# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 05:19 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 4MHJ |
| Title | : | Crystal structure of Fab H5M9 in complex with influenza virus hemagglutinin from A/goose/Guangdong/1/96 (H5N1) |
| Authors | : | Zhu, X.; Wilson, I.A. |
| Deposited on | : | 2013-08-29 |
| Resolution | : | 6.98 Å(reported) |

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

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

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

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

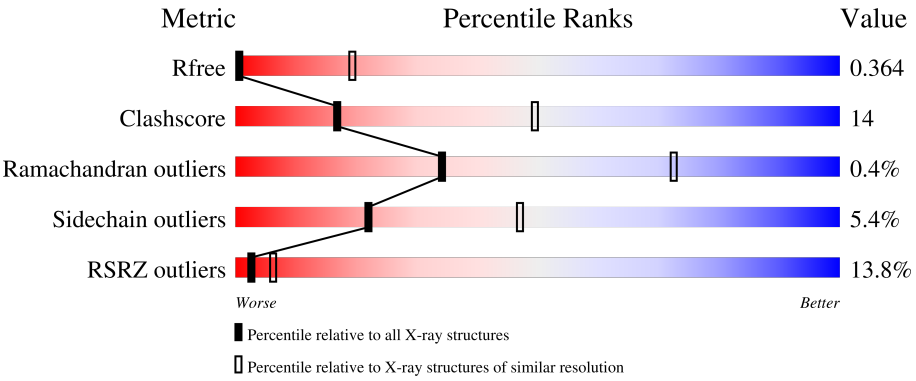
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.98 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1004 (10.00-3.90) |
| Clashscore | 141614 | 1069 (10.00-3.90) |
| Ramachandran outliers | 138981 | 1002 (10.00-3.90) |
| Sidechain outliers | 138945 | 1002 (10.00-3.86) |
| RSRZ outliers | 127900 | 1004 (9.50-3.80) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 334 | 9% 73% 22% |
| 1 | C | 334 | 13% 73% 22% |
| 1 | G | 334 | 11% 72% 23% |
| 1 | M | 334 | 10% 75% 20% |
| 1 | O | 334 | 14% 72% 22% 5% |

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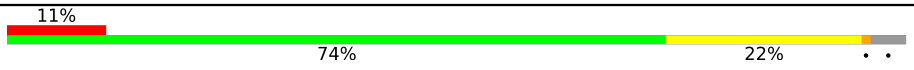
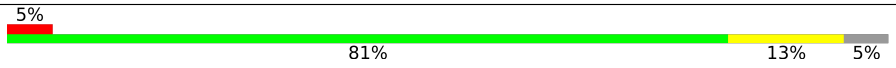
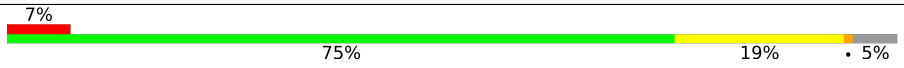
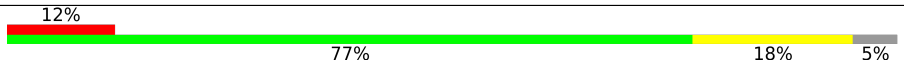
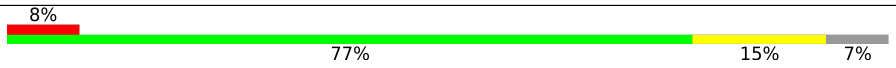
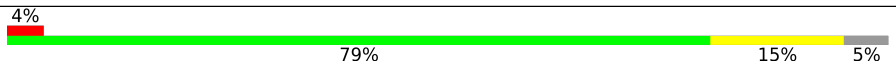
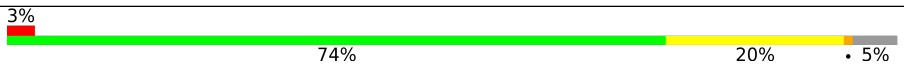
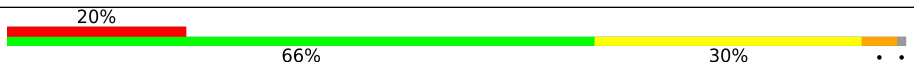
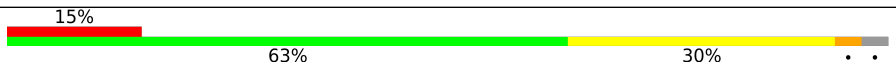
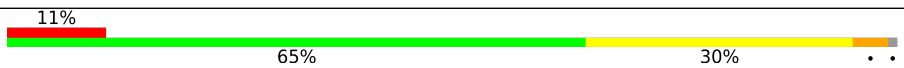
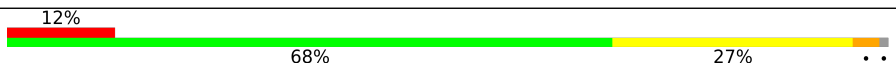
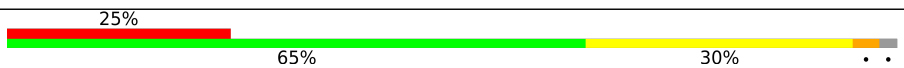
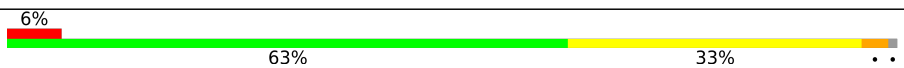
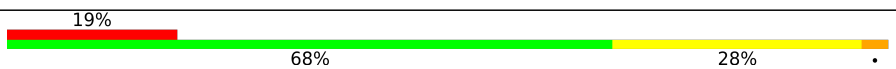
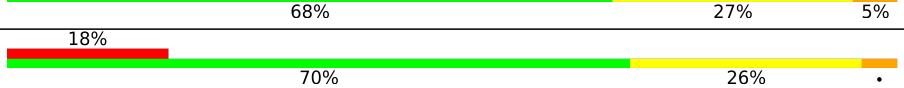
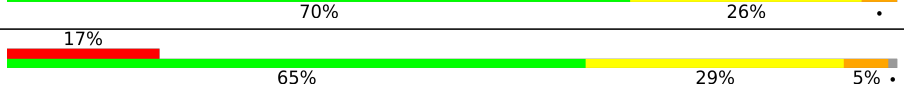
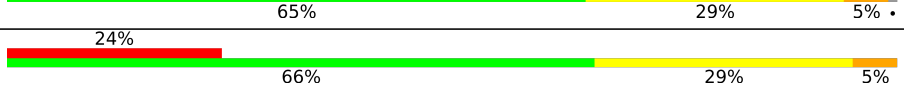
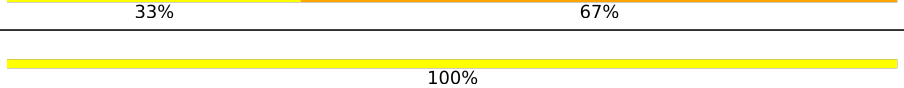
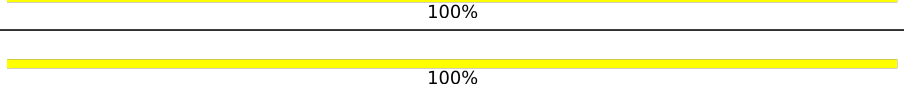
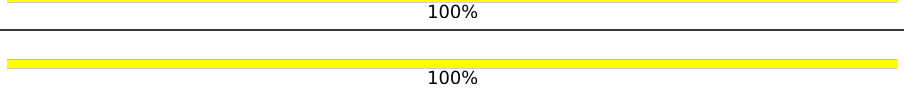
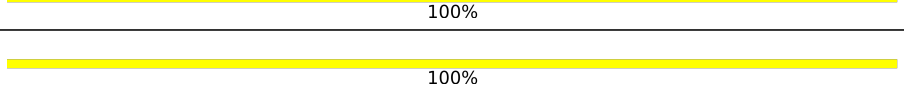
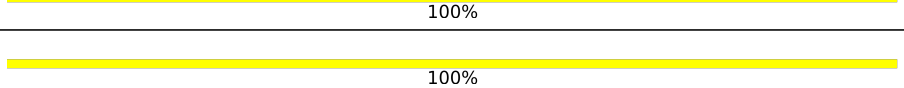
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | S | 334 |   |
| 2 | B | 182 |   |
| 2 | D | 182 |   |
| 2 | I | 182 |   |
| 2 | N | 182 |   |
| 2 | P | 182 |   |
| 2 | U | 182 |   |
| 3 | E | 218 |   |
| 3 | J | 218 |   |
| 3 | L | 218 |   |
| 3 | Q | 218 |   |
| 3 | V | 218 |   |
| 3 | X | 218 |   |
| 4 | F | 222 |   |
| 4 | H | 222 |   |
| 4 | K | 222 |   |
| 4 | R | 222 |   |
| 4 | T | 222 |   |
| 4 | W | 222 |   |
| 5 | Y | 3 |   |
| 5 | d | 3 |   |
| 5 | f | 3 |   |
| 6 | Z | 8 |   |
| 7 | a | 2 |   |
| 7 | c | 2 |   |

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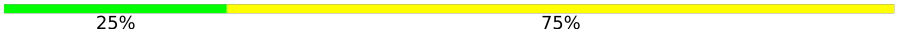
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | b | 3 |   |
| 9 | e | 4 |   |

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 |
|---|---|---|---|---|---|---|---|
| 10 | NAG | A | 2004 | - | - | - | X |
| 10 | NAG | P | 2001 | - | - | - | X |
| 10 | NAG | S | 2004 | - | - | - | X |
| 5 | NAG | Y | 2 | - | - | - | X |
| 5 | MAN | Y | 3 | - | - | - | X |
| 5 | NAG | d | 1 | - | - | - | X |
| 5 | MAN | d | 3 | - | - | - | X |
| 6 | MAN | Z | 5 | - | - | - | X |
| 7 | NAG | c | 1 | - | - | - | X |
| 7 | NAG | c | 2 | - | - | - | X |
| 8 | BMA | b | 3 | - | - | - | X |
| 9 | NAG | e | 1 | - | - | - | X |
| 9 | MAN | e | 4 | - | - | - | X |

## 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 43995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 322 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2542 | 1603 | 440 | 484 | 15 | | | |
| 1 | C | 321 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2533 | 1598 | 438 | 482 | 15 | | | |
| 1 | G | 321 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2530 | 1594 | 439 | 482 | 15 | | | |
| 1 | M | 322 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2542 | 1603 | 440 | 484 | 15 | | | |
| 1 | O | 318 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2514 | 1587 | 435 | 477 | 15 | | | |
| 1 | S | 322 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2542 | 1603 | 440 | 484 | 15 | | | |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 7 | ALA | - | expression tag | UNP Q9Q0U6 |
| A | 8 | ASP | - | expression tag | UNP Q9Q0U6 |
| A | 9 | PRO | - | expression tag | UNP Q9Q0U6 |
| A | 10 | GLY | - | expression tag | UNP Q9Q0U6 |
| C | 7 | ALA | - | expression tag | UNP Q9Q0U6 |
| C | 8 | ASP | - | expression tag | UNP Q9Q0U6 |
| C | 9 | PRO | - | expression tag | UNP Q9Q0U6 |
| C | 10 | GLY | - | expression tag | UNP Q9Q0U6 |
| G | 7 | ALA | - | expression tag | UNP Q9Q0U6 |
| G | 8 | ASP | - | expression tag | UNP Q9Q0U6 |
| G | 9 | PRO | - | expression tag | UNP Q9Q0U6 |
| G | 10 | GLY | - | expression tag | UNP Q9Q0U6 |
| M | 7 | ALA | - | expression tag | UNP Q9Q0U6 |
| M | 8 | ASP | - | expression tag | UNP Q9Q0U6 |
| M | 9 | PRO | - | expression tag | UNP Q9Q0U6 |
| M | 10 | GLY | - | expression tag | UNP Q9Q0U6 |
| O | 7 | ALA | - | expression tag | UNP Q9Q0U6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| O | 8 | ASP | - | expression tag | UNP Q9Q0U6 |
| O | 9 | PRO | - | expression tag | UNP Q9Q0U6 |
| O | 10 | GLY | - | expression tag | UNP Q9Q0U6 |
| S | 7 | ALA | - | expression tag | UNP Q9Q0U6 |
| S | 8 | ASP | - | expression tag | UNP Q9Q0U6 |
| S | 9 | PRO | - | expression tag | UNP Q9Q0U6 |
| S | 10 | GLY | - | expression tag | UNP Q9Q0U6 |

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1393 | 866 | 239 | 280 | 8 | | | |
| 2 | D | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1393 | 866 | 239 | 280 | 8 | | | |
| 2 | N | 169 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1363 | 846 | 233 | 276 | 8 | | | |
| 2 | P | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1393 | 866 | 239 | 280 | 8 | | | |
| 2 | I | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1403 | 872 | 242 | 281 | 8 | | | |
| 2 | U | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1403 | 872 | 242 | 281 | 8 | | | |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 176 | SER | - | expression tag | UNP Q9Q0U6 |
| B | 177 | GLY | - | expression tag | UNP Q9Q0U6 |
| B | 178 | ARG | - | expression tag | UNP Q9Q0U6 |
| B | 179 | LEU | - | expression tag | UNP Q9Q0U6 |
| B | 180 | VAL | - | expression tag | UNP Q9Q0U6 |
| B | 181 | PRO | - | expression tag | UNP Q9Q0U6 |
| B | 182 | ARG | - | expression tag | UNP Q9Q0U6 |
| D | 176 | SER | - | expression tag | UNP Q9Q0U6 |
| D | 177 | GLY | - | expression tag | UNP Q9Q0U6 |
| D | 178 | ARG | - | expression tag | UNP Q9Q0U6 |
| D | 179 | LEU | - | expression tag | UNP Q9Q0U6 |
| D | 180 | VAL | - | expression tag | UNP Q9Q0U6 |
| D | 181 | PRO | - | expression tag | UNP Q9Q0U6 |
| D | 182 | ARG | - | expression tag | UNP Q9Q0U6 |
| N | 176 | SER | - | expression tag | UNP Q9Q0U6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| N | 177 | GLY | - | expression tag | UNP Q9Q0U6 |
| N | 178 | ARG | - | expression tag | UNP Q9Q0U6 |
| N | 179 | LEU | - | expression tag | UNP Q9Q0U6 |
| N | 180 | VAL | - | expression tag | UNP Q9Q0U6 |
| N | 181 | PRO | - | expression tag | UNP Q9Q0U6 |
| N | 182 | ARG | - | expression tag | UNP Q9Q0U6 |
| P | 176 | SER | - | expression tag | UNP Q9Q0U6 |
| P | 177 | GLY | - | expression tag | UNP Q9Q0U6 |
| P | 178 | ARG | - | expression tag | UNP Q9Q0U6 |
| P | 179 | LEU | - | expression tag | UNP Q9Q0U6 |
| P | 180 | VAL | - | expression tag | UNP Q9Q0U6 |
| P | 181 | PRO | - | expression tag | UNP Q9Q0U6 |
| P | 182 | ARG | - | expression tag | UNP Q9Q0U6 |
| I | 176 | SER | - | expression tag | UNP Q9Q0U6 |
| I | 177 | GLY | - | expression tag | UNP Q9Q0U6 |
| I | 178 | ARG | - | expression tag | UNP Q9Q0U6 |
| I | 179 | LEU | - | expression tag | UNP Q9Q0U6 |
| I | 180 | VAL | - | expression tag | UNP Q9Q0U6 |
| I | 181 | PRO | - | expression tag | UNP Q9Q0U6 |
| I | 182 | ARG | - | expression tag | UNP Q9Q0U6 |
| U | 176 | SER | - | expression tag | UNP Q9Q0U6 |
| U | 177 | GLY | - | expression tag | UNP Q9Q0U6 |
| U | 178 | ARG | - | expression tag | UNP Q9Q0U6 |
| U | 179 | LEU | - | expression tag | UNP Q9Q0U6 |
| U | 180 | VAL | - | expression tag | UNP Q9Q0U6 |
| U | 181 | PRO | - | expression tag | UNP Q9Q0U6 |
| U | 182 | ARG | - | expression tag | UNP Q9Q0U6 |

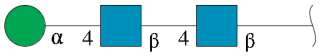
- Molecule 3 is a protein called H5M9 antibody, light chain (kappa).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | L | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1666 | 1032 | 289 | 339 | 6 | | | |
| 3 | E | 216 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1672 | 1035 | 290 | 341 | 6 | | | |
| 3 | J | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1634 | 1015 | 280 | 333 | 6 | | | |
| 3 | X | 216 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1672 | 1035 | 290 | 341 | 6 | | | |
| 3 | Q | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1665 | 1031 | 289 | 339 | 6 | | | |
| 3 | V | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1655 | 1026 | 285 | 338 | 6 | | | |

- Molecule 4 is a protein called H5M9 antibody, heavy chain (IgG1).

