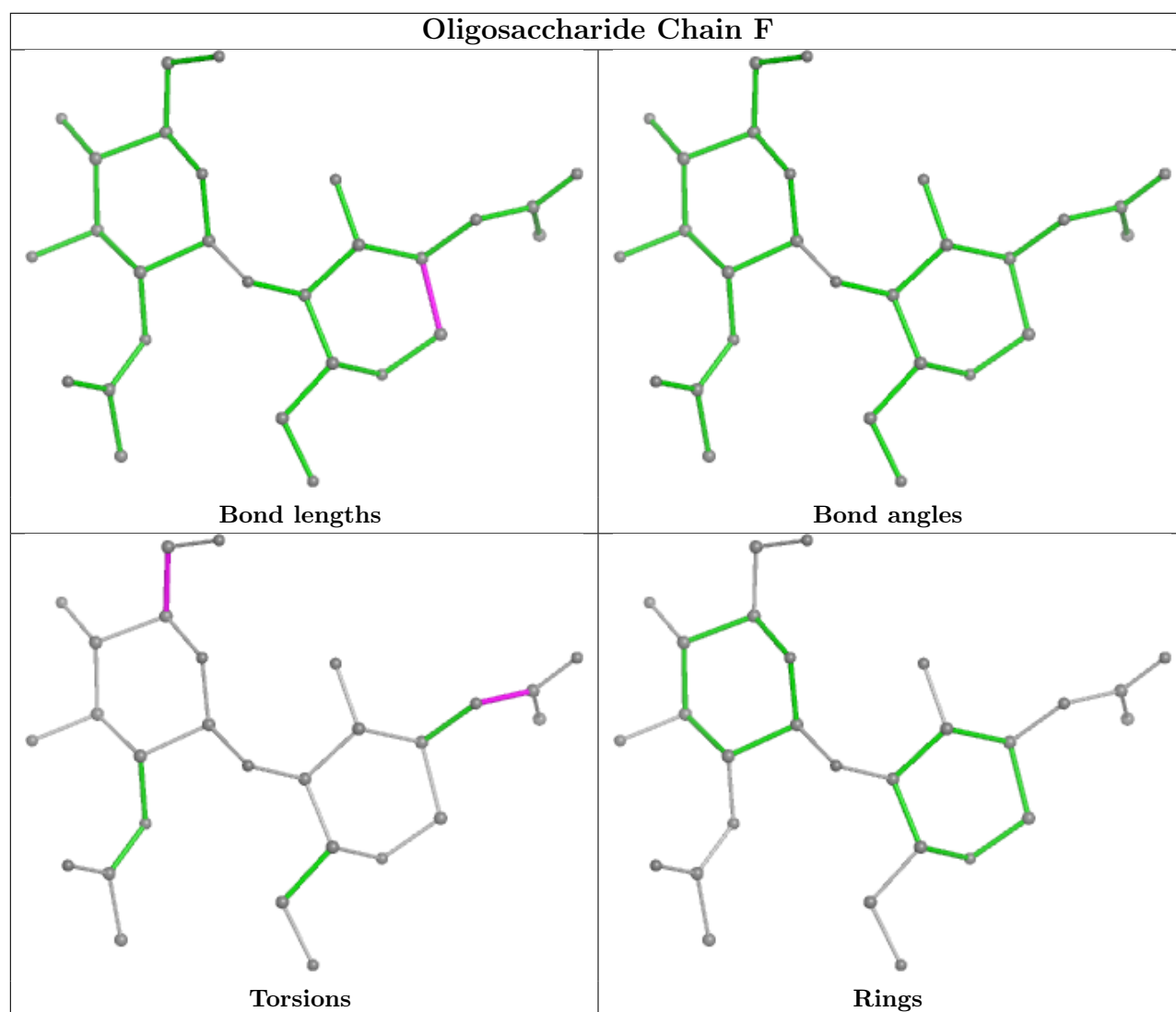
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | G | 1 | NAG | O5-C5-C6-O6 |
| 3 | G | 2 | NAG | O5-C5-C6-O6 |
| 3 | G | 1 | NAG | C4-C5-C6-O6 |
| 3 | F | 2 | NAG | O5-C5-C6-O6 |
| 3 | F | 2 | NAG | C4-C5-C6-O6 |
| 3 | J | 1 | NAG | C4-C5-C6-O6 |
| 3 | F | 1 | NAG | C8-C7-N2-C2 |
| 3 | F | 1 | NAG | O7-C7-N2-C2 |
| 3 | G | 1 | NAG | C8-C7-N2-C2 |
| 3 | G | 1 | NAG | O7-C7-N2-C2 |
| 3 | H | 2 | NAG | C8-C7-N2-C2 |
| 3 | H | 2 | NAG | O7-C7-N2-C2 |
| 3 | I | 1 | NAG | C8-C7-N2-C2 |
| 3 | I | 1 | NAG | O7-C7-N2-C2 |
| 3 | G | 2 | NAG | C4-C5-C6-O6 |
| 3 | I | 1 | NAG | O5-C5-C6-O6 |
| 3 | I | 2 | NAG | O5-C5-C6-O6 |
| 3 | J | 1 | NAG | O5-C5-C6-O6 |
| 3 | H | 1 | NAG | O5-C5-C6-O6 |
| 3 | H | 1 | NAG | C4-C5-C6-O6 |
| 3 | I | 1 | NAG | C4-C5-C6-O6 |
| 3 | I | 2 | NAG | C4-C5-C6-O6 |

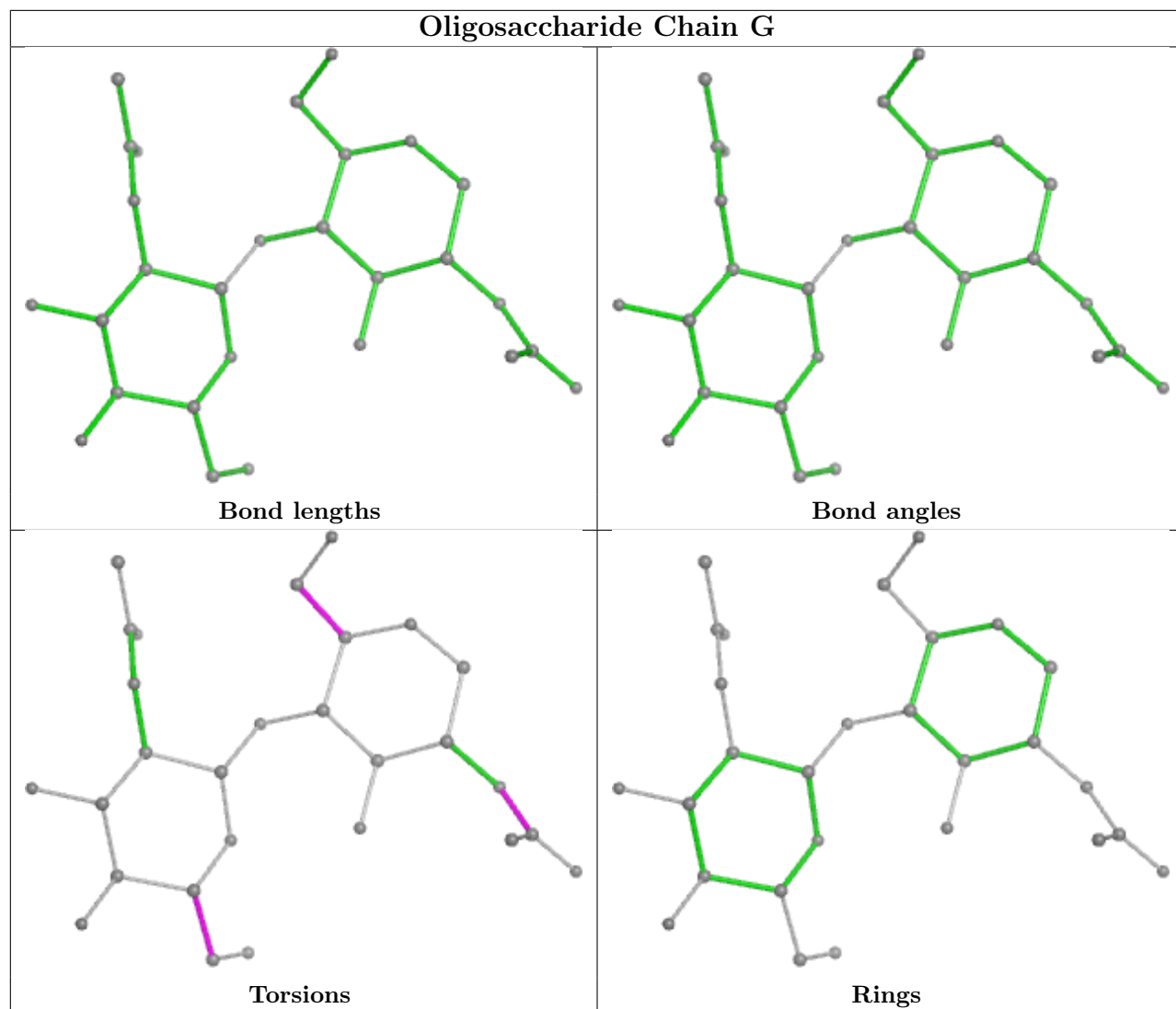
There are no ring outliers.