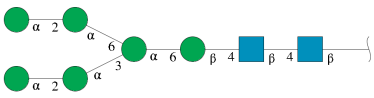
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | H | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1675 | 1059 | 276 | 331 | 9 | | | |
| 4 | F | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1675 | 1059 | 276 | 331 | 9 | | | |
| 4 | K | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1674 | 1057 | 276 | 332 | 9 | | | |
| 4 | T | 220 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1666 | 1054 | 274 | 329 | 9 | | | |
| 4 | R | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1675 | 1059 | 276 | 331 | 9 | | | |
| 4 | W | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1675 | 1059 | 276 | 331 | 9 | | | |

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | Y | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 5 | d | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 5 | f | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

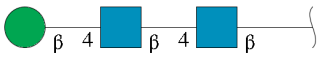



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | Z | 8 | Total | C | N | O | 0 | 0 | 0 |
| | | | 94 | 52 | 2 | 40 | | | |

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | a | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 7 | c | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

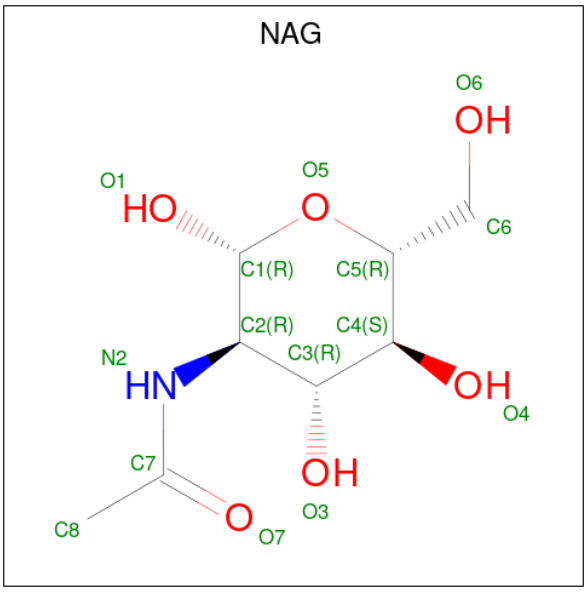



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | b | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | e | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

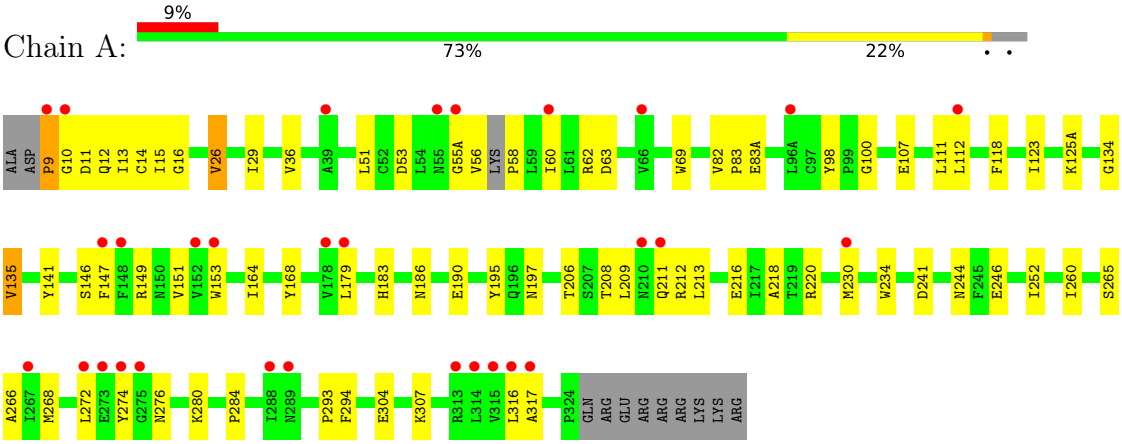



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 10 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 10 | C | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 10 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 10 | O | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 10 | P | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 10 | S | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

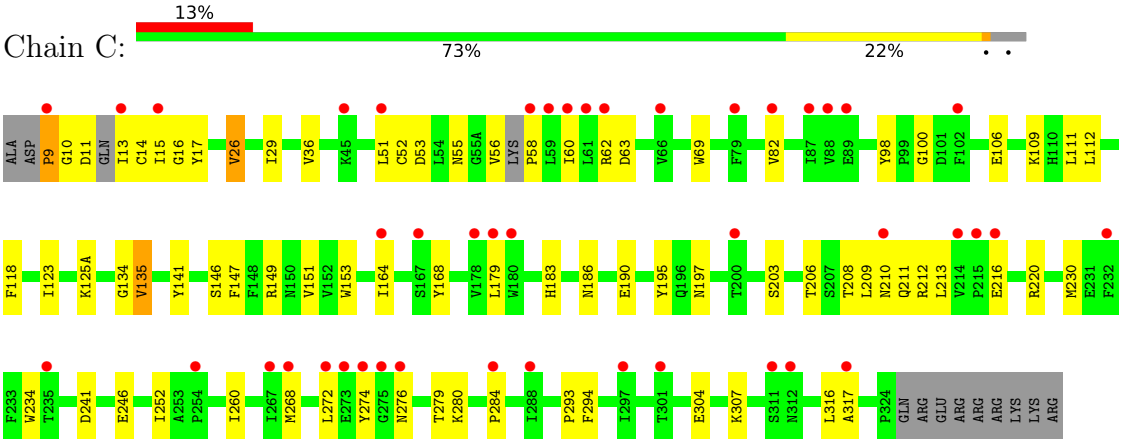
# 3 Residue-property plots (i)

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

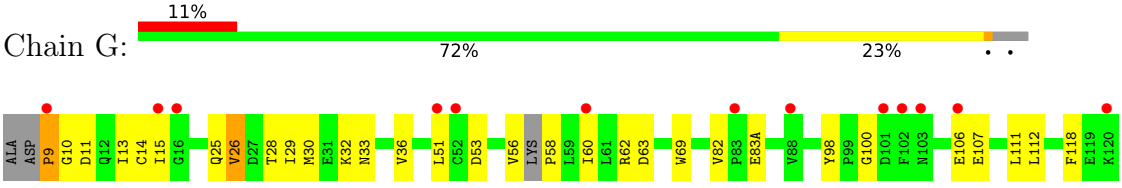
• Molecule 1: Hemagglutinin HA1 chain

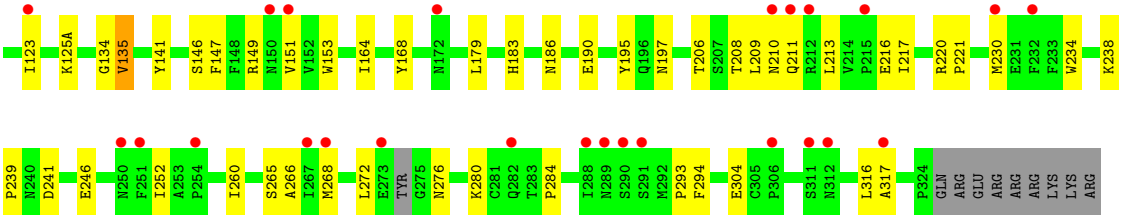



• Molecule 1: Hemagglutinin HA1 chain

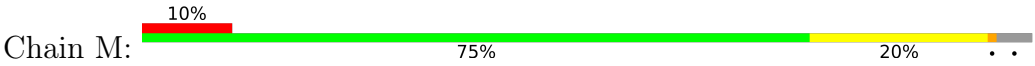


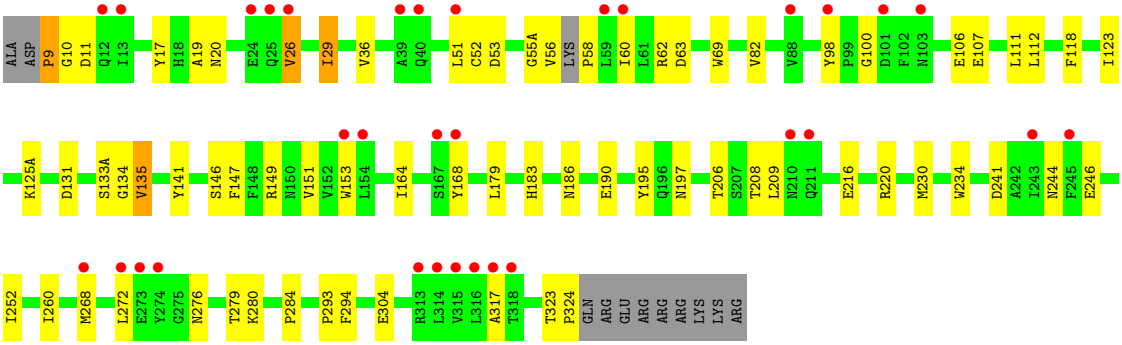

• Molecule 1: Hemagglutinin HA1 chain



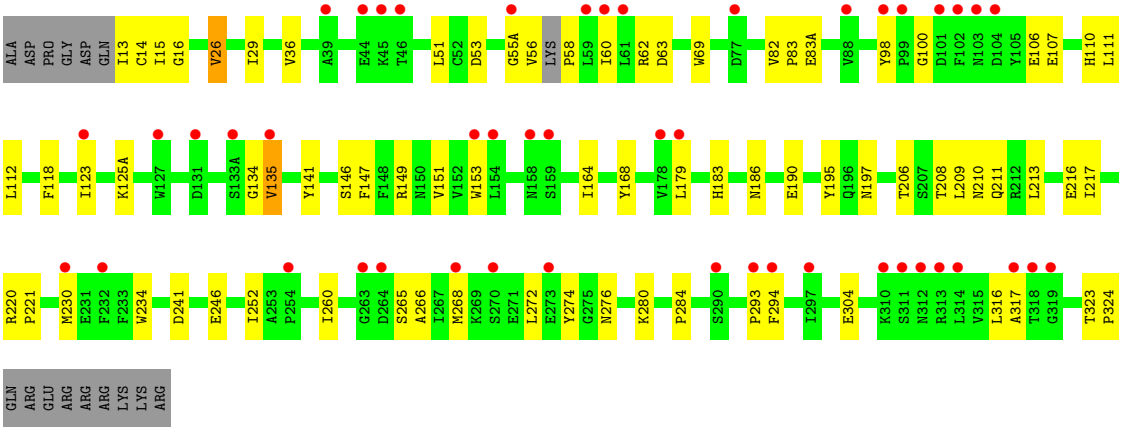



• Molecule 1: Hemagglutinin HA1 chain

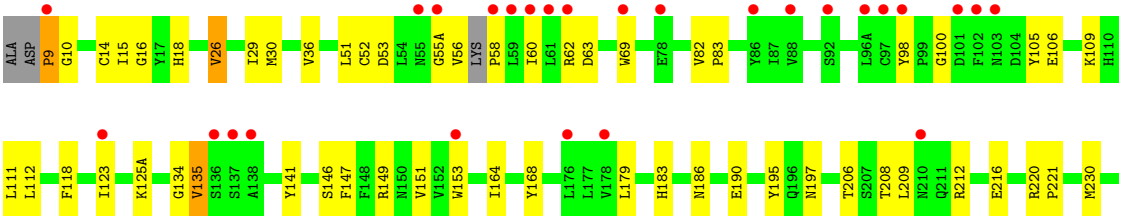


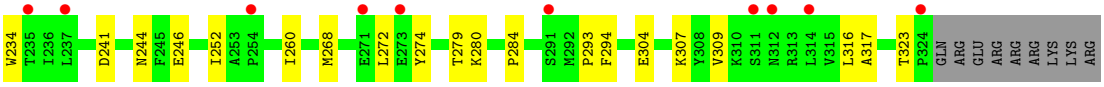




• Molecule 1: Hemagglutinin HA1 chain

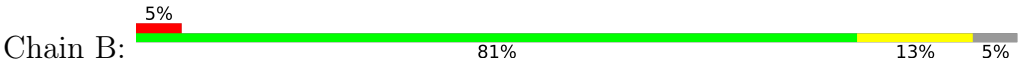



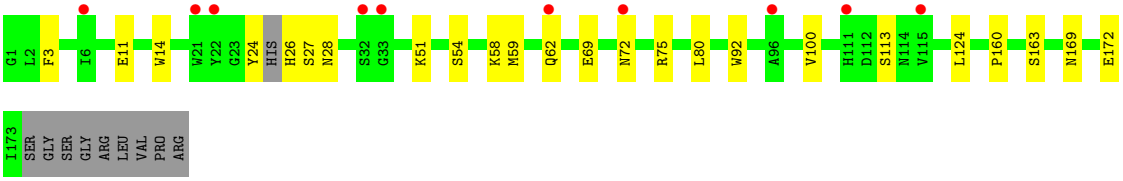

• Molecule 1: Hemagglutinin HA1 chain

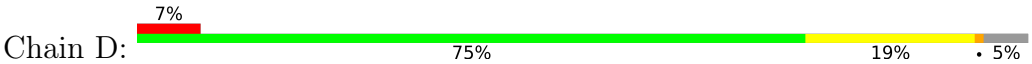


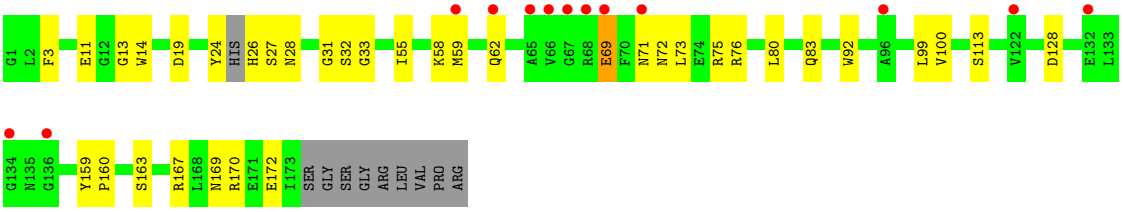

• Molecule 2: Hemagglutinin HA2 chain



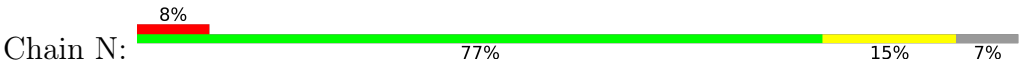



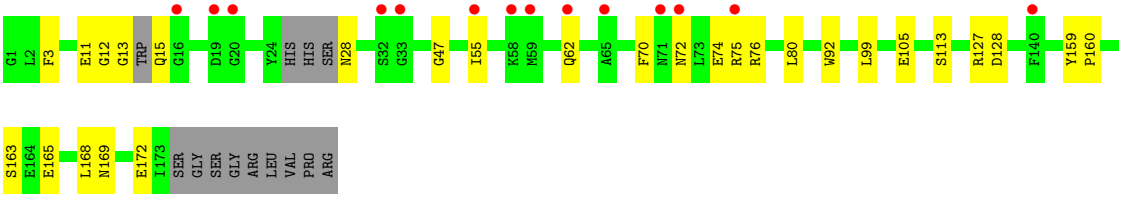

• Molecule 2: Hemagglutinin HA2 chain



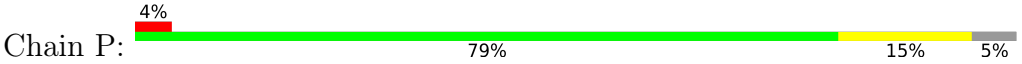



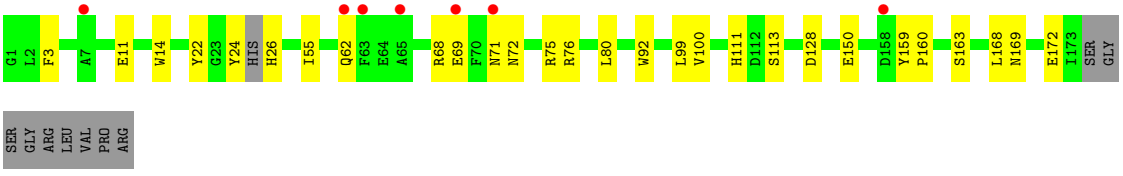

• Molecule 2: Hemagglutinin HA2 chain



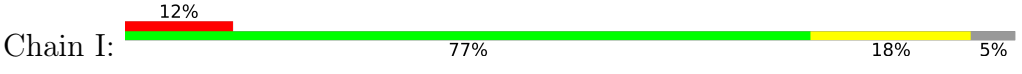



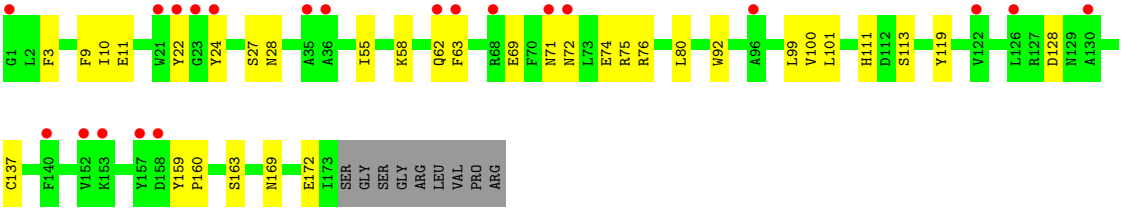

• Molecule 2: Hemagglutinin HA2 chain



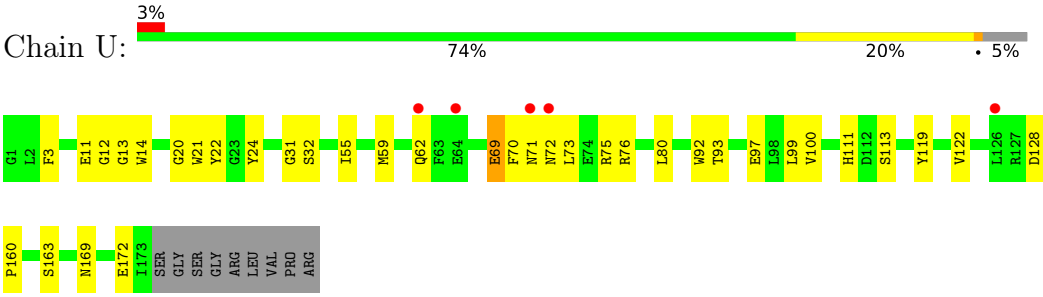




• Molecule 2: Hemagglutinin HA2 chain

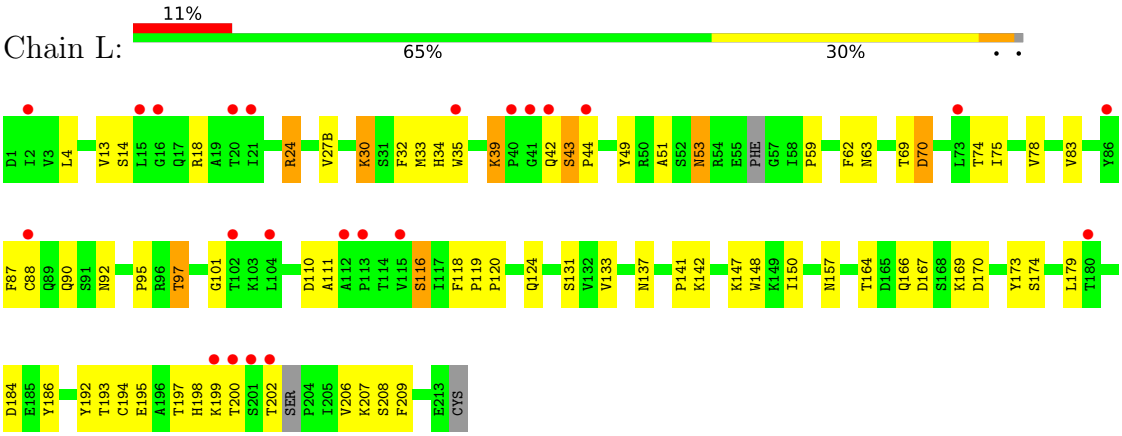




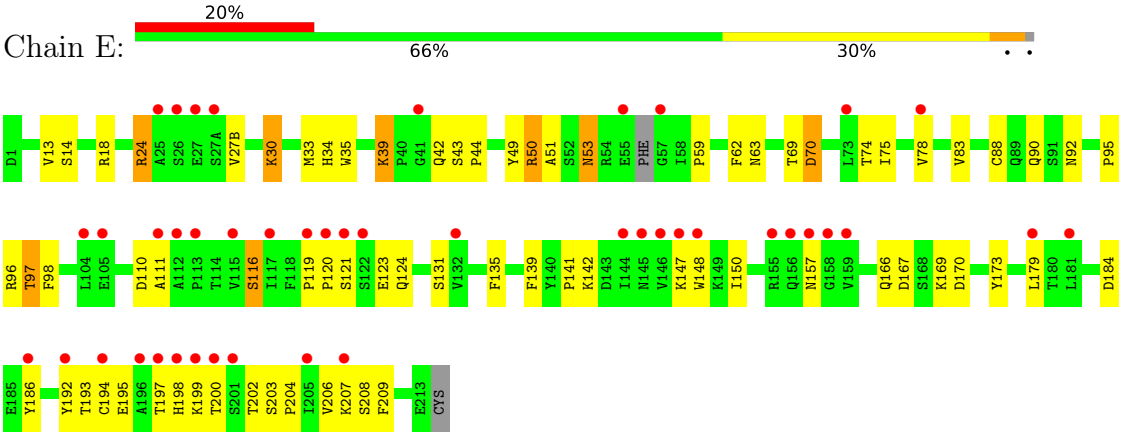

• Molecule 2: Hemagglutinin HA2 chain



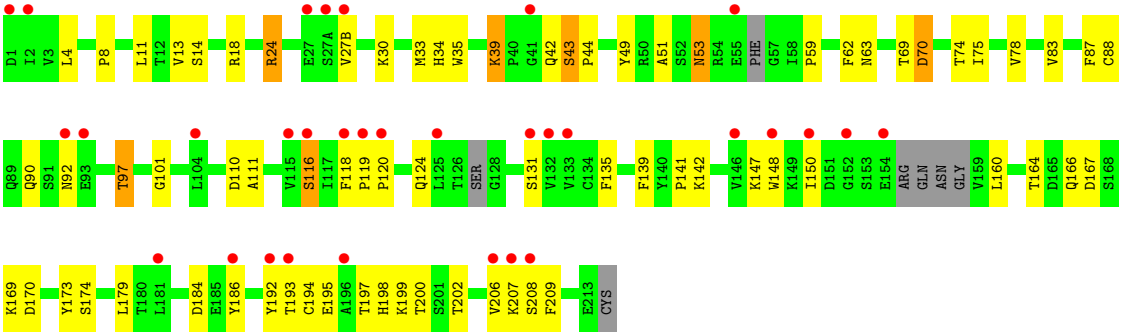

• Molecule 3: H5M9 antibody, light chain (kappa)




• Molecule 3: H5M9 antibody, light chain (kappa)

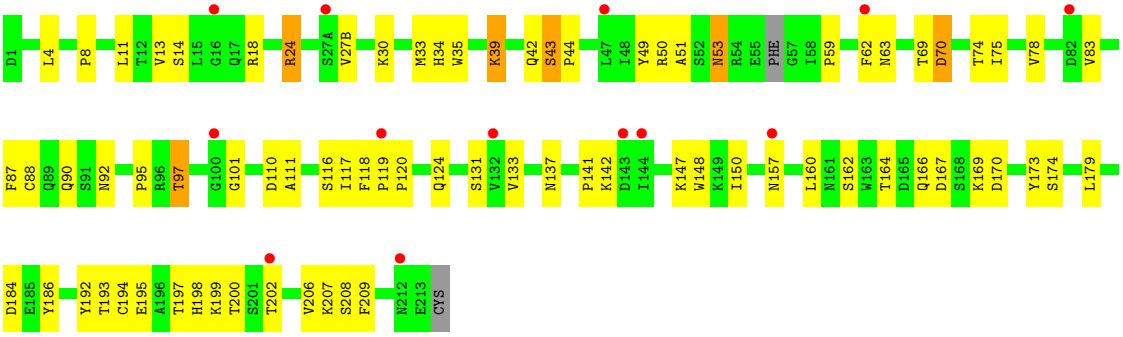



• Molecule 3: H5M9 antibody, light chain (kappa)



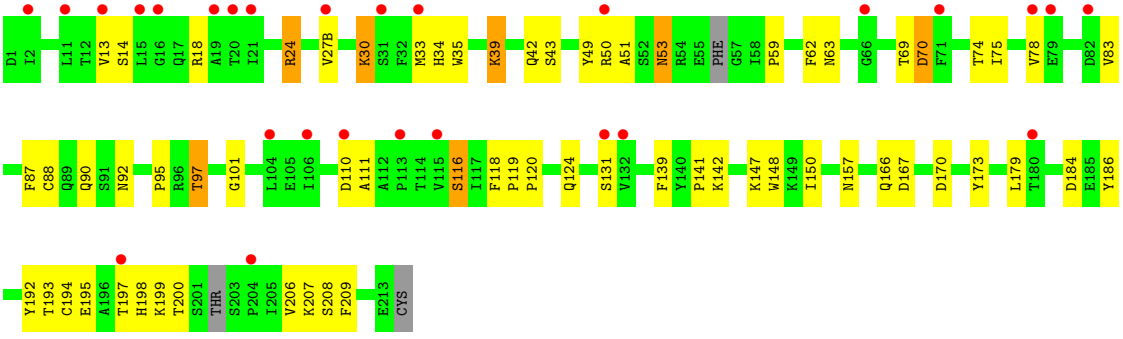

• Molecule 3: H5M9 antibody, light chain (kappa)

Chain X:

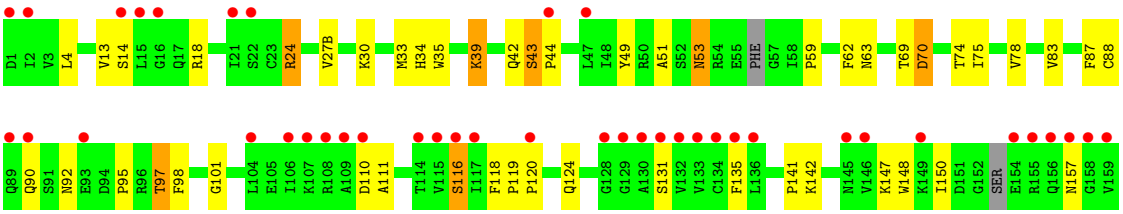

• Molecule 3: H5M9 antibody, light chain (kappa)

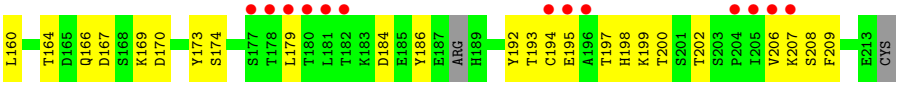
Chain Q:


• Molecule 3: H5M9 antibody, light chain (kappa)