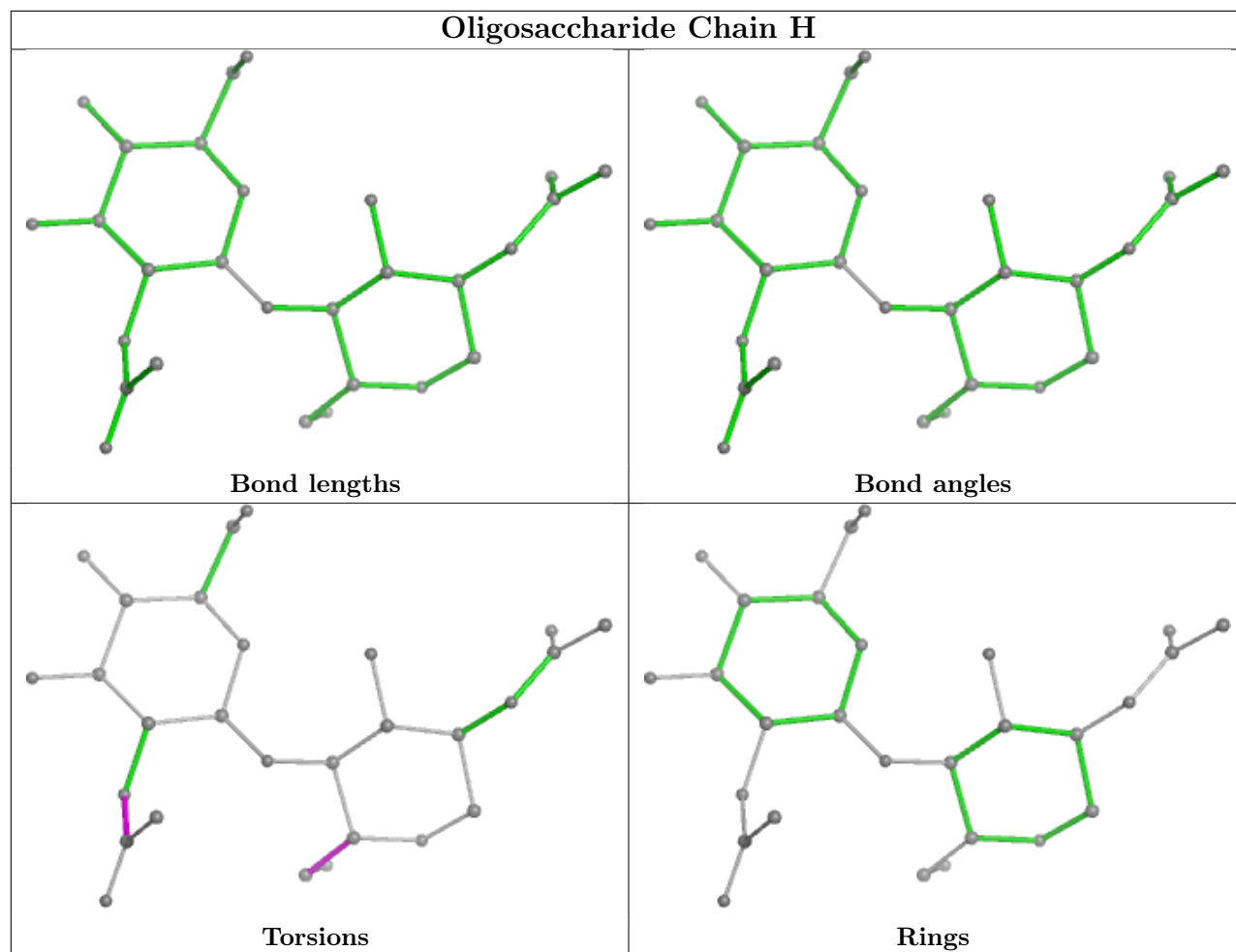
3 monomers are involved in 5 short contacts:

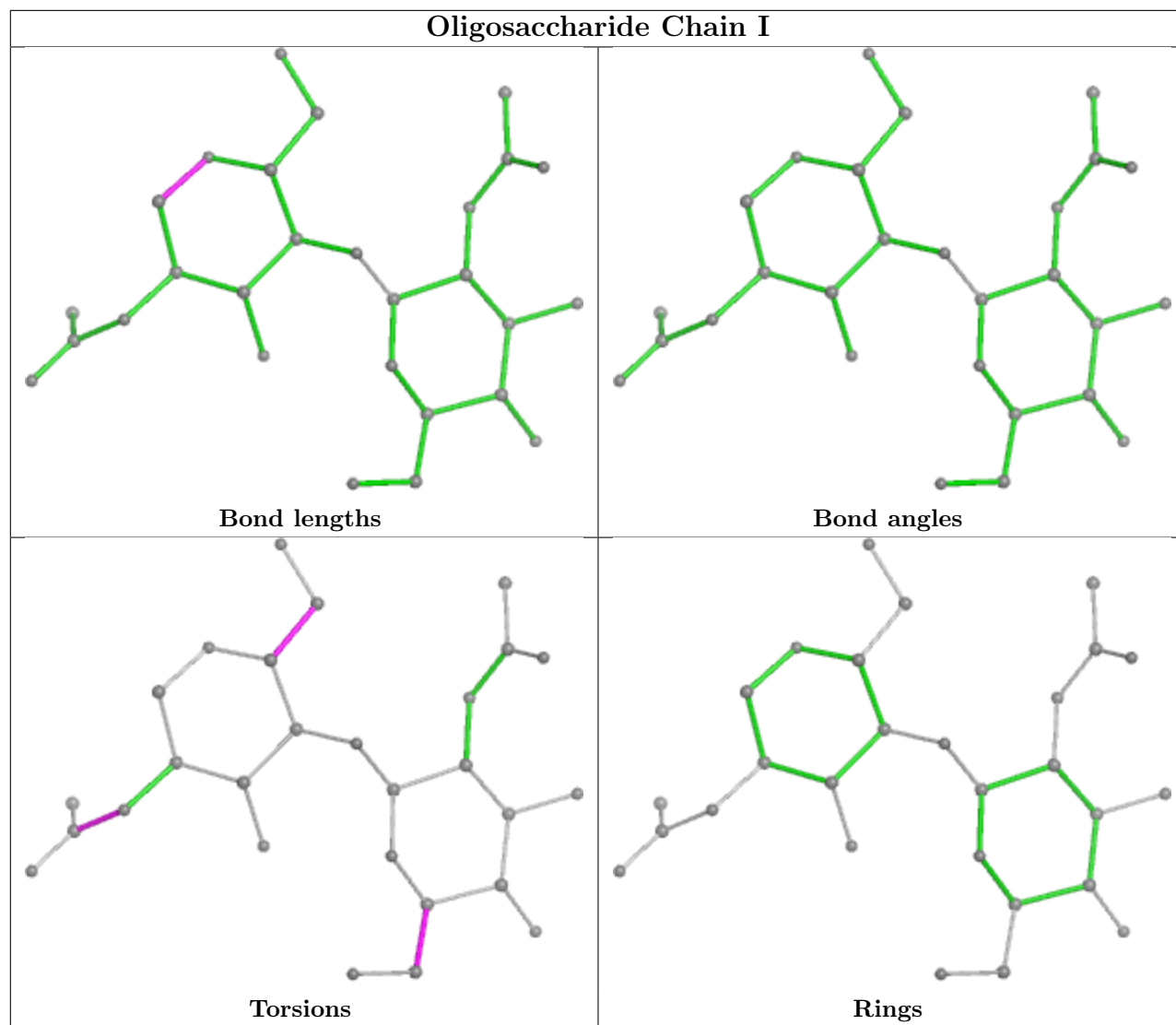
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | I | 1 | NAG | 1 | 0 |
| 3 | F | 1 | NAG | 2 | 0 |
| 3 | J | 1 | NAG | 2 | 0 |