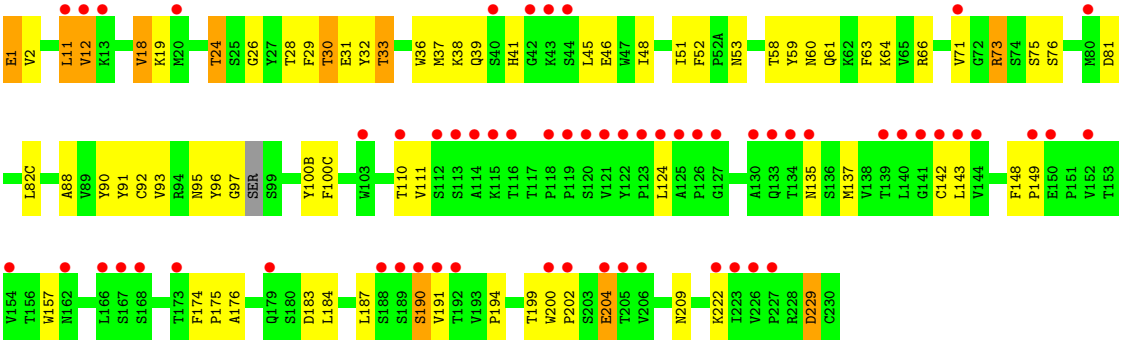
Chain V:



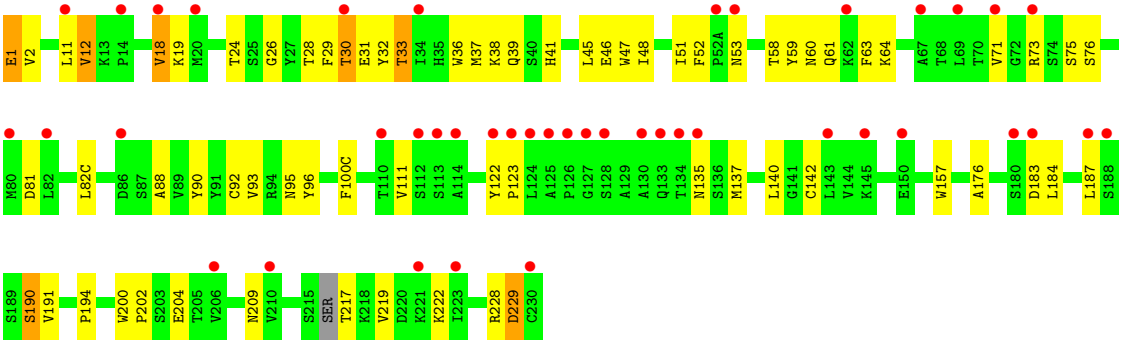

• Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain H:

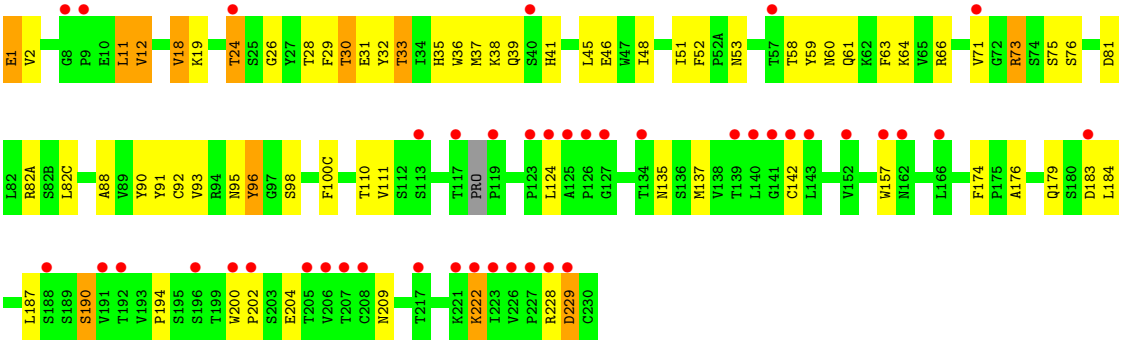

• Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain F:

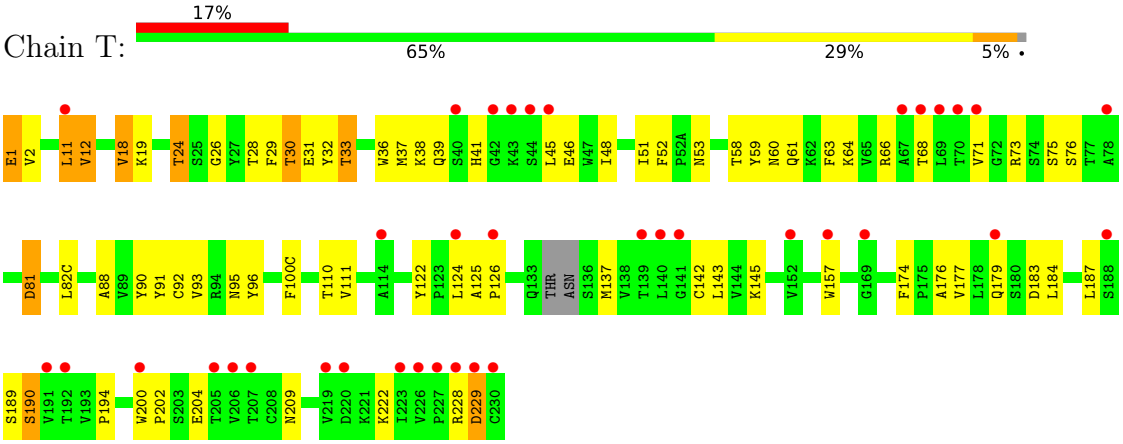

• Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain K:

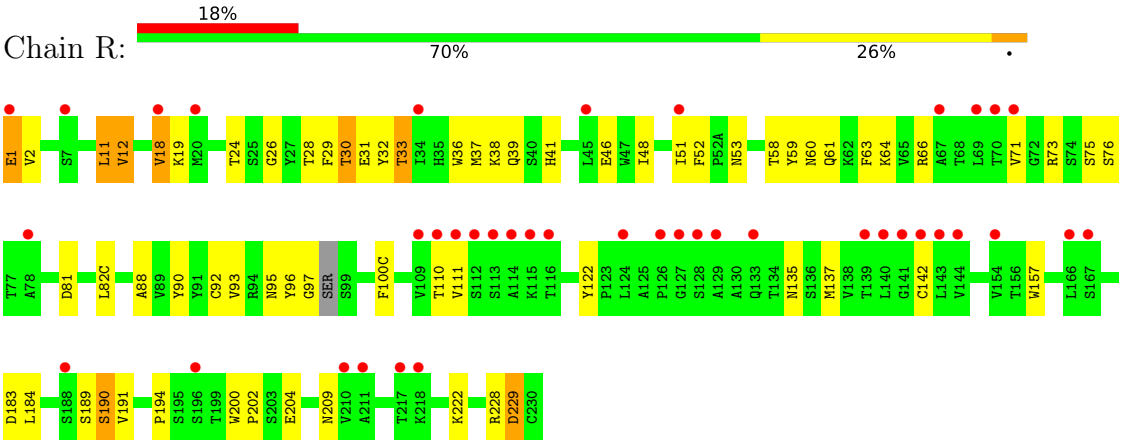

• Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain T:



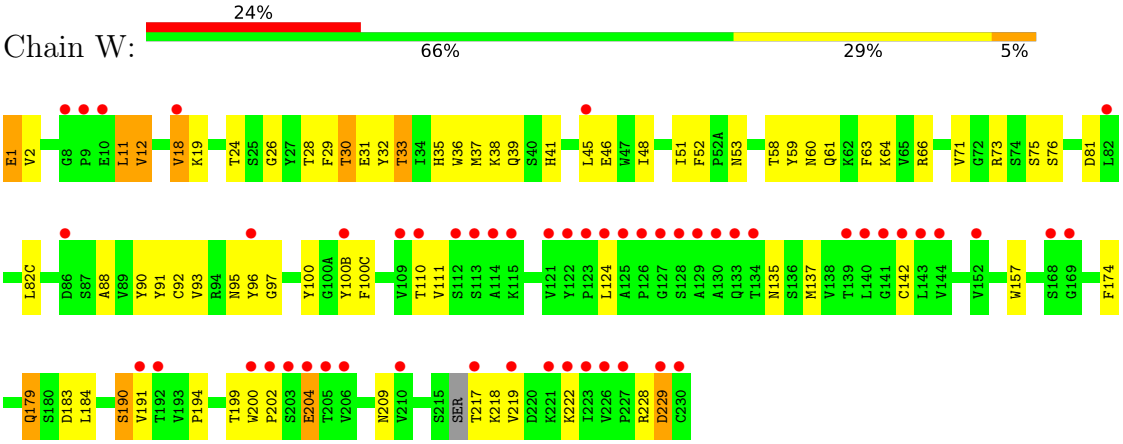

• Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain R:




• Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain W:

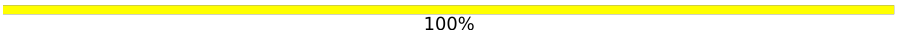



• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

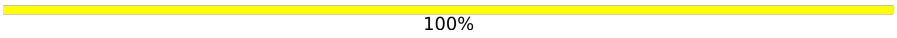
Chain d:





• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

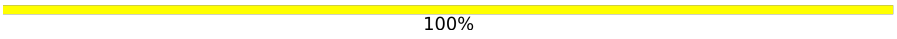
Chain f:





• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

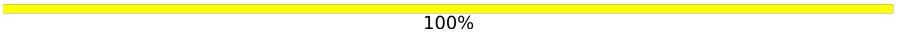
Chain Z:





• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

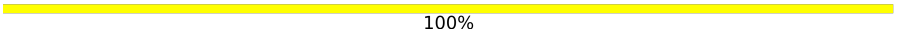
Chain a:





• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:





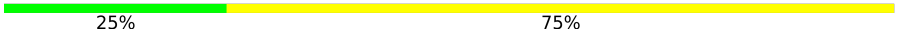
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:




# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 31 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 199.55Å 199.55Å 466.89Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 50.08 – 6.98<br>50.03 – 6.98 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 92.7 (50.08-6.98)<br>93.0 (50.03-6.98) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.14 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.56 (at 6.68Å) | Xtriage |
| Refinement program | REFMAC 5.7.0032 | Depositor |
| R, $R_{free}$ | 0.377 , 0.387<br>0.368 , 0.364 | Depositor<br>DCC |
| $R_{free}$ test set | 843 reflections (5.10%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 375.9 | Xtriage |
| Anisotropy | 0.537 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 214.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.45$, $< L^2 > = 0.27$ | Xtriage |
| Estimated twinning fraction | 0.045 for -h,-k,l | Xtriage |
| $F_o$,$F_c$ correlation | 0.78 | EDS |
| Total number of atoms | 43995 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 89.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.47 | 0/2606 | 0.67 | 1/3542 (0.0%) |
| 1 | C | 0.47 | 0/2596 | 0.67 | 1/3527 (0.0%) |
| 1 | G | 0.47 | 0/2592 | 0.67 | 1/3521 (0.0%) |
| 1 | M | 0.47 | 0/2606 | 0.67 | 1/3542 (0.0%) |
| 1 | O | 0.46 | 0/2577 | 0.66 | 0/3503 |
| 1 | S | 0.47 | 0/2606 | 0.67 | 1/3542 (0.0%) |
| 2 | B | 0.50 | 0/1418 | 0.65 | 0/1906 |
| 2 | D | 0.50 | 0/1418 | 0.65 | 0/1906 |
| 2 | I | 0.49 | 0/1430 | 0.65 | 0/1924 |
| 2 | N | 0.50 | 0/1384 | 0.65 | 0/1857 |
| 2 | P | 0.50 | 0/1418 | 0.65 | 0/1906 |
| 2 | U | 0.50 | 0/1430 | 0.65 | 0/1924 |
| 3 | E | 0.64 | 0/1707 | 0.74 | 0/2313 |
| 3 | J | 0.64 | 0/1667 | 0.75 | 0/2257 |
| 3 | L | 0.65 | 0/1700 | 0.74 | 0/2301 |
| 3 | Q | 0.65 | 0/1699 | 0.74 | 0/2300 |
| 3 | V | 0.64 | 0/1688 | 0.74 | 0/2285 |
| 3 | X | 0.64 | 0/1707 | 0.74 | 0/2313 |
| 4 | F | 0.62 | 0/1720 | 0.77 | 0/2350 |
| 4 | H | 0.62 | 0/1720 | 0.77 | 0/2350 |
| 4 | K | 0.62 | 0/1718 | 0.77 | 0/2345 |
| 4 | R | 0.62 | 0/1720 | 0.77 | 0/2350 |
| 4 | T | 0.61 | 0/1711 | 0.77 | 0/2337 |
| 4 | W | 0.62 | 0/1720 | 0.77 | 0/2350 |
| All | All | 0.55 | 0/44558 | 0.71 | 5/60451 (0.0%) |

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 |
|---|---|---|---|
| 3 | E | 0 | 1 |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 9 | PRO | CA-N-CD | -8.46 | 99.65 | 111.50 |
| 1 | C | 9 | PRO | CA-N-CD | -8.46 | 99.66 | 111.50 |
| 1 | G | 9 | PRO | CA-N-CD | -8.46 | 99.66 | 111.50 |
| 1 | M | 9 | PRO | CA-N-CD | -8.44 | 99.68 | 111.50 |
| 1 | S | 9 | PRO | CA-N-CD | -8.44 | 99.68 | 111.50 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | E | 50 | ARG | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2542 | 0 | 2464 | 74 | 0 |
| 1 | C | 2533 | 0 | 2455 | 75 | 0 |
| 1 | G | 2530 | 0 | 2453 | 68 | 0 |
| 1 | M | 2542 | 0 | 2464 | 77 | 0 |
| 1 | O | 2514 | 0 | 2440 | 75 | 0 |
| 1 | S | 2542 | 0 | 2463 | 73 | 0 |
| 2 | B | 1393 | 0 | 1295 | 24 | 0 |
| 2 | D | 1393 | 0 | 1295 | 55 | 0 |
| 2 | I | 1403 | 0 | 1302 | 36 | 0 |
| 2 | N | 1363 | 0 | 1272 | 54 | 0 |
| 2 | P | 1393 | 0 | 1294 | 35 | 0 |
| 2 | U | 1403 | 0 | 1302 | 46 | 0 |
| 3 | E | 1672 | 0 | 1597 | 57 | 0 |
| 3 | J | 1634 | 0 | 1560 | 77 | 0 |
| 3 | L | 1666 | 0 | 1592 | 70 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | Q | 1665 | 0 | 1589 | 57 | 0 |
| 3 | V | 1655 | 0 | 1577 | 76 | 0 |
| 3 | X | 1672 | 0 | 1597 | 77 | 0 |
| 4 | F | 1675 | 0 | 1626 | 61 | 0 |
| 4 | H | 1675 | 0 | 1626 | 75 | 0 |
| 4 | K | 1674 | 0 | 1625 | 79 | 0 |
| 4 | R | 1675 | 0 | 1626 | 60 | 0 |
| 4 | T | 1666 | 0 | 1618 | 79 | 0 |
| 4 | W | 1675 | 0 | 1626 | 100 | 0 |
| 5 | Y | 39 | 0 | 34 | 1 | 0 |
| 5 | d | 39 | 0 | 34 | 0 | 0 |
| 5 | f | 39 | 0 | 34 | 0 | 0 |
| 6 | Z | 94 | 0 | 79 | 0 | 0 |
| 7 | a | 28 | 0 | 25 | 0 | 0 |
| 7 | c | 28 | 0 | 25 | 0 | 0 |
| 8 | b | 39 | 0 | 34 | 0 | 0 |
| 9 | e | 50 | 0 | 43 | 0 | 0 |
| 10 | A | 14 | 0 | 13 | 0 | 0 |
| 10 | C | 14 | 0 | 13 | 0 | 0 |
| 10 | M | 14 | 0 | 13 | 0 | 0 |
| 10 | O | 14 | 0 | 13 | 0 | 0 |
| 10 | P | 14 | 0 | 13 | 2 | 0 |
| 10 | S | 14 | 0 | 13 | 0 | 0 |
| All | All | 43995 | 0 | 42144 | 1200 | 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 14.

All (1200) 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) |
|---|---|---|---|
| 4:H:31:GLU:HG3 | 4:H:32:TYR:CD1 | 1.57 | 1.40 |
| 4:K:31:GLU:HG3 | 4:K:32:TYR:CD1 | 1.57 | 1.39 |
| 4:W:31:GLU:HG3 | 4:W:32:TYR:CD1 | 1.57 | 1.39 |
| 3:V:164:THR:HG23 | 4:W:174:PHE:CD1 | 1.59 | 1.38 |
| 4:R:31:GLU:HG3 | 4:R:32:TYR:CD1 | 1.57 | 1.38 |
| 4:F:31:GLU:HG3 | 4:F:32:TYR:CD1 | 1.57 | 1.37 |
| 4:T:31:GLU:HG3 | 4:T:32:TYR:CD1 | 1.57 | 1.37 |
| 4:R:31:GLU:HG3 | 4:R:32:TYR:CE1 | 1.79 | 1.17 |
| 1:O:274:TYR:CE2 | 4:R:97:GLY:HA2 | 1.81 | 1.16 |
| 4:F:31:GLU:HG3 | 4:F:32:TYR:CE1 | 1.79 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:W:31:GLU:HG3 | 4:W:32:TYR:CE1 | 1.79 | 1.16 |
| 4:H:31:GLU:HG3 | 4:H:32:TYR:CE1 | 1.79 | 1.15 |
| 4:K:31:GLU:HG3 | 4:K:32:TYR:CE1 | 1.79 | 1.15 |
| 4:T:31:GLU:HG3 | 4:T:32:TYR:CE1 | 1.79 | 1.15 |
| 1:G:316:LEU:HD21 | 2:I:100:VAL:HG22 | 1.29 | 1.14 |
| 3:J:164:THR:HG23 | 4:K:174:PHE:CD1 | 1.83 | 1.12 |
| 3:V:43:SER:HB3 | 4:W:91:TYR:CE1 | 1.84 | 1.11 |
| 3:X:117:ILE:HG22 | 3:X:207:LYS:HG3 | 1.29 | 1.11 |
| 2:D:76:ARG:NH2 | 2:I:74:GLU:OE2 | 1.89 | 1.06 |
| 4:W:31:GLU:CG | 4:W:32:TYR:CE1 | 2.39 | 1.05 |
| 4:T:31:GLU:CG | 4:T:32:TYR:CE1 | 2.39 | 1.05 |
| 4:H:31:GLU:CG | 4:H:32:TYR:CE1 | 2.39 | 1.05 |
| 4:R:31:GLU:CG | 4:R:32:TYR:CE1 | 2.39 | 1.05 |
| 4:F:31:GLU:CG | 4:F:32:TYR:CE1 | 2.39 | 1.04 |
| 4:K:31:GLU:CG | 4:K:32:TYR:CE1 | 2.39 | 1.04 |
| 4:K:31:GLU:CD | 4:K:32:TYR:CE1 | 2.32 | 1.04 |
| 1:G:9:PRO:HD2 | 1:G:10:GLY:H | 1.23 | 1.03 |
| 4:W:31:GLU:CD | 4:W:32:TYR:CE1 | 2.32 | 1.03 |
| 1:S:9:PRO:HD2 | 1:S:10:GLY:H | 1.23 | 1.03 |
| 4:F:31:GLU:CD | 4:F:32:TYR:CE1 | 2.32 | 1.03 |
| 4:H:31:GLU:CD | 4:H:32:TYR:CE1 | 2.32 | 1.03 |
| 4:R:31:GLU:CD | 4:R:32:TYR:CE1 | 2.32 | 1.03 |
| 4:T:31:GLU:CD | 4:T:32:TYR:CE1 | 2.32 | 1.03 |
| 1:C:9:PRO:HD2 | 1:C:10:GLY:H | 1.23 | 1.02 |
| 1:O:274:TYR:HE2 | 4:R:97:GLY:HA2 | 1.13 | 1.01 |
| 4:T:68:THR:HB | 4:T:81:ASP:OD2 | 1.61 | 1.01 |
| 4:K:31:GLU:CG | 4:K:32:TYR:CD1 | 2.44 | 1.00 |
| 4:F:31:GLU:CG | 4:F:32:TYR:CD1 | 2.44 | 1.00 |
| 4:W:31:GLU:CG | 4:W:32:TYR:CD1 | 2.44 | 1.00 |
| 1:M:9:PRO:HD2 | 1:M:10:GLY:H | 1.23 | 1.00 |
| 4:R:31:GLU:CG | 4:R:32:TYR:CD1 | 2.44 | 1.00 |
| 4:H:31:GLU:CG | 4:H:32:TYR:CD1 | 2.44 | 1.00 |
| 4:T:31:GLU:CG | 4:T:32:TYR:CD1 | 2.44 | 0.99 |
| 4:W:33:THR:HB | 4:W:52:PHE:CD1 | 1.96 | 0.99 |
| 4:R:31:GLU:OE2 | 4:R:32:TYR:HE1 | 1.47 | 0.98 |
| 1:A:9:PRO:HD2 | 1:A:10:GLY:H | 1.23 | 0.98 |
| 4:F:31:GLU:OE2 | 4:F:32:TYR:HE1 | 1.47 | 0.98 |
| 3:V:164:THR:CG2 | 4:W:174:PHE:CD1 | 2.46 | 0.97 |
| 4:K:31:GLU:OE2 | 4:K:32:TYR:HE1 | 1.47 | 0.97 |
| 4:W:31:GLU:OE2 | 4:W:32:TYR:HE1 | 1.47 | 0.97 |
| 4:T:31:GLU:OE2 | 4:T:32:TYR:HE1 | 1.46 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:316:LEU:CD2 | 2:I:100:VAL:HG22 | 1.94 | 0.97 |
| 4:H:31:GLU:OE2 | 4:H:32:TYR:HE1 | 1.47 | 0.97 |
| 2:D:167:ARG:HG2 | 2:D:170:ARG:NH2 | 1.80 | 0.96 |
| 1:O:274:TYR:OH | 4:R:97:GLY:HA3 | 1.67 | 0.95 |
| 3:L:43:SER:HB3 | 4:H:91:TYR:CE1 | 2.01 | 0.95 |
| 2:N:168:LEU:HD12 | 2:N:169:ASN:N | 1.81 | 0.94 |
| 3:Q:119:PRO:HB2 | 4:R:228:ARG:HH21 | 1.31 | 0.94 |
| 1:M:17:TYR:CE2 | 2:N:13:GLY:CA | 2.50 | 0.94 |
| 2:N:76:ARG:HH12 | 2:P:68:ARG:HG2 | 1.32 | 0.93 |
| 1:S:274:TYR:HD2 | 4:W:31:GLU:O | 1.51 | 0.93 |
| 1:M:276:ASN:ND2 | 4:T:52:PHE:CE1 | 2.38 | 0.92 |
| 3:V:164:THR:HG23 | 4:W:174:PHE:HD1 | 1.00 | 0.92 |
| 3:J:8:PRO:HB3 | 3:X:11:LEU:CD1 | 1.99 | 0.92 |
| 2:D:32:SER:O | 4:W:217:THR:HG23 | 1.71 | 0.90 |
| 3:X:117:ILE:CG2 | 3:X:207:LYS:HG3 | 2.01 | 0.90 |
| 1:O:274:TYR:OH | 4:R:97:GLY:CA | 2.20 | 0.89 |
| 3:L:44:PRO:HG2 | 4:H:45:LEU:HD11 | 1.54 | 0.88 |
| 1:M:17:TYR:CZ | 2:N:12:GLY:C | 2.47 | 0.88 |
| 1:M:17:TYR:CE2 | 2:N:13:GLY:HA3 | 2.07 | 0.88 |
| 2:D:167:ARG:HG2 | 2:D:170:ARG:HH21 | 1.36 | 0.88 |
| 3:J:164:THR:HG23 | 4:K:174:PHE:HD1 | 1.36 | 0.88 |
| 2:N:76:ARG:NH1 | 2:P:68:ARG:HG2 | 1.91 | 0.86 |
| 1:M:9:PRO:HD2 | 1:M:10:GLY:N | 1.91 | 0.85 |
| 1:G:9:PRO:HD2 | 1:G:10:GLY:N | 1.91 | 0.85 |
| 1:S:9:PRO:HD2 | 1:S:10:GLY:N | 1.91 | 0.85 |
| 3:V:174:SER:HB2 | 4:W:174:PHE:HE1 | 1.42 | 0.85 |
| 3:J:119:PRO:HB2 | 4:K:228:ARG:HH21 | 1.40 | 0.85 |
| 3:J:160:LEU:HD11 | 4:K:179:GLN:OE1 | 1.77 | 0.85 |
| 1:A:9:PRO:HD2 | 1:A:10:GLY:N | 1.91 | 0.84 |
| 4:F:31:GLU:CD | 4:F:32:TYR:HE1 | 1.78 | 0.84 |
| 2:U:32:SER:O | 4:F:217:THR:HA | 1.76 | 0.84 |
| 1:C:9:PRO:HD2 | 1:C:10:GLY:N | 1.91 | 0.84 |
| 1:C:11:ASP:OD1 | 2:D:28:ASN:HA | 1.77 | 0.84 |
| 3:X:117:ILE:HG22 | 3:X:207:LYS:CG | 2.08 | 0.84 |
| 3:V:43:SER:HB3 | 4:W:91:TYR:HE1 | 1.34 | 0.84 |
| 3:V:119:PRO:HB2 | 4:W:228:ARG:HH21 | 1.44 | 0.83 |
| 4:H:31:GLU:CD | 4:H:32:TYR:HE1 | 1.78 | 0.83 |
| 1:G:11:ASP:OD1 | 2:I:28:ASN:HA | 1.78 | 0.83 |
| 4:W:31:GLU:CD | 4:W:32:TYR:HE1 | 1.78 | 0.83 |
| 1:G:276:ASN:O | 4:K:98:SER:HB3 | 1.78 | 0.82 |
| 3:X:160:LEU:HD11 | 4:T:179:GLN:OE1 | 1.79 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:V:160:LEU:HD21 | 4:W:179:GLN:HE21 | 1.42 | 0.82 |
| 1:A:83:PRO:CG | 4:H:100(B):TYR:OH | 2.28 | 0.82 |
| 3:J:43:SER:HB3 | 4:K:91:TYR:CE1 | 2.13 | 0.82 |
| 3:X:118:PHE:CD2 | 4:T:124:LEU:HB3 | 2.14 | 0.82 |
| 4:R:31:GLU:CD | 4:R:32:TYR:HE1 | 1.78 | 0.81 |
| 1:A:274:TYR:OH | 4:H:97:GLY:HA3 | 1.80 | 0.81 |
| 2:N:165:GLU:HA | 2:N:168:LEU:CD2 | 2.10 | 0.81 |
| 1:A:274:TYR:OH | 4:H:97:GLY:CA | 2.29 | 0.81 |
| 1:M:17:TYR:CZ | 2:N:13:GLY:N | 2.48 | 0.81 |
| 3:X:160:LEU:HD11 | 4:T:179:GLN:CD | 2.01 | 0.81 |
| 1:M:107:GLU:OE2 | 2:U:76:ARG:HG3 | 1.81 | 0.81 |
| 1:G:25:GLN:OE1 | 1:G:33:ASN:OD1 | 1.99 | 0.80 |
| 3:V:44:PRO:HG2 | 4:W:45:LEU:HD11 | 1.62 | 0.80 |
| 1:O:274:TYR:CE2 | 4:R:97:GLY:CA | 2.65 | 0.79 |
| 4:K:28:THR:O | 4:K:31:GLU:HG2 | 1.83 | 0.79 |
| 1:S:105:TYR:CZ | 1:S:109:LYS:HE3 | 2.16 | 0.79 |
| 2:N:76:ARG:HH11 | 2:N:76:ARG:HG2 | 1.44 | 0.79 |
| 4:F:28:THR:O | 4:F:31:GLU:HG2 | 1.83 | 0.79 |
| 3:J:118:PHE:CD2 | 4:K:124:LEU:HB3 | 2.17 | 0.78 |
| 4:T:28:THR:O | 4:T:31:GLU:HG2 | 1.83 | 0.78 |
| 1:S:83:PRO:CG | 4:W:100(B):TYR:OH | 2.32 | 0.78 |
| 4:R:28:THR:O | 4:R:31:GLU:HG2 | 1.83 | 0.78 |
| 3:V:174:SER:HB2 | 4:W:174:PHE:CE1 | 2.18 | 0.78 |
| 3:J:8:PRO:HB3 | 3:X:11:LEU:HD11 | 1.64 | 0.78 |
| 1:M:118:PHE:HE1 | 1:M:260:ILE:HD13 | 1.49 | 0.78 |
| 4:K:31:GLU:CD | 4:K:32:TYR:HE1 | 1.78 | 0.78 |
| 4:W:28:THR:O | 4:W:31:GLU:HG2 | 1.82 | 0.78 |
| 1:G:118:PHE:HE1 | 1:G:260:ILE:HD13 | 1.49 | 0.78 |
| 1:M:206:THR:HB | 1:M:209:LEU:HB3 | 1.66 | 0.78 |
| 4:H:28:THR:O | 4:H:31:GLU:HG2 | 1.83 | 0.78 |
| 1:G:206:THR:HB | 1:G:209:LEU:HB3 | 1.66 | 0.77 |
| 1:S:15:ILE:HD11 | 2:U:122:VAL:HG21 | 1.66 | 0.77 |
| 1:M:17:TYR:OH | 2:N:12:GLY:C | 2.23 | 0.77 |
| 1:G:206:THR:HG22 | 1:G:208:THR:H | 1.50 | 0.77 |
| 4:T:31:GLU:CD | 4:T:32:TYR:HE1 | 1.78 | 0.77 |
| 1:G:316:LEU:HD23 | 2:I:100:VAL:HG13 | 1.65 | 0.77 |
| 1:A:206:THR:HG22 | 1:A:208:THR:H | 1.50 | 0.77 |
| 3:J:120:PRO:HB3 | 3:J:131:SER:H | 1.50 | 0.77 |
| 4:W:48:ILE:HA | 4:W:63:PHE:HD2 | 1.49 | 0.77 |
| 1:M:206:THR:HG22 | 1:M:208:THR:H | 1.50 | 0.77 |
| 1:O:118:PHE:HE1 | 1:O:260:ILE:HD13 | 1.49 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:206:THR:HB | 1:A:209:LEU:HB3 | 1.66 | 0.77 |