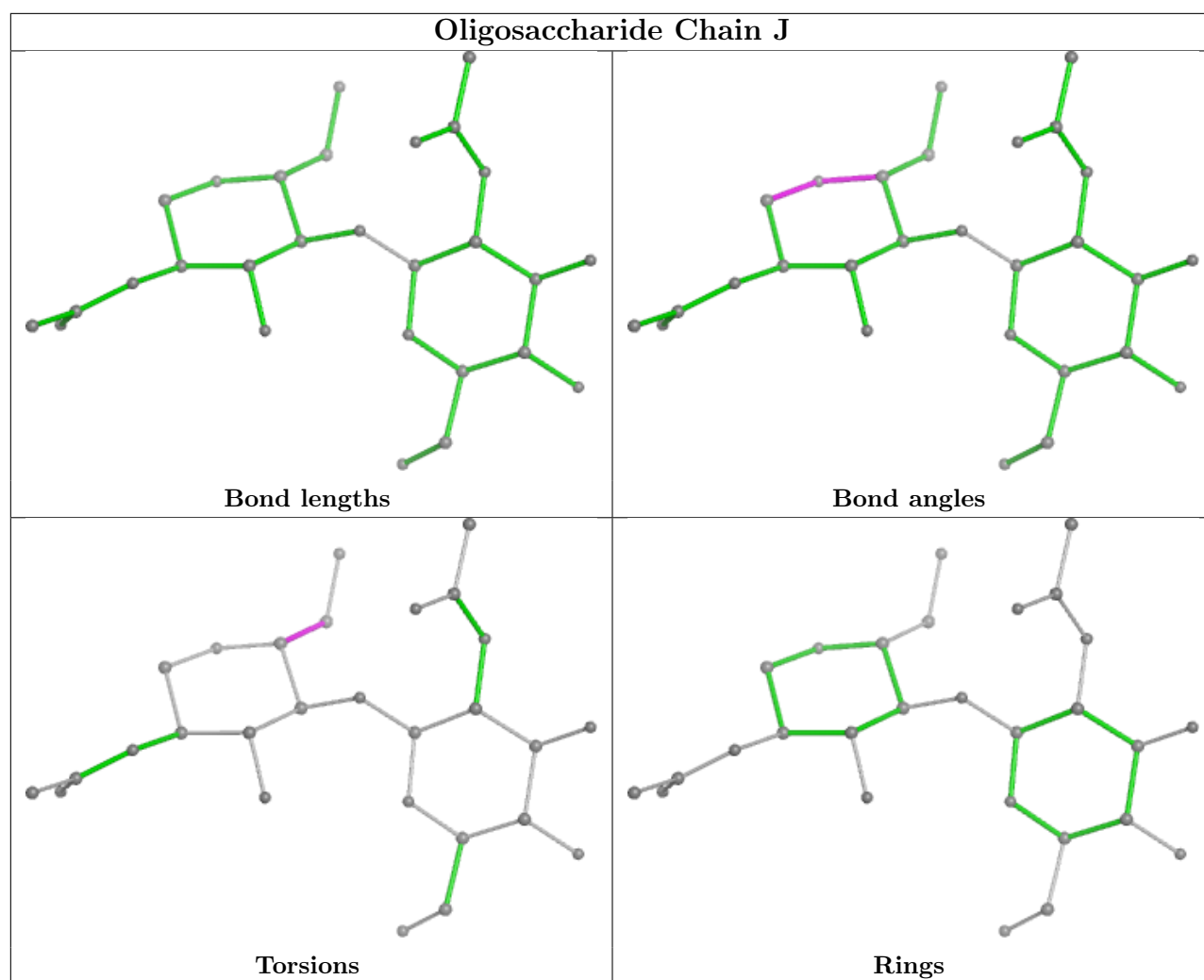
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

33 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 | $\# Z > 2$ |
| 4 | NAG | A | 1307 | 1 | 14,14,15 | 1.66 | 2 (14%) | 17,19,21 | 2.00 | 1 (5%) |
| 4 | NAG | B | 1304 | 1 | 14,14,15 | 1.81 | 2 (14%) | 17,19,21 | 1.12 | 2 (11%) |
| 4 | NAG | B | 1306 | - | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.38 | 0 |
| 4 | NAG | B | 1301 | - | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.46 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAG | A | 1306 | - | 14,14,15 | 0.63 | 0 | 17,19,21 | 0.45 | 0 |
| 4 | NAG | B | 1308 | 1 | 14,14,15 | 1.17 | 2 (14%) | 17,19,21 | 0.94 | 1 (5%) |
| 4 | NAG | C | 1305 | 1 | 14,14,15 | 2.18 | 1 (7%) | 17,19,21 | 2.18 | 1 (5%) |
| 4 | NAG | B | 1309 | 1 | 14,14,15 | 1.06 | 1 (7%) | 17,19,21 | 0.69 | 0 |
| 4 | NAG | A | 1304 | 1 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.43 | 0 |
| 4 | NAG | A | 1301 | - | 14,14,15 | 0.89 | 1 (7%) | 17,19,21 | 0.66 | 0 |
| 4 | NAG | A | 1312 | - | 14,14,15 | 0.65 | 1 (7%) | 17,19,21 | 0.77 | 1 (5%) |
| 4 | NAG | B | 1310 | 1 | 14,14,15 | 3.30 | 2 (14%) | 17,19,21 | 2.13 | 1 (5%) |
| 4 | NAG | C | 1303 | 1 | 14,14,15 | 0.87 | 1 (7%) | 17,19,21 | 0.66 | 1 (5%) |
| 4 | NAG | A | 1309 | 1 | 14,14,15 | 1.29 | 1 (7%) | 17,19,21 | 1.02 | 1 (5%) |
| 4 | NAG | B | 1313 | 1 | 14,14,15 | 0.98 | 1 (7%) | 17,19,21 | 0.69 | 1 (5%) |
| 4 | NAG | A | 1310 | 1 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.35 | 0 |
| 4 | NAG | B | 1312 | - | 14,14,15 | 2.78 | 2 (14%) | 17,19,21 | 1.04 | 1 (5%) |
| 4 | NAG | C | 1306 | 1 | 14,14,15 | 2.34 | 2 (14%) | 17,19,21 | 1.28 | 1 (5%) |
| 4 | NAG | C | 1301 | 1 | 14,14,15 | 0.92 | 1 (7%) | 17,19,21 | 0.95 | 1 (5%) |
| 4 | NAG | A | 1308 | 1 | 14,14,15 | 0.47 | 0 | 17,19,21 | 1.37 | 1 (5%) |
| 4 | NAG | C | 1304 | - | 14,14,15 | 1.00 | 2 (14%) | 17,19,21 | 1.45 | 3 (17%) |
| 4 | NAG | B | 1302 | - | 14,14,15 | 0.56 | 0 | 17,19,21 | 0.44 | 0 |
| 4 | NAG | A | 1313 | 1 | 14,14,15 | 0.74 | 1 (7%) | 17,19,21 | 0.41 | 0 |
| 4 | NAG | B | 1303 | - | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.52 | 0 |
| 4 | NAG | C | 1302 | 1 | 14,14,15 | 0.51 | 0 | 17,19,21 | 1.10 | 2 (11%) |
| 4 | NAG | A | 1302 | - | 14,14,15 | 0.16 | 0 | 17,19,21 | 0.61 | 0 |
| 4 | NAG | B | 1305 | - | 14,14,15 | 0.69 | 1 (7%) | 17,19,21 | 0.51 | 0 |
| 4 | NAG | B | 1307 | - | 14,14,15 | 0.61 | 0 | 17,19,21 | 0.73 | 1 (5%) |
| 4 | NAG | A | 1311 | 1 | 14,14,15 | 1.76 | 2 (14%) | 17,19,21 | 1.44 | 1 (5%) |
| 4 | NAG | B | 1311 | 1 | 14,14,15 | 1.66 | 2 (14%) | 17,19,21 | 1.35 | 2 (11%) |
| 4 | NAG | A | 1314 | 1 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.46 | 0 |
| 4 | NAG | A | 1305 | 1 | 14,14,15 | 1.74 | 2 (14%) | 17,19,21 | 0.66 | 0 |
| 4 | NAG | A | 1303 | - | 14,14,15 | 1.41 | 2 (14%) | 17,19,21 | 1.02 | 2 (11%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 4 | NAG | A | 1307 | 1 | - | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 4 | NAG | B | 1304 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1306 | - | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1301 | - | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1306 | - | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1308 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | C | 1305 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1309 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1304 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1301 | - | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1312 | - | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1310 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | C | 1303 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1309 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1313 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1310 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1312 | - | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | C | 1306 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | C | 1301 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1308 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | C | 1304 | - | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1302 | - | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1313 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1303 | - | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | C | 1302 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1302 | - | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1305 | - | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1307 | - | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1311 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1311 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1314 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1305 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1303 | - | - | 1/6/23/26 | 0/1/1/1 |