| 4:H:48:ILE:HA | 4:H:63:PHE:HD2 | 1.49 | 0.76 |
| 1:O:106:GLU:OE2 | 2:P:71:ASN:HB3 | 1.85 | 0.76 |
| 1:C:206:THR:HB | 1:C:209:LEU:HB3 | 1.66 | 0.76 |
| 1:G:106:GLU:CD | 2:I:71:ASN:HB3 | 2.05 | 0.76 |
| 3:L:120:PRO:HB3 | 3:L:131:SER:H | 1.50 | 0.76 |
| 3:Q:120:PRO:HB3 | 3:Q:131:SER:H | 1.50 | 0.76 |
| 1:S:206:THR:HG22 | 1:S:208:THR:H | 1.50 | 0.76 |
| 1:O:206:THR:HG22 | 1:O:208:THR:H | 1.50 | 0.76 |
| 4:T:48:ILE:HA | 4:T:63:PHE:HD2 | 1.50 | 0.76 |
| 4:F:48:ILE:HA | 4:F:63:PHE:HD2 | 1.50 | 0.76 |
| 3:X:120:PRO:HB3 | 3:X:131:SER:H | 1.50 | 0.76 |
| 4:R:48:ILE:HA | 4:R:63:PHE:HD2 | 1.49 | 0.76 |
| 1:O:206:THR:HB | 1:O:209:LEU:HB3 | 1.66 | 0.76 |
| 1:S:206:THR:HB | 1:S:209:LEU:HB3 | 1.66 | 0.76 |
| 4:K:48:ILE:HA | 4:K:63:PHE:HD2 | 1.49 | 0.76 |
| 1:O:316:LEU:HD21 | 2:P:100:VAL:HG22 | 1.69 | 0.75 |
| 1:S:118:PHE:HE1 | 1:S:260:ILE:HD13 | 1.49 | 0.75 |
| 1:A:11:ASP:OD1 | 2:B:28:ASN:HA | 1.86 | 0.75 |
| 1:A:118:PHE:HE1 | 1:A:260:ILE:HD13 | 1.49 | 0.75 |
| 1:C:11:ASP:CG | 2:D:28:ASN:HA | 2.06 | 0.75 |
| 1:C:118:PHE:HE1 | 1:C:260:ILE:HD13 | 1.49 | 0.75 |
| 1:G:276:ASN:ND2 | 4:K:52:PHE:CE1 | 2.55 | 0.75 |
| 1:C:206:THR:HG22 | 1:C:208:THR:H | 1.50 | 0.74 |
| 3:L:137:ASN:ND2 | 4:H:174:PHE:HZ | 1.85 | 0.74 |
| 3:E:120:PRO:HB3 | 3:E:131:SER:H | 1.50 | 0.74 |
| 3:V:120:PRO:HB3 | 3:V:131:SER:H | 1.50 | 0.74 |
| 3:J:8:PRO:CB | 3:X:11:LEU:HD12 | 2.17 | 0.74 |
| 4:W:33:THR:HB | 4:W:52:PHE:CE1 | 2.21 | 0.74 |
| 1:M:276:ASN:HD21 | 4:T:31:GLU:C | 1.91 | 0.74 |
| 1:O:216:GLU:O | 1:O:220:ARG:NH2 | 2.21 | 0.74 |
| 1:C:16:GLY:N | 2:D:14:TRP:CH2 | 2.56 | 0.74 |
| 1:M:216:GLU:O | 1:M:220:ARG:NH2 | 2.21 | 0.73 |
| 1:M:11:ASP:CG | 2:N:28:ASN:HA | 2.09 | 0.73 |
| 1:G:276:ASN:O | 4:K:98:SER:CB | 2.36 | 0.73 |
| 1:A:56:VAL:HG21 | 3:L:30:LYS:NZ | 2.03 | 0.73 |
| 2:D:76:ARG:NE | 1:G:107:GLU:OE2 | 2.20 | 0.73 |
| 1:S:274:TYR:OH | 4:W:97:GLY:HA2 | 1.88 | 0.73 |
| 2:N:74:GLU:OE2 | 2:U:76:ARG:NH2 | 2.21 | 0.73 |
| 1:G:216:GLU:O | 1:G:220:ARG:NH2 | 2.21 | 0.73 |
| 1:O:13:ILE:HA | 2:P:26:HIS:HA | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:J:8:PRO:CB | 3:X:11:LEU:CD1 | 2.67 | 0.73 |
| 1:S:83:PRO:CB | 4:W:100(B):TYR:OH | 2.36 | 0.72 |
| 1:A:216:GLU:O | 1:A:220:ARG:NH2 | 2.21 | 0.72 |
| 1:C:15:ILE:C | 2:D:14:TRP:CH2 | 2.63 | 0.72 |
| 1:M:17:TYR:CE1 | 2:N:12:GLY:O | 2.43 | 0.72 |
| 2:N:165:GLU:HA | 2:N:168:LEU:HD21 | 1.70 | 0.72 |
| 1:S:216:GLU:O | 1:S:220:ARG:NH2 | 2.21 | 0.72 |
| 1:C:216:GLU:O | 1:C:220:ARG:NH2 | 2.21 | 0.72 |
| 1:C:220:ARG:NE | 1:G:210:ASN:OD1 | 2.22 | 0.72 |
| 3:V:160:LEU:HD11 | 4:W:179:GLN:HG2 | 1.73 | 0.71 |
| 2:D:80:LEU:HD11 | 2:I:80:LEU:HD22 | 1.72 | 0.71 |
| 1:A:274:TYR:CE2 | 4:H:97:GLY:HA2 | 2.26 | 0.71 |
| 1:G:106:GLU:OE2 | 2:I:71:ASN:HB3 | 1.91 | 0.71 |
| 1:M:9:PRO:CD | 1:M:10:GLY:H | 2.02 | 0.71 |
| 1:G:9:PRO:CD | 1:G:10:GLY:H | 2.02 | 0.70 |
| 1:S:307:LYS:HD3 | 2:U:59:MET:O | 1.91 | 0.70 |
| 1:S:9:PRO:CD | 1:S:10:GLY:H | 2.02 | 0.70 |
| 1:S:55(A):GLY:HA2 | 4:W:100:TYR:HB2 | 1.74 | 0.70 |
| 1:S:106:GLU:OE2 | 2:U:71:ASN:HB3 | 1.91 | 0.70 |
| 1:O:274:TYR:CZ | 4:R:97:GLY:CA | 2.75 | 0.69 |
| 1:M:17:TYR:CD2 | 2:N:13:GLY:HA3 | 2.27 | 0.69 |
| 1:C:118:PHE:CE1 | 1:C:260:ILE:HD13 | 2.28 | 0.69 |
| 1:C:9:PRO:CD | 1:C:10:GLY:H | 2.02 | 0.69 |
| 4:K:31:GLU:OE2 | 4:K:32:TYR:CE1 | 2.36 | 0.69 |
| 1:M:62:ARG:HG2 | 1:M:63:ASP:N | 2.08 | 0.69 |
| 3:V:43:SER:HA | 4:W:91:TYR:OH | 1.93 | 0.69 |
| 4:T:31:GLU:OE2 | 4:T:32:TYR:CE1 | 2.36 | 0.69 |
| 1:O:118:PHE:CE1 | 1:O:260:ILE:HD13 | 2.28 | 0.68 |
| 1:C:62:ARG:HG2 | 1:C:63:ASP:N | 2.08 | 0.68 |
| 1:S:118:PHE:CE1 | 1:S:260:ILE:HD13 | 2.28 | 0.68 |
| 1:S:274:TYR:OH | 4:W:97:GLY:CA | 2.40 | 0.68 |
| 4:W:33:THR:HB | 4:W:52:PHE:HD1 | 1.54 | 0.68 |
| 2:P:150:GLU:HB2 | 10:P:2001:NAG:H62 | 1.74 | 0.68 |
| 3:V:98:PHE:CD1 | 4:W:45:LEU:O | 2.46 | 0.68 |
| 1:A:62:ARG:HG2 | 1:A:63:ASP:N | 2.08 | 0.68 |
| 1:G:118:PHE:CE1 | 1:G:260:ILE:HD13 | 2.28 | 0.68 |
| 1:G:62:ARG:HG2 | 1:G:63:ASP:N | 2.08 | 0.68 |
| 1:O:56:VAL:HG21 | 3:Q:30:LYS:NZ | 2.08 | 0.68 |
| 1:M:118:PHE:CE1 | 1:M:260:ILE:HD13 | 2.28 | 0.68 |
| 1:O:62:ARG:HG2 | 1:O:63:ASP:N | 2.08 | 0.68 |
| 1:S:62:ARG:HG2 | 1:S:63:ASP:N | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:107:GLU:OE2 | 2:I:76:ARG:NE | 2.25 | 0.68 |
| 1:A:212:ARG:NH2 | 1:G:217:ILE:O | 2.25 | 0.68 |
| 4:T:68:THR:CB | 4:T:81:ASP:OD2 | 2.41 | 0.68 |
| 2:N:76:ARG:NH1 | 2:N:76:ARG:HG2 | 2.08 | 0.67 |
| 3:J:90:GLN:HE21 | 3:J:97:THR:CG2 | 2.08 | 0.67 |
| 1:O:15:ILE:C | 2:P:14:TRP:CH2 | 2.67 | 0.67 |
| 3:X:90:GLN:HE21 | 3:X:97:THR:CG2 | 2.08 | 0.67 |
| 3:Q:90:GLN:HE21 | 3:Q:97:THR:CG2 | 2.08 | 0.67 |
| 1:A:118:PHE:CE1 | 1:A:260:ILE:HD13 | 2.28 | 0.67 |
| 3:E:90:GLN:HE21 | 3:E:97:THR:CG2 | 2.08 | 0.67 |
| 3:L:90:GLN:HE21 | 3:L:97:THR:CG2 | 2.08 | 0.67 |
| 3:V:90:GLN:HE21 | 3:V:97:THR:CG2 | 2.08 | 0.67 |
| 2:D:76:ARG:NH1 | 2:I:74:GLU:OE1 | 2.27 | 0.67 |
| 3:X:164:THR:HG23 | 4:T:174:PHE:CD1 | 2.30 | 0.67 |
| 1:A:83:PRO:HG3 | 4:H:100(B):TYR:OH | 1.94 | 0.67 |
| 1:C:13:ILE:HA | 2:D:26:HIS:HA | 1.78 | 0.66 |
| 1:S:106:GLU:CD | 2:U:71:ASN:HB3 | 2.16 | 0.66 |
| 1:M:107:GLU:OE2 | 2:U:76:ARG:CG | 2.43 | 0.66 |
| 1:M:17:TYR:CZ | 2:N:13:GLY:CA | 2.78 | 0.65 |
| 1:A:244:ASN:ND2 | 1:G:221:PRO:HD3 | 2.12 | 0.65 |
| 3:X:133:VAL:HG21 | 4:T:143:LEU:HD13 | 1.78 | 0.65 |
| 1:M:9:PRO:CD | 1:M:10:GLY:N | 2.59 | 0.65 |
| 1:M:17:TYR:OH | 2:N:12:GLY:CA | 2.44 | 0.65 |
| 1:S:274:TYR:CD2 | 4:W:31:GLU:O | 2.42 | 0.65 |
| 1:A:216:GLU:HB3 | 1:C:212:ARG:HB3 | 1.79 | 0.65 |
| 1:M:276:ASN:ND2 | 4:T:52:PHE:HE1 | 1.94 | 0.65 |
| 1:O:16:GLY:N | 2:P:14:TRP:CH2 | 2.64 | 0.65 |
| 3:J:44:PRO:HG2 | 4:K:45:LEU:HD11 | 1.79 | 0.65 |
| 1:C:9:PRO:CD | 1:C:10:GLY:N | 2.59 | 0.64 |
| 1:O:106:GLU:CD | 2:P:71:ASN:HB3 | 2.17 | 0.64 |
| 2:D:80:LEU:HD21 | 2:I:80:LEU:HD21 | 1.79 | 0.64 |
| 4:H:31:GLU:OE2 | 4:H:32:TYR:CE1 | 2.36 | 0.64 |
| 1:A:56:VAL:HG21 | 3:L:30:LYS:HZ2 | 1.61 | 0.64 |
| 1:G:123:ILE:HD11 | 1:G:168:TYR:CZ | 2.33 | 0.64 |
| 1:M:123:ILE:HD11 | 1:M:168:TYR:CZ | 2.33 | 0.64 |
| 4:K:12:VAL:HG21 | 4:K:82(C):LEU:HD13 | 1.80 | 0.64 |
| 4:W:31:GLU:OE2 | 4:W:32:TYR:CE1 | 2.36 | 0.64 |
| 1:A:123:ILE:HD11 | 1:A:168:TYR:CZ | 2.33 | 0.64 |
| 4:W:12:VAL:HG21 | 4:W:82(C):LEU:HD13 | 1.80 | 0.64 |
| 4:T:12:VAL:HG21 | 4:T:82(C):LEU:HD13 | 1.80 | 0.64 |
| 1:S:123:ILE:HD11 | 1:S:168:TYR:CZ | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:63:ASN:HB3 | 3:E:74:THR:HB | 1.80 | 0.64 |
| 1:A:9:PRO:CD | 1:A:10:GLY:N | 2.59 | 0.64 |
| 3:V:160:LEU:CD1 | 4:W:179:GLN:HG2 | 2.27 | 0.64 |
| 1:C:123:ILE:HD11 | 1:C:168:TYR:CZ | 2.33 | 0.64 |
| 1:M:17:TYR:CD2 | 2:N:13:GLY:CA | 2.81 | 0.63 |
| 4:H:12:VAL:HG21 | 4:H:82(C):LEU:HD13 | 1.80 | 0.63 |
| 1:C:316:LEU:HD21 | 2:D:100:VAL:HG22 | 1.79 | 0.63 |
| 3:J:43:SER:HB3 | 4:K:91:TYR:HE1 | 1.63 | 0.63 |
| 3:J:119:PRO:HB2 | 4:K:228:ARG:NH2 | 2.13 | 0.63 |
| 3:V:164:THR:CG2 | 4:W:174:PHE:HD1 | 1.94 | 0.63 |
| 1:A:218:ALA:HB2 | 1:C:203:SER:HB2 | 1.80 | 0.63 |
| 1:O:123:ILE:HD11 | 1:O:168:TYR:CZ | 2.33 | 0.63 |
| 3:J:119:PRO:CB | 4:K:228:ARG:HH21 | 2.11 | 0.63 |
| 4:W:18:VAL:HG22 | 4:W:82(C):LEU:HD11 | 1.81 | 0.63 |
| 1:G:9:PRO:CD | 1:G:10:GLY:N | 2.59 | 0.63 |
| 4:F:18:VAL:HG22 | 4:F:82(C):LEU:HD11 | 1.81 | 0.63 |
| 4:R:18:VAL:HG22 | 4:R:82(C):LEU:HD11 | 1.81 | 0.63 |
| 1:A:12:GLN:O | 2:B:27:SER:N | 2.32 | 0.63 |
| 1:A:274:TYR:HE2 | 4:H:97:GLY:HA2 | 1.63 | 0.63 |
| 4:H:18:VAL:HG22 | 4:H:82(C):LEU:HD11 | 1.81 | 0.63 |
| 2:N:80:LEU:HD22 | 2:U:80:LEU:HD11 | 1.81 | 0.62 |
| 4:F:12:VAL:HG21 | 4:F:82(C):LEU:HD13 | 1.80 | 0.62 |
| 3:L:63:ASN:HB3 | 3:L:74:THR:HB | 1.80 | 0.62 |
| 3:X:63:ASN:HB3 | 3:X:74:THR:HB | 1.80 | 0.62 |
| 3:V:174:SER:CB | 4:W:174:PHE:CE1 | 2.81 | 0.62 |
| 4:R:12:VAL:HG21 | 4:R:82(C):LEU:HD13 | 1.80 | 0.62 |
| 1:O:55(A):GLY:O | 3:Q:50:ARG:NH2 | 2.33 | 0.62 |
| 3:Q:63:ASN:HB3 | 3:Q:74:THR:HB | 1.80 | 0.62 |
| 4:T:18:VAL:HG22 | 4:T:82(C):LEU:HD11 | 1.81 | 0.62 |
| 1:S:9:PRO:CD | 1:S:10:GLY:N | 2.59 | 0.62 |
| 3:L:118:PHE:CD2 | 4:H:124:LEU:HB3 | 2.35 | 0.62 |
| 3:V:63:ASN:HB3 | 3:V:74:THR:HB | 1.80 | 0.62 |
| 3:J:63:ASN:HB3 | 3:J:74:THR:HB | 1.80 | 0.62 |
| 1:C:276:ASN:HD21 | 4:F:32:TYR:HA | 1.64 | 0.62 |
| 3:Q:119:PRO:HB2 | 4:R:228:ARG:NH2 | 2.11 | 0.62 |
| 1:S:323:THR:HG21 | 2:U:12:GLY:HA2 | 1.82 | 0.62 |
| 4:K:18:VAL:HG22 | 4:K:82(C):LEU:HD11 | 1.81 | 0.61 |
| 1:M:17:TYR:CE2 | 2:N:13:GLY:N | 2.68 | 0.61 |
| 3:L:137:ASN:HD21 | 4:H:174:PHE:HZ | 1.48 | 0.61 |
| 2:D:80:LEU:HD21 | 2:I:80:LEU:CD2 | 2.30 | 0.61 |
| 1:O:274:TYR:CZ | 4:R:97:GLY:HA2 | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:293:PRO:HG2 | 1:M:294:PHE:HD1 | 1.66 | 0.61 |
| 1:A:16:GLY:N | 2:B:14:TRP:CH2 | 2.68 | 0.61 |
| 1:C:293:PRO:HG2 | 1:C:294:PHE:HD1 | 1.66 | 0.61 |
| 2:D:32:SER:O | 4:W:217:THR:CG2 | 2.46 | 0.61 |
| 1:O:293:PRO:HG2 | 1:O:294:PHE:HD1 | 1.66 | 0.61 |
| 1:G:293:PRO:HG2 | 1:G:294:PHE:HD1 | 1.66 | 0.61 |
| 1:O:276:ASN:OD1 | 4:R:33:THR:HG22 | 1.99 | 0.61 |
| 3:L:174:SER:CB | 4:H:174:PHE:HE1 | 2.14 | 0.61 |
| 4:K:200:TRP:CD1 | 4:K:202:PRO:HA | 2.36 | 0.61 |
| 2:P:80:LEU:HD21 | 2:U:80:LEU:CD2 | 2.31 | 0.61 |
| 4:R:200:TRP:CD1 | 4:R:202:PRO:HA | 2.36 | 0.61 |
| 4:W:48:ILE:HA | 4:W:63:PHE:CD2 | 2.35 | 0.61 |
| 1:S:83:PRO:HB2 | 4:W:100(B):TYR:OH | 2.00 | 0.60 |
| 1:M:186:ASN:ND2 | 1:M:190:GLU:OE1 | 2.33 | 0.60 |
| 1:A:293:PRO:HG2 | 1:A:294:PHE:HD1 | 1.66 | 0.60 |
| 3:J:164:THR:CG2 | 4:K:174:PHE:CD1 | 2.74 | 0.60 |
| 3:J:174:SER:HB2 | 4:K:174:PHE:CE1 | 2.36 | 0.60 |
| 4:H:200:TRP:CD1 | 4:H:202:PRO:HA | 2.36 | 0.60 |
| 1:O:83:PRO:HB3 | 3:Q:49:TYR:CE2 | 2.36 | 0.60 |
| 1:O:217:ILE:O | 1:S:212:ARG:NH2 | 2.31 | 0.60 |
| 2:N:168:LEU:HD12 | 2:N:168:LEU:C | 2.20 | 0.60 |
| 1:O:56:VAL:CG2 | 3:Q:30:LYS:NZ | 2.64 | 0.60 |
| 4:K:48:ILE:HA | 4:K:63:PHE:CD2 | 2.35 | 0.60 |
| 4:T:200:TRP:CD1 | 4:T:202:PRO:HA | 2.36 | 0.60 |
| 1:A:268:MET:HG3 | 1:A:284:PRO:HG3 | 1.84 | 0.60 |
| 3:L:164:THR:HG23 | 4:H:174:PHE:HD1 | 1.66 | 0.60 |
| 4:T:48:ILE:HA | 4:T:63:PHE:CD2 | 2.36 | 0.60 |
| 4:W:200:TRP:CD1 | 4:W:202:PRO:HA | 2.36 | 0.60 |
| 3:L:164:THR:HG23 | 4:H:174:PHE:CD1 | 2.37 | 0.60 |
| 1:O:14:CYS:O | 2:P:24:TYR:HA | 2.02 | 0.60 |
| 1:C:268:MET:HG3 | 1:C:284:PRO:HG3 | 1.84 | 0.60 |
| 1:A:83(A):GLU:N | 3:L:49:TYR:OH | 2.28 | 0.59 |
| 3:X:44:PRO:HG2 | 4:T:45:LEU:HD11 | 1.84 | 0.59 |
| 3:X:124:GLN:HB2 | 4:T:122:TYR:CE1 | 2.37 | 0.59 |
| 1:S:268:MET:HG3 | 1:S:284:PRO:HG3 | 1.84 | 0.59 |
| 1:S:293:PRO:HG2 | 1:S:294:PHE:HD1 | 1.66 | 0.59 |
| 3:E:90:GLN:HE21 | 3:E:97:THR:HG23 | 1.68 | 0.59 |
| 3:Q:90:GLN:HE21 | 3:Q:97:THR:HG23 | 1.68 | 0.59 |
| 3:V:174:SER:CB | 4:W:174:PHE:HE1 | 2.13 | 0.59 |
| 4:K:1:GLU:O | 4:K:26:GLY:HA3 | 2.03 | 0.59 |
| 4:T:39:GLN:O | 4:T:88:ALA:HB1 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:186:ASN:ND2 | 1:A:190:GLU:OE1 | 2.33 | 0.59 |
| 3:X:90:GLN:HE21 | 3:X:97:THR:HG23 | 1.68 | 0.59 |
| 4:K:19:LYS:NZ | 4:K:81:ASP:HB2 | 2.18 | 0.59 |
| 1:G:268:MET:HG3 | 1:G:284:PRO:HG3 | 1.84 | 0.59 |
| 3:J:160:LEU:CD1 | 4:K:179:GLN:OE1 | 2.49 | 0.59 |
| 3:X:119:PRO:HB2 | 4:T:228:ARG:HH21 | 1.68 | 0.59 |
| 3:E:123:GLU:OE1 | 4:F:123:PRO:CD | 2.51 | 0.59 |
| 3:V:43:SER:CB | 4:W:91:TYR:CE1 | 2.75 | 0.59 |
| 2:U:72:ASN:OD1 | 2:U:75:ARG:NH2 | 2.36 | 0.59 |
| 3:J:174:SER:HB2 | 4:K:174:PHE:HE1 | 1.68 | 0.59 |
| 4:R:39:GLN:O | 4:R:88:ALA:HB1 | 2.03 | 0.59 |
| 4:W:1:GLU:O | 4:W:26:GLY:HA3 | 2.02 | 0.59 |
| 4:R:19:LYS:NZ | 4:R:81:ASP:HB2 | 2.18 | 0.59 |
| 1:O:83:PRO:HB3 | 3:Q:49:TYR:HE2 | 1.66 | 0.59 |
| 4:H:19:LYS:NZ | 4:H:81:ASP:HB2 | 2.18 | 0.59 |
| 4:K:39:GLN:O | 4:K:88:ALA:HB1 | 2.03 | 0.59 |
| 4:K:200:TRP:CG | 4:K:202:PRO:HA | 2.38 | 0.59 |
| 2:D:72:ASN:OD1 | 2:D:75:ARG:NH2 | 2.36 | 0.58 |
| 1:M:268:MET:HG3 | 1:M:284:PRO:HG3 | 1.84 | 0.58 |
| 2:N:72:ASN:OD1 | 2:N:75:ARG:NH2 | 2.36 | 0.58 |
| 1:O:268:MET:HG3 | 1:O:284:PRO:HG3 | 1.84 | 0.58 |
| 4:F:1:GLU:O | 4:F:26:GLY:HA3 | 2.03 | 0.58 |
| 4:F:19:LYS:NZ | 4:F:81:ASP:HB2 | 2.18 | 0.58 |
| 4:F:200:TRP:CD1 | 4:F:202:PRO:HA | 2.36 | 0.58 |
| 4:R:1:GLU:O | 4:R:26:GLY:HA3 | 2.02 | 0.58 |
| 3:V:164:THR:HG23 | 4:W:174:PHE:CE1 | 2.31 | 0.58 |
| 4:H:39:GLN:O | 4:H:88:ALA:HB1 | 2.03 | 0.58 |
| 3:L:90:GLN:HE21 | 3:L:97:THR:HG23 | 1.68 | 0.58 |
| 3:X:160:LEU:CD1 | 4:T:179:GLN:CD | 2.70 | 0.58 |
| 4:W:19:LYS:NZ | 4:W:81:ASP:HB2 | 2.18 | 0.58 |
| 4:W:200:TRP:CG | 4:W:202:PRO:HA | 2.38 | 0.58 |
| 2:P:72:ASN:OD1 | 2:P:75:ARG:NH2 | 2.36 | 0.58 |
| 3:J:90:GLN:HE21 | 3:J:97:THR:HG23 | 1.68 | 0.58 |
| 3:V:174:SER:HB3 | 4:W:174:PHE:CZ | 2.39 | 0.58 |
| 2:I:72:ASN:OD1 | 2:I:75:ARG:NH2 | 2.36 | 0.58 |
| 4:H:200:TRP:CG | 4:H:202:PRO:HA | 2.39 | 0.58 |
| 4:F:39:GLN:O | 4:F:88:ALA:HB1 | 2.03 | 0.58 |
| 1:M:107:GLU:OE1 | 2:U:75:ARG:HB2 | 2.03 | 0.58 |
| 3:Q:124:GLN:HG3 | 4:R:122:TYR:CE2 | 2.39 | 0.58 |
| 4:H:1:GLU:O | 4:H:26:GLY:HA3 | 2.02 | 0.58 |
| 4:R:200:TRP:CG | 4:R:202:PRO:HA | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:V:90:GLN:HE21 | 3:V:97:THR:HG23 | 1.68 | 0.58 |
| 4:K:190:SER:O | 4:K:190:SER:OG | 2.22 | 0.58 |
| 4:R:48:ILE:HA | 4:R:63:PHE:CD2 | 2.36 | 0.58 |
| 4:F:31:GLU:OE2 | 4:F:32:TYR:CE1 | 2.36 | 0.58 |
| 4:R:31:GLU:OE2 | 4:R:32:TYR:CE1 | 2.36 | 0.58 |
| 4:T:1:GLU:O | 4:T:26:GLY:HA3 | 2.03 | 0.58 |
| 4:W:190:SER:O | 4:W:190:SER:OG | 2.22 | 0.58 |
| 1:A:9:PRO:CD | 1:A:10:GLY:H | 2.02 | 0.58 |
| 1:M:276:ASN:OD1 | 4:T:32:TYR:HA | 2.02 | 0.58 |
| 3:V:118:PHE:CD2 | 4:W:124:LEU:HB3 | 2.39 | 0.58 |
| 3:V:135:PHE:CZ | 4:W:124:LEU:HD13 | 2.39 | 0.58 |
| 1:A:316:LEU:HD21 | 2:B:100:VAL:HG22 | 1.86 | 0.57 |
| 1:C:62:ARG:HG2 | 1:C:63:ASP:H | 1.70 | 0.57 |
| 2:D:33:GLY:HA2 | 4:W:217:THR:HA | 1.85 | 0.57 |
| 4:F:190:SER:O | 4:F:190:SER:OG | 2.21 | 0.57 |
| 1:G:186:ASN:ND2 | 1:G:190:GLU:OE1 | 2.33 | 0.57 |
| 4:T:200:TRP:CG | 4:T:202:PRO:HA | 2.38 | 0.57 |
| 4:W:39:GLN:O | 4:W:88:ALA:HB1 | 2.03 | 0.57 |
| 1:M:11:ASP:CB | 2:N:28:ASN:HA | 2.34 | 0.57 |
| 4:F:48:ILE:HA | 4:F:63:PHE:CD2 | 2.36 | 0.57 |
| 1:S:307:LYS:NZ | 2:U:59:MET:HB2 | 2.19 | 0.57 |
| 3:V:98:PHE:CD2 | 4:W:45:LEU:HB2 | 2.39 | 0.57 |
| 4:F:200:TRP:CG | 4:F:202:PRO:HA | 2.38 | 0.57 |
| 4:R:59:TYR:HD2 | 4:R:64:LYS:HD3 | 1.70 | 0.57 |
| 1:G:62:ARG:HG2 | 1:G:63:ASP:H | 1.70 | 0.57 |
| 4:R:157:TRP:HE1 | 4:R:189:SER:HG | 1.52 | 0.57 |