All (32) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | B | 1310 | NAG | O5-C1 | 11.92 | 1.62 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | B | 1312 | NAG | O5-C1 | 9.95 | 1.59 | 1.43 |
| 4 | C | 1306 | NAG | O5-C1 | 8.02 | 1.56 | 1.43 |
| 4 | C | 1305 | NAG | O5-C1 | 7.93 | 1.56 | 1.43 |
| 4 | B | 1304 | NAG | C1-C2 | 6.29 | 1.61 | 1.52 |
| 4 | A | 1311 | NAG | O5-C1 | 5.92 | 1.53 | 1.43 |
| 4 | A | 1305 | NAG | O5-C1 | 5.72 | 1.52 | 1.43 |
| 4 | A | 1307 | NAG | O5-C1 | 5.68 | 1.52 | 1.43 |
| 4 | B | 1311 | NAG | O5-C1 | -4.89 | 1.35 | 1.43 |
| 4 | A | 1309 | NAG | O5-C1 | 4.73 | 1.51 | 1.43 |
| 4 | A | 1303 | NAG | C1-C2 | -3.68 | 1.46 | 1.52 |
| 4 | A | 1303 | NAG | O5-C1 | -3.67 | 1.37 | 1.43 |
| 4 | B | 1311 | NAG | C1-C2 | -3.48 | 1.47 | 1.52 |
| 4 | B | 1309 | NAG | C1-C2 | 3.44 | 1.57 | 1.52 |
| 4 | C | 1301 | NAG | O5-C1 | -3.39 | 1.38 | 1.43 |
| 4 | C | 1306 | NAG | C1-C2 | 3.32 | 1.57 | 1.52 |
| 4 | B | 1308 | NAG | O5-C1 | 3.29 | 1.49 | 1.43 |
| 4 | B | 1313 | NAG | C1-C2 | -3.23 | 1.47 | 1.52 |
| 4 | C | 1303 | NAG | O5-C1 | -2.89 | 1.39 | 1.43 |
| 4 | A | 1305 | NAG | C1-C2 | 2.88 | 1.56 | 1.52 |
| 4 | B | 1308 | NAG | C1-C2 | 2.82 | 1.56 | 1.52 |
| 4 | A | 1301 | NAG | O5-C1 | -2.71 | 1.39 | 1.43 |
| 4 | B | 1310 | NAG | C1-C2 | 2.59 | 1.56 | 1.52 |
| 4 | C | 1304 | NAG | O5-C1 | -2.57 | 1.39 | 1.43 |
| 4 | A | 1311 | NAG | C1-C2 | 2.57 | 1.56 | 1.52 |
| 4 | A | 1313 | NAG | O5-C1 | -2.53 | 1.39 | 1.43 |
| 4 | B | 1304 | NAG | O5-C1 | 2.37 | 1.47 | 1.43 |
| 4 | B | 1305 | NAG | O5-C1 | -2.34 | 1.40 | 1.43 |
| 4 | A | 1307 | NAG | C1-C2 | 2.20 | 1.55 | 1.52 |
| 4 | A | 1312 | NAG | O5-C1 | -2.11 | 1.40 | 1.43 |
| 4 | C | 1304 | NAG | C1-C2 | -2.10 | 1.49 | 1.52 |
| 4 | B | 1312 | NAG | C1-C2 | 2.06 | 1.55 | 1.52 |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 4 | C | 1305 | NAG | C1-O5-C5 | 8.40 | 123.57 | 112.19 |
| 4 | B | 1310 | NAG | C1-O5-C5 | 8.22 | 123.33 | 112.19 |
| 4 | A | 1307 | NAG | C1-O5-C5 | 7.87 | 122.86 | 112.19 |
| 4 | A | 1311 | NAG | C1-O5-C5 | 5.35 | 119.44 | 112.19 |
| 4 | A | 1308 | NAG | C1-O5-C5 | 5.23 | 119.28 | 112.19 |
| 4 | C | 1306 | NAG | C1-O5-C5 | 4.32 | 118.05 | 112.19 |
| 4 | C | 1304 | NAG | C1-O5-C5 | 3.86 | 117.42 | 112.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4 | A | 1309 | NAG | C1-O5-C5 | 3.83 | 117.38 | 112.19 |
| 4 | B | 1311 | NAG | O5-C5-C4 | -3.27 | 102.88 | 110.83 |
| 4 | B | 1304 | NAG | C2-N2-C7 | 3.08 | 127.28 | 122.90 |
| 4 | B | 1308 | NAG | C1-O5-C5 | 3.06 | 116.33 | 112.19 |
| 4 | C | 1301 | NAG | C1-O5-C5 | 2.96 | 116.20 | 112.19 |
| 4 | B | 1311 | NAG | C1-O5-C5 | -2.88 | 108.29 | 112.19 |
| 4 | C | 1302 | NAG | O5-C5-C4 | -2.73 | 104.18 | 110.83 |
| 4 | B | 1312 | NAG | C1-O5-C5 | 2.67 | 115.81 | 112.19 |
| 4 | B | 1304 | NAG | C1-C2-N2 | 2.61 | 114.95 | 110.49 |
| 4 | A | 1303 | NAG | C2-N2-C7 | 2.59 | 126.59 | 122.90 |
| 4 | C | 1304 | NAG | C3-C4-C5 | 2.39 | 114.51 | 110.24 |
| 4 | C | 1304 | NAG | C4-C3-C2 | -2.37 | 107.54 | 111.02 |
| 4 | A | 1303 | NAG | C1-C2-N2 | -2.22 | 106.69 | 110.49 |
| 4 | B | 1307 | NAG | C2-N2-C7 | 2.20 | 126.04 | 122.90 |
| 4 | C | 1302 | NAG | C3-C4-C5 | -2.17 | 106.37 | 110.24 |
| 4 | A | 1312 | NAG | C1-O5-C5 | 2.15 | 115.10 | 112.19 |
| 4 | B | 1313 | NAG | C1-O5-C5 | -2.03 | 109.44 | 112.19 |
| 4 | C | 1303 | NAG | C1-O5-C5 | 2.00 | 114.90 | 112.19 |

There are no chirality outliers.

All (62) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 4 | B | 1307 | NAG | C3-C2-N2-C7 |
| 4 | C | 1306 | NAG | C1-C2-N2-C7 |
| 4 | A | 1304 | NAG | C4-C5-C6-O6 |
| 4 | A | 1302 | NAG | O5-C5-C6-O6 |
| 4 | B | 1309 | NAG | O5-C5-C6-O6 |
| 4 | C | 1304 | NAG | O5-C5-C6-O6 |
| 4 | B | 1307 | NAG | O5-C5-C6-O6 |
| 4 | C | 1306 | NAG | O5-C5-C6-O6 |
| 4 | A | 1304 | NAG | O5-C5-C6-O6 |
| 4 | A | 1306 | NAG | O5-C5-C6-O6 |
| 4 | B | 1307 | NAG | C4-C5-C6-O6 |
| 4 | C | 1304 | NAG | C4-C5-C6-O6 |
| 4 | A | 1302 | NAG | C4-C5-C6-O6 |
| 4 | A | 1307 | NAG | O5-C5-C6-O6 |
| 4 | A | 1314 | NAG | O5-C5-C6-O6 |
| 4 | B | 1309 | NAG | C4-C5-C6-O6 |
| 4 | A | 1301 | NAG | C1-C2-N2-C7 |
| 4 | C | 1306 | NAG | C4-C5-C6-O6 |
| 4 | A | 1309 | NAG | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 4 | A | 1305 | NAG | O5-C5-C6-O6 |
| 4 | A | 1312 | NAG | O5-C5-C6-O6 |
| 4 | A | 1302 | NAG | C8-C7-N2-C2 |
| 4 | A | 1302 | NAG | O7-C7-N2-C2 |
| 4 | B | 1303 | NAG | C8-C7-N2-C2 |
| 4 | B | 1303 | NAG | O7-C7-N2-C2 |
| 4 | B | 1304 | NAG | C8-C7-N2-C2 |
| 4 | B | 1304 | NAG | O7-C7-N2-C2 |
| 4 | B | 1308 | NAG | C8-C7-N2-C2 |
| 4 | B | 1308 | NAG | O7-C7-N2-C2 |
| 4 | C | 1305 | NAG | C8-C7-N2-C2 |
| 4 | C | 1305 | NAG | O7-C7-N2-C2 |
| 4 | A | 1313 | NAG | O5-C5-C6-O6 |
| 4 | A | 1306 | NAG | C4-C5-C6-O6 |
| 4 | A | 1314 | NAG | C4-C5-C6-O6 |
| 4 | A | 1305 | NAG | C4-C5-C6-O6 |
| 4 | C | 1302 | NAG | O5-C5-C6-O6 |
| 4 | A | 1313 | NAG | C4-C5-C6-O6 |
| 4 | A | 1301 | NAG | O5-C5-C6-O6 |
| 4 | A | 1312 | NAG | C4-C5-C6-O6 |
| 4 | A | 1309 | NAG | O5-C5-C6-O6 |
| 4 | B | 1302 | NAG | C1-C2-N2-C7 |
| 4 | A | 1303 | NAG | C1-C2-N2-C7 |
| 4 | A | 1312 | NAG | C1-C2-N2-C7 |
| 4 | B | 1308 | NAG | O5-C5-C6-O6 |
| 4 | C | 1303 | NAG | O5-C5-C6-O6 |
| 4 | B | 1302 | NAG | C3-C2-N2-C7 |
| 4 | B | 1304 | NAG | C3-C2-N2-C7 |
| 4 | B | 1310 | NAG | C3-C2-N2-C7 |
| 4 | A | 1307 | NAG | C4-C5-C6-O6 |
| 4 | B | 1301 | NAG | C4-C5-C6-O6 |
| 4 | B | 1312 | NAG | C1-C2-N2-C7 |
| 4 | B | 1301 | NAG | O5-C5-C6-O6 |
| 4 | A | 1301 | NAG | C3-C2-N2-C7 |
| 4 | A | 1307 | NAG | C3-C2-N2-C7 |
| 4 | B | 1311 | NAG | O5-C5-C6-O6 |
| 4 | A | 1301 | NAG | C4-C5-C6-O6 |
| 4 | B | 1311 | NAG | C4-C5-C6-O6 |
| 4 | C | 1303 | NAG | C1-C2-N2-C7 |
| 4 | C | 1301 | NAG | C4-C5-C6-O6 |
| 4 | A | 1312 | NAG | C3-C2-N2-C7 |
| 4 | B | 1312 | NAG | C3-C2-N2-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 4 | C | 1303 | NAG | C3-C2-N2-C7 |

There are no ring outliers.

16 monomers are involved in 49 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | B | 1304 | NAG | 4 | 0 |
| 4 | B | 1301 | NAG | 2 | 0 |
| 4 | A | 1306 | NAG | 2 | 0 |
| 4 | A | 1301 | NAG | 4 | 0 |
| 4 | B | 1310 | NAG | 9 | 0 |
| 4 | C | 1303 | NAG | 1 | 0 |
| 4 | A | 1309 | NAG | 2 | 0 |
| 4 | C | 1306 | NAG | 2 | 0 |
| 4 | C | 1301 | NAG | 1 | 0 |
| 4 | C | 1304 | NAG | 4 | 0 |
| 4 | B | 1302 | NAG | 2 | 0 |
| 4 | A | 1313 | NAG | 1 | 0 |
| 4 | A | 1302 | NAG | 2 | 0 |
| 4 | B | 1305 | NAG | 2 | 0 |
| 4 | B | 1307 | NAG | 7 | 0 |
| 4 | A | 1303 | NAG | 4 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | C | 3 |
| 1 | A | 3 |
| 1 | B | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | C | 332:ILE | C | 333:THR | N | 6.23 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|------------|--------|--------------|
| 1 | C | 527:PRO | C | 528:LYS | N | 4.26 |
| 1 | B | 481:ASN | C | 482:GLY | N | 3.38 |
| 1 | C | 528:LYS | C | 529:LYS | N | 3.28 |
| 1 | A | 527:PRO | C | 528:LYS | N | 3.23 |
| 1 | A | 458:LYS | C | 459[A]:SER | N | 3.12 |
| 1 | A | 458:LYS | C | 459[B]:SER | N | 3.07 |

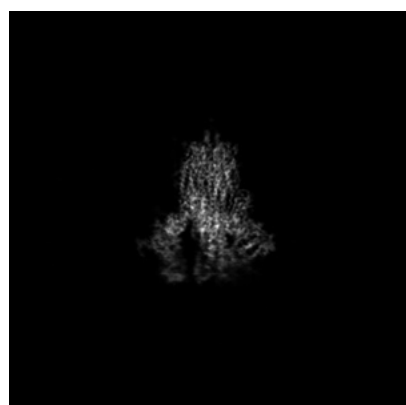
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14314. These allow visual inspection of the internal detail of the map and identification of artifacts.

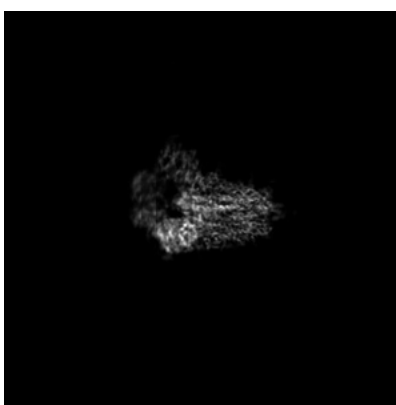
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 246



Y Index: 246



Z Index: 246

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 249



Y Index: 238

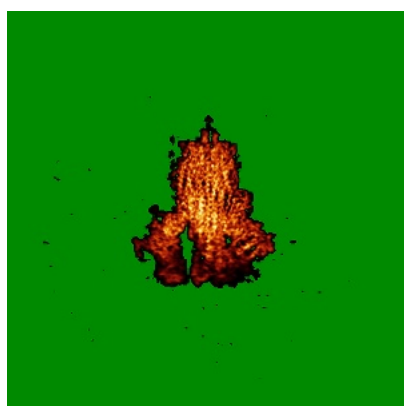


Z Index: 222

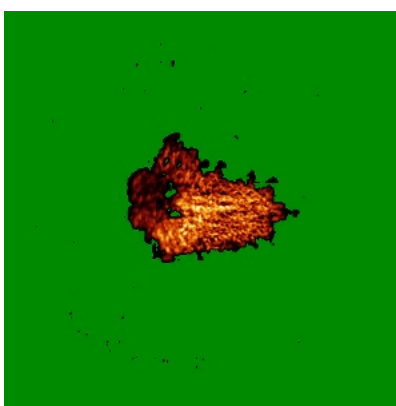
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

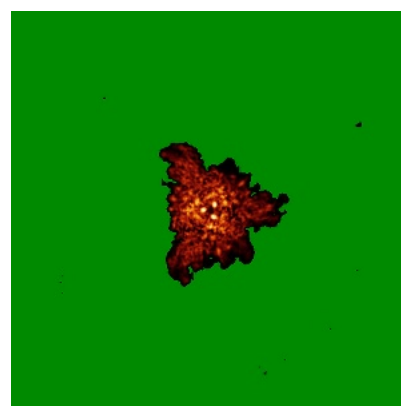
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

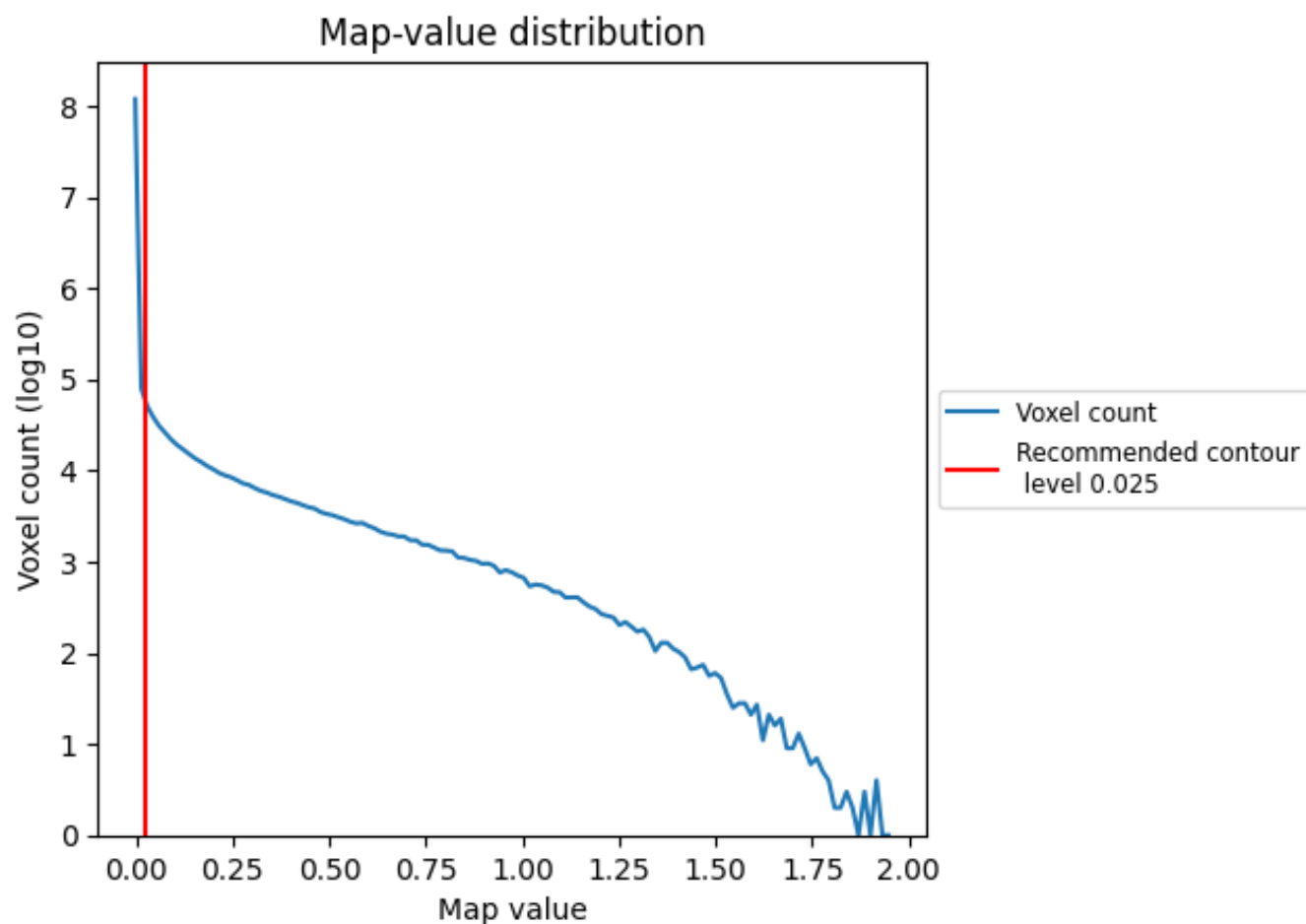
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

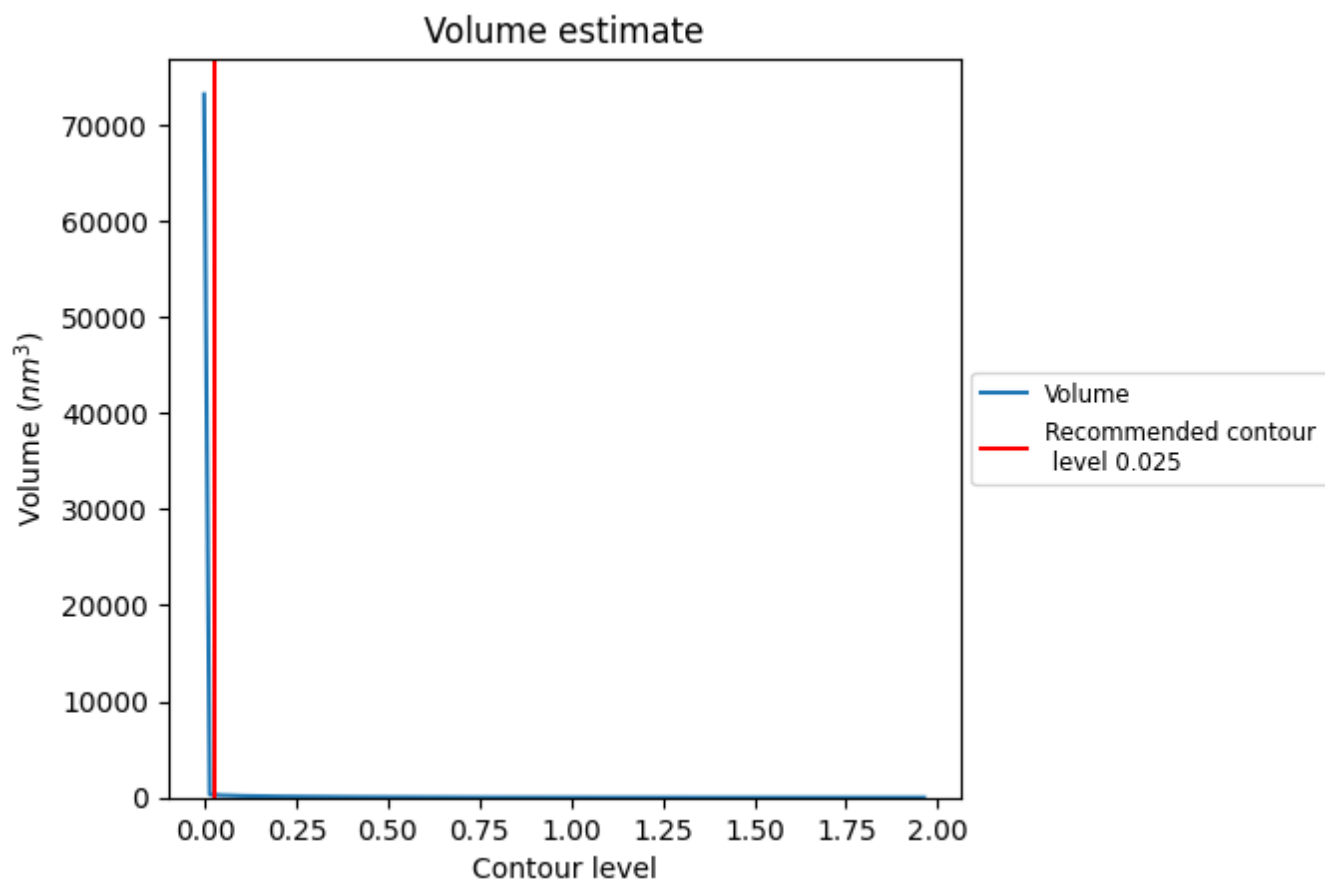
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

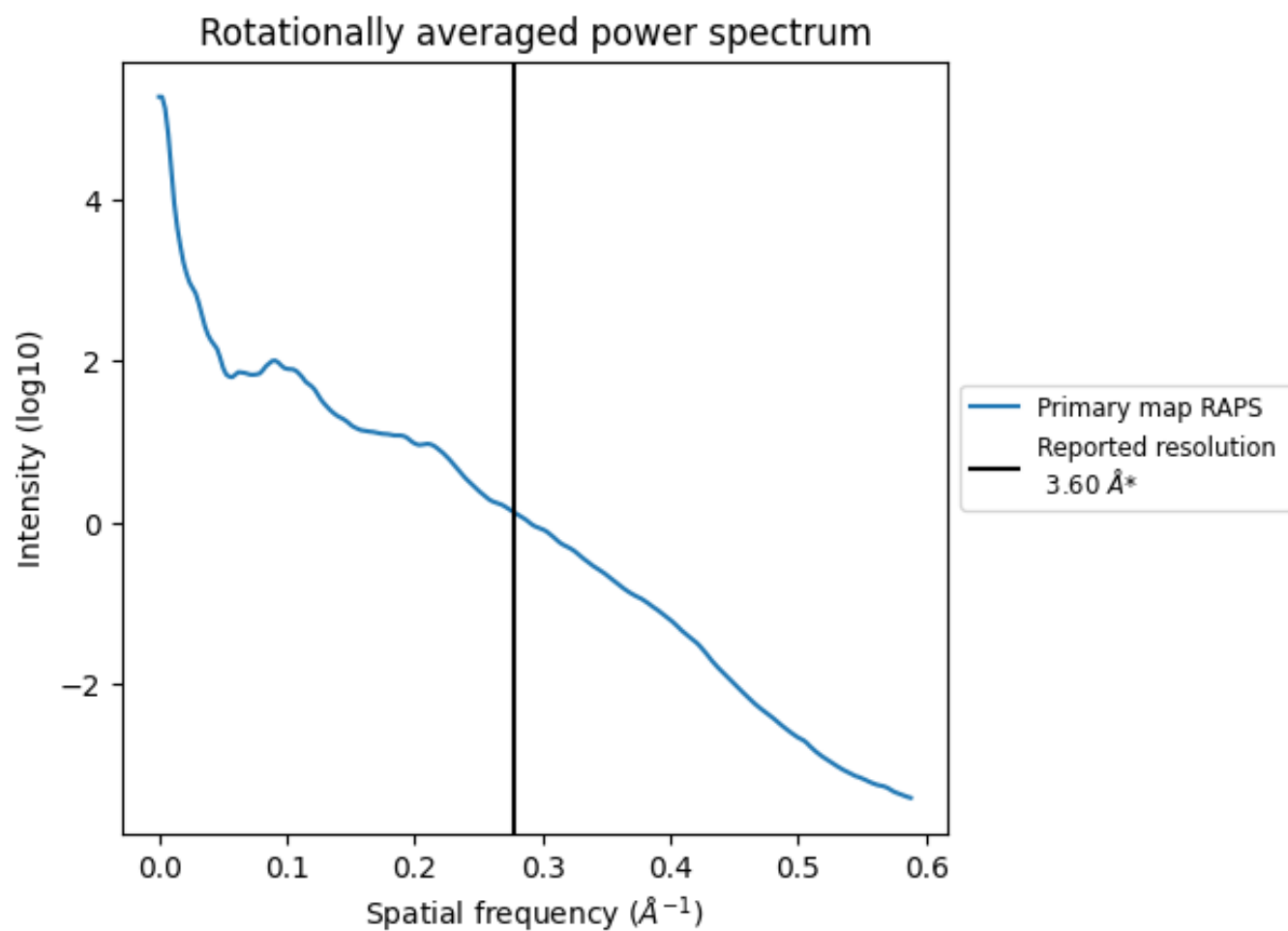
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm^3 ; this corresponds to an approximate mass of 256 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

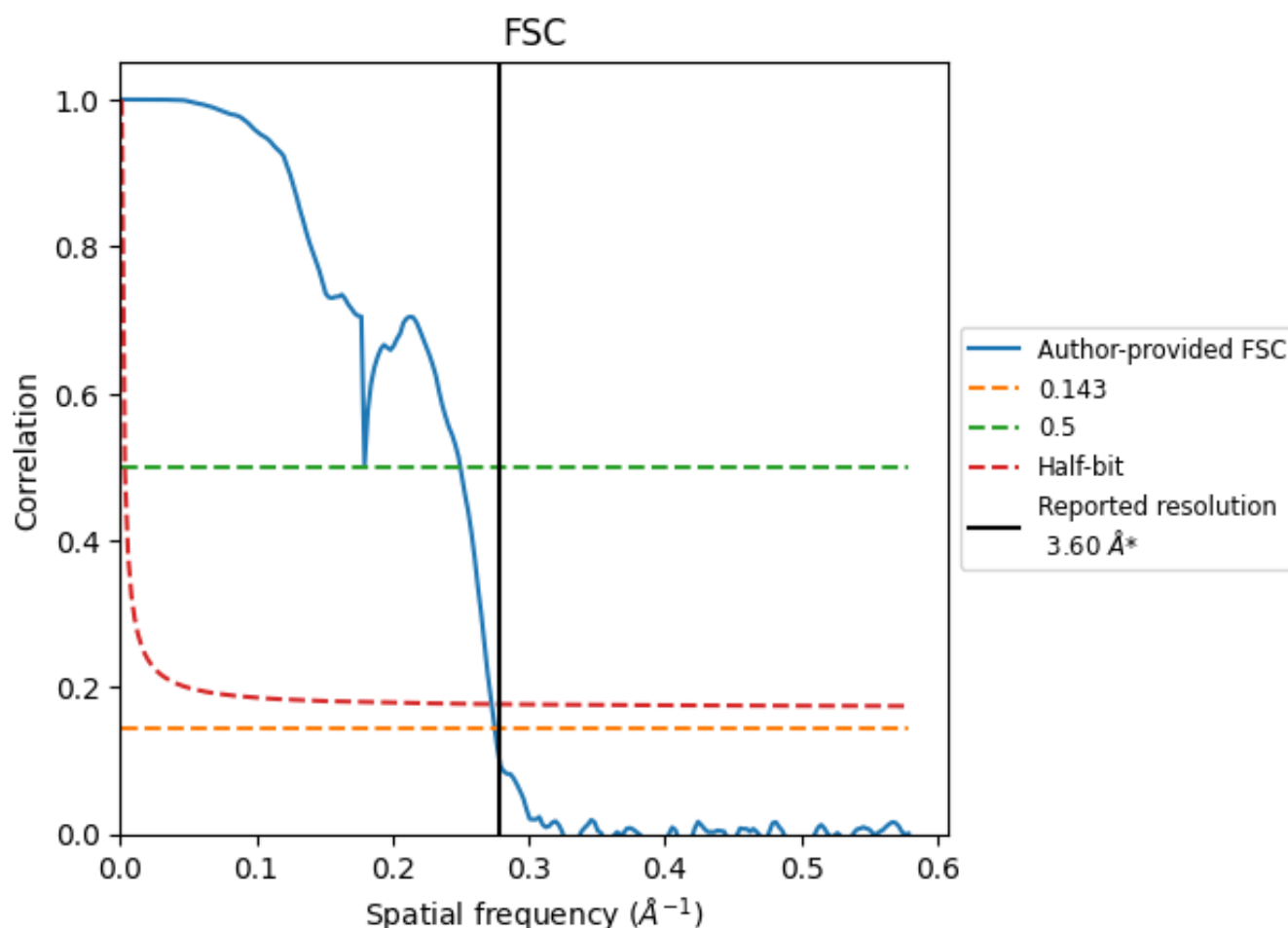


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

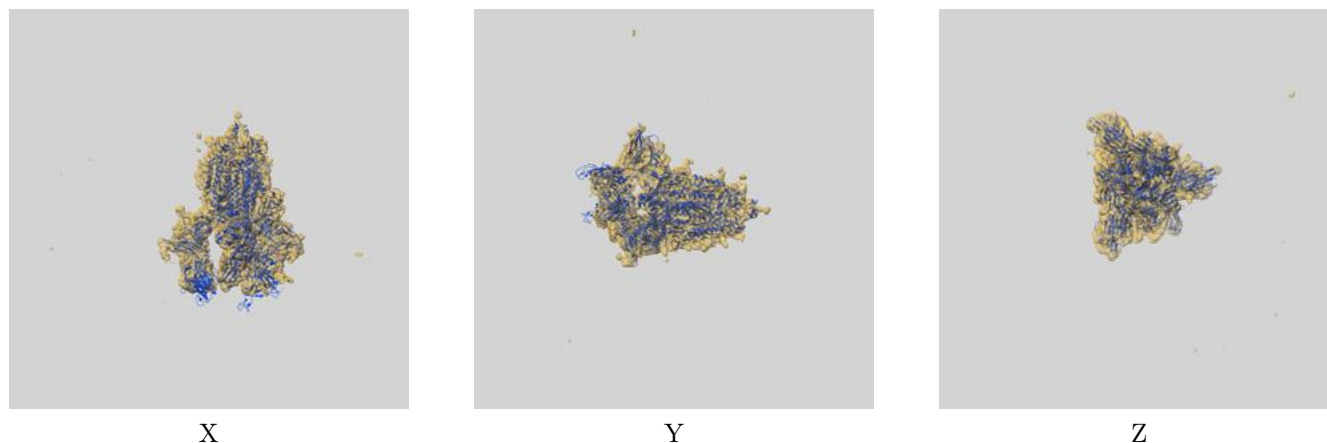
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.60 | - | - |
| Author-provided FSC curve | 3.64 | 4.00 | 3.67 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

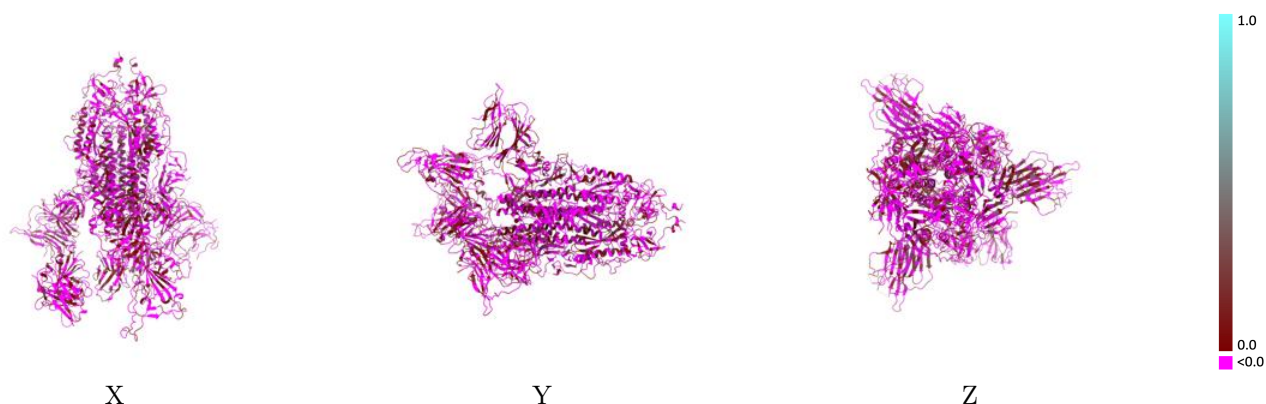
This section contains information regarding the fit between EMDB map EMD-14314 and PDB model 7R4Q. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



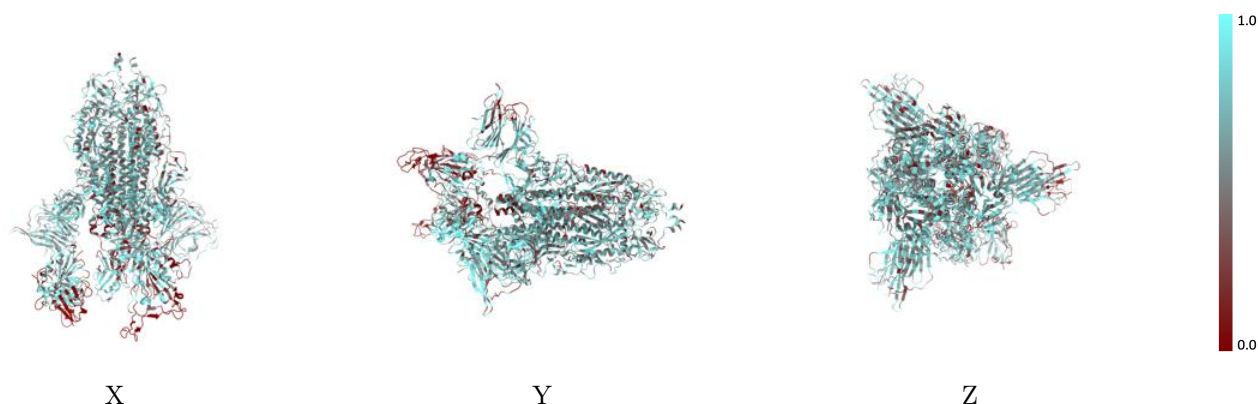
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



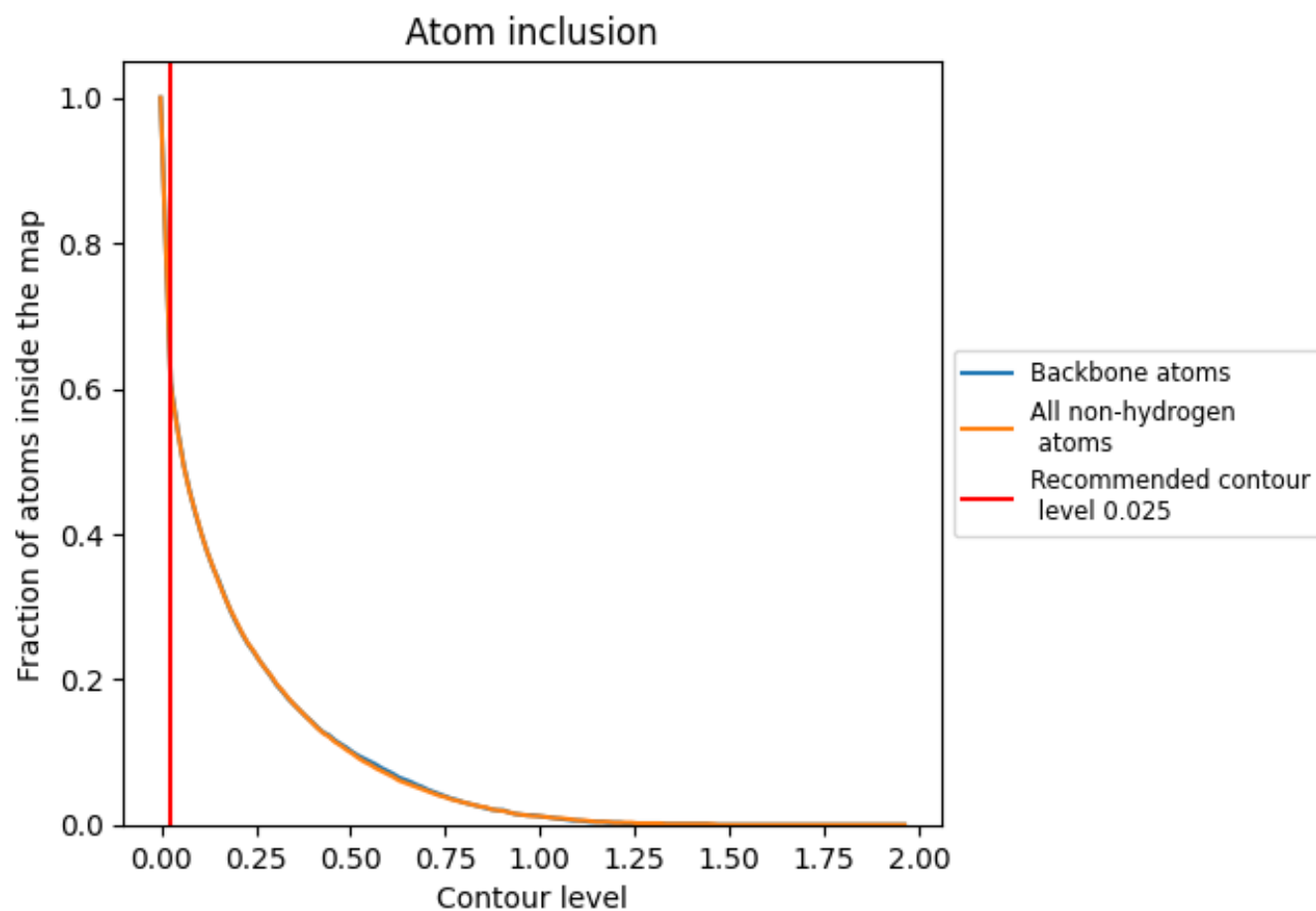
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|---------------------|
| All | <div></div> 0.6070 | <div></div> -0.0140 |
| A | <div></div> 0.5970 | <div></div> -0.0160 |
| B | <div></div> 0.6360 | <div></div> -0.0170 |
| C | <div></div> 0.6050 | <div></div> -0.0140 |
| D | <div></div> 0.4740 | <div></div> -0.0100 |
| E | <div></div> 0.6520 | <div></div> 0.0220 |
| F | <div></div> 0.5000 | <div></div> -0.0690 |
| G | <div></div> 0.2140 | <div></div> -0.0520 |
| H | <div></div> 0.1430 | <div></div> -0.1320 |
| I | <div></div> 0.8930 | <div></div> 0.2040 |
| J | <div></div> 0.3570 | <div></div> 0.1110 |

1.0
0.0
<0.0