| 2:D:76:ARG:HH12 | 2:I:74:GLU:CD | 2.08 | 0.57 |
| 3:E:116:SER:HA | 3:E:207:LYS:HD2 | 1.87 | 0.57 |
| 3:V:116:SER:HA | 3:V:207:LYS:HD2 | 1.87 | 0.57 |
| 4:H:48:ILE:HA | 4:H:63:PHE:CD2 | 2.36 | 0.57 |
| 1:O:186:ASN:ND2 | 1:O:190:GLU:OE1 | 2.33 | 0.57 |
| 3:L:43:SER:HB3 | 4:H:91:TYR:HE1 | 1.66 | 0.57 |
| 2:B:72:ASN:OD1 | 2:B:75:ARG:NH2 | 2.36 | 0.57 |
| 2:P:80:LEU:HD21 | 2:U:80:LEU:HD21 | 1.86 | 0.57 |
| 3:L:116:SER:HA | 3:L:207:LYS:HD2 | 1.87 | 0.57 |
| 3:X:174:SER:CB | 4:T:174:PHE:HE1 | 2.17 | 0.57 |
| 3:Q:116:SER:HA | 3:Q:207:LYS:HD2 | 1.87 | 0.57 |
| 4:H:59:TYR:HD2 | 4:H:64:LYS:HD3 | 1.70 | 0.57 |
| 3:V:119:PRO:CB | 4:W:228:ARG:HH21 | 2.16 | 0.56 |
| 1:A:83:PRO:HB3 | 3:L:49:TYR:HE2 | 1.70 | 0.56 |
| 2:B:80:LEU:HD22 | 2:I:80:LEU:HD11 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:62:ARG:HG2 | 1:O:63:ASP:H | 1.70 | 0.56 |
| 3:E:192:TYR:HB2 | 3:E:209:PHE:CE1 | 2.41 | 0.56 |
| 1:A:83:PRO:HG2 | 4:H:100(B):TYR:OH | 2.05 | 0.56 |
| 3:Q:192:TYR:HB2 | 3:Q:209:PHE:CE1 | 2.41 | 0.56 |
| 3:V:192:TYR:HB2 | 3:V:209:PHE:CE1 | 2.41 | 0.56 |
| 4:T:59:TYR:HD2 | 4:T:64:LYS:HD3 | 1.70 | 0.56 |
| 1:A:11:ASP:CG | 2:B:28:ASN:HA | 2.25 | 0.56 |
| 1:G:83(A):GLU:OE1 | 3:J:53:ASN:ND2 | 2.39 | 0.56 |
| 1:A:307:LYS:HD3 | 2:B:59:MET:O | 2.06 | 0.56 |
| 2:D:33:GLY:CA | 4:W:217:THR:HA | 2.36 | 0.56 |
| 1:S:62:ARG:HG2 | 1:S:63:ASP:H | 1.70 | 0.56 |
| 3:L:192:TYR:HB2 | 3:L:209:PHE:CE1 | 2.41 | 0.56 |
| 3:V:98:PHE:CE2 | 4:W:45:LEU:HB2 | 2.41 | 0.56 |
| 1:M:29:ILE:HD12 | 2:N:105:GLU:OE1 | 2.06 | 0.56 |
| 3:J:192:TYR:HB2 | 3:J:209:PHE:CE1 | 2.41 | 0.56 |
| 1:G:14:CYS:O | 2:I:24:TYR:HA | 2.06 | 0.56 |
| 1:M:62:ARG:HG2 | 1:M:63:ASP:H | 1.70 | 0.56 |
| 3:J:116:SER:HA | 3:J:207:LYS:HD2 | 1.87 | 0.56 |
| 1:A:15:ILE:C | 2:B:14:TRP:CH2 | 2.79 | 0.55 |
| 1:A:293:PRO:HG2 | 1:A:294:PHE:CD1 | 2.42 | 0.55 |
| 1:C:293:PRO:HG2 | 1:C:294:PHE:CD1 | 2.41 | 0.55 |
| 3:L:110:ASP:OD2 | 3:L:199:LYS:HE2 | 2.07 | 0.55 |
| 4:W:59:TYR:HD2 | 4:W:64:LYS:HD3 | 1.70 | 0.55 |
| 1:M:293:PRO:HG2 | 1:M:294:PHE:CD1 | 2.42 | 0.55 |
| 1:S:186:ASN:ND2 | 1:S:190:GLU:OE1 | 2.33 | 0.55 |
| 1:S:293:PRO:HG2 | 1:S:294:PHE:CD1 | 2.41 | 0.55 |
| 3:L:174:SER:HB2 | 4:H:174:PHE:HE1 | 1.71 | 0.55 |
| 3:X:110:ASP:OD2 | 3:X:199:LYS:HE2 | 2.07 | 0.55 |
| 3:X:192:TYR:HB2 | 3:X:209:PHE:CE1 | 2.41 | 0.55 |
| 2:U:31:GLY:HA3 | 4:F:219:VAL:HG22 | 1.86 | 0.55 |
| 4:F:59:TYR:HD2 | 4:F:64:LYS:HD3 | 1.70 | 0.55 |
| 1:S:18:HIS:N | 2:U:21:TRP:O | 2.34 | 0.55 |
| 1:S:100:GLY:HA3 | 1:S:230:MET:O | 2.07 | 0.55 |
| 3:E:110:ASP:OD2 | 3:E:199:LYS:HE2 | 2.07 | 0.55 |
| 4:H:37:MET:HE3 | 4:H:46:GLU:O | 2.07 | 0.55 |
| 1:G:293:PRO:HG2 | 1:G:294:PHE:CD1 | 2.41 | 0.55 |
| 3:V:119:PRO:HB2 | 4:W:228:ARG:NH2 | 2.17 | 0.55 |
| 4:K:19:LYS:HZ3 | 4:K:81:ASP:HB2 | 1.70 | 0.55 |
| 4:K:59:TYR:HD2 | 4:K:64:LYS:HD3 | 1.70 | 0.55 |
| 1:S:105:TYR:OH | 1:S:109:LYS:HE3 | 2.06 | 0.55 |
| 3:E:123:GLU:OE1 | 4:F:123:PRO:HD2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:110:ASP:OD2 | 3:Q:199:LYS:HE2 | 2.07 | 0.55 |
| 1:A:62:ARG:HG2 | 1:A:63:ASP:H | 1.70 | 0.55 |
| 1:O:293:PRO:HG2 | 1:O:294:PHE:CD1 | 2.42 | 0.55 |
| 4:T:68:THR:HB | 4:T:81:ASP:CG | 2.26 | 0.55 |
| 1:S:15:ILE:HG13 | 2:U:119:TYR:HA | 1.89 | 0.55 |
| 1:C:100:GLY:HA3 | 1:C:230:MET:O | 2.07 | 0.54 |
| 1:M:220:ARG:NH2 | 1:O:210:ASN:OD1 | 2.40 | 0.54 |
| 3:V:110:ASP:OD2 | 3:V:199:LYS:HE2 | 2.07 | 0.54 |
| 4:K:37:MET:HE3 | 4:K:46:GLU:O | 2.06 | 0.54 |
| 1:M:69:TRP:HZ3 | 1:M:112:LEU:HD21 | 1.73 | 0.54 |
| 1:M:100:GLY:HA3 | 1:M:230:MET:O | 2.07 | 0.54 |
| 1:C:16:GLY:N | 2:D:14:TRP:CZ3 | 2.76 | 0.54 |
| 2:D:167:ARG:CG | 2:D:170:ARG:HH21 | 2.14 | 0.54 |
| 1:G:69:TRP:HZ3 | 1:G:112:LEU:HD21 | 1.73 | 0.54 |
| 1:A:100:GLY:HA3 | 1:A:230:MET:O | 2.07 | 0.54 |
| 1:A:183:HIS:HB2 | 1:A:252:ILE:HD11 | 1.90 | 0.54 |
| 1:C:186:ASN:ND2 | 1:C:190:GLU:OE1 | 2.33 | 0.54 |
| 1:O:183:HIS:HB2 | 1:O:252:ILE:HD11 | 1.90 | 0.54 |
| 4:T:81:ASP:OD1 | 4:T:81:ASP:C | 2.45 | 0.54 |
| 1:O:100:GLY:HA3 | 1:O:230:MET:O | 2.07 | 0.54 |
| 3:L:124:GLN:NE2 | 3:L:131:SER:OG | 2.38 | 0.54 |
| 3:J:110:ASP:OD2 | 3:J:199:LYS:HE2 | 2.07 | 0.54 |
| 3:X:35:TRP:CZ3 | 3:X:88:CYS:HB3 | 2.43 | 0.54 |
| 1:G:100:GLY:HA3 | 1:G:230:MET:O | 2.07 | 0.54 |
| 1:O:56:VAL:HG21 | 3:Q:30:LYS:HZ1 | 1.72 | 0.54 |
| 1:O:274:TYR:CZ | 4:R:97:GLY:HA3 | 2.39 | 0.54 |
| 1:S:69:TRP:HZ3 | 1:S:112:LEU:HD21 | 1.73 | 0.54 |
| 3:J:49:TYR:CE1 | 3:J:53:ASN:HB2 | 2.43 | 0.54 |
| 3:X:164:THR:HG23 | 4:T:174:PHE:HD1 | 1.69 | 0.54 |
| 4:H:190:SER:O | 4:H:190:SER:OG | 2.22 | 0.54 |
| 1:A:51:LEU:HD13 | 1:A:272:LEU:HB2 | 1.90 | 0.54 |
| 3:X:160:LEU:CD1 | 4:T:179:GLN:OE1 | 2.52 | 0.54 |
| 1:C:183:HIS:HB2 | 1:C:252:ILE:HD11 | 1.90 | 0.54 |
| 1:S:51:LEU:HD13 | 1:S:272:LEU:HB2 | 1.90 | 0.54 |
| 1:M:183:HIS:HB2 | 1:M:252:ILE:HD11 | 1.90 | 0.53 |
| 3:Q:49:TYR:CE1 | 3:Q:53:ASN:HB2 | 2.43 | 0.53 |
| 3:V:124:GLN:NE2 | 3:V:131:SER:OG | 2.38 | 0.53 |
| 1:C:69:TRP:HZ3 | 1:C:112:LEU:HD21 | 1.73 | 0.53 |
| 3:L:35:TRP:CZ3 | 3:L:88:CYS:HB3 | 2.43 | 0.53 |
| 3:E:35:TRP:CZ3 | 3:E:88:CYS:HB3 | 2.43 | 0.53 |
| 3:E:98:PHE:CE1 | 4:F:37:MET:HE1 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:J:35:TRP:CZ3 | 3:J:88:CYS:HB3 | 2.43 | 0.53 |
| 3:X:193:THR:HG23 | 3:X:208:SER:HB3 | 1.90 | 0.53 |
| 3:Q:193:THR:HG23 | 3:Q:208:SER:HB3 | 1.90 | 0.53 |
| 3:V:164:THR:HG22 | 4:W:174:PHE:HA | 1.89 | 0.53 |
| 3:V:193:THR:HG23 | 3:V:208:SER:HB3 | 1.90 | 0.53 |
| 1:G:51:LEU:HD13 | 1:G:272:LEU:HB2 | 1.90 | 0.53 |
| 3:L:49:TYR:CE1 | 3:L:53:ASN:HB2 | 2.43 | 0.53 |
| 3:E:49:TYR:CE1 | 3:E:53:ASN:HB2 | 2.43 | 0.53 |
| 3:X:137:ASN:ND2 | 4:T:174:PHE:HZ | 2.06 | 0.53 |
| 3:X:193:THR:HG22 | 3:X:194:CYS:H | 1.74 | 0.53 |
| 3:Q:35:TRP:CZ3 | 3:Q:88:CYS:HB3 | 2.43 | 0.53 |
| 3:Q:124:GLN:HB2 | 4:R:122:TYR:CD1 | 2.43 | 0.53 |
| 3:V:49:TYR:CE1 | 3:V:53:ASN:HB2 | 2.43 | 0.53 |
| 1:G:183:HIS:HB2 | 1:G:252:ILE:HD11 | 1.90 | 0.53 |
| 1:O:69:TRP:HZ3 | 1:O:112:LEU:HD21 | 1.72 | 0.53 |
| 3:X:174:SER:HB2 | 4:T:174:PHE:HE1 | 1.74 | 0.53 |
| 3:L:193:THR:HG22 | 3:L:194:CYS:H | 1.74 | 0.53 |
| 3:J:174:SER:HB3 | 4:K:174:PHE:CZ | 2.43 | 0.53 |
| 3:L:147:LYS:HE3 | 3:L:195:GLU:HB3 | 1.91 | 0.53 |
| 3:X:49:TYR:CE1 | 3:X:53:ASN:HB2 | 2.43 | 0.53 |
| 3:V:35:TRP:CZ3 | 3:V:88:CYS:HB3 | 2.43 | 0.53 |
| 1:A:26:VAL:HG11 | 1:A:317:ALA:HB2 | 1.91 | 0.53 |
| 1:C:276:ASN:ND2 | 4:F:52:PHE:CE1 | 2.76 | 0.53 |
| 3:L:141:PRO:HD2 | 3:L:198:HIS:HE1 | 1.74 | 0.53 |
| 1:O:26:VAL:HG11 | 1:O:317:ALA:HB2 | 1.91 | 0.53 |
| 3:J:141:PRO:HD2 | 3:J:198:HIS:HE1 | 1.74 | 0.53 |
| 1:G:26:VAL:HG11 | 1:G:317:ALA:HB2 | 1.91 | 0.53 |
| 1:M:26:VAL:HG11 | 1:M:317:ALA:HB2 | 1.91 | 0.53 |
| 1:S:26:VAL:HG11 | 1:S:317:ALA:HB2 | 1.91 | 0.53 |
| 3:X:147:LYS:HE3 | 3:X:195:GLU:HB3 | 1.91 | 0.53 |
| 4:R:33:THR:CG2 | 4:R:95:ASN:HD22 | 2.22 | 0.53 |
| 4:R:37:MET:HE3 | 4:R:46:GLU:O | 2.09 | 0.53 |
| 1:S:183:HIS:HB2 | 1:S:252:ILE:HD11 | 1.90 | 0.52 |
| 3:E:147:LYS:HE3 | 3:E:195:GLU:HB3 | 1.91 | 0.52 |
| 3:X:141:PRO:HD2 | 3:X:198:HIS:HE1 | 1.74 | 0.52 |
| 1:A:69:TRP:HZ3 | 1:A:112:LEU:HD21 | 1.73 | 0.52 |
| 3:E:141:PRO:HD2 | 3:E:198:HIS:HE1 | 1.74 | 0.52 |
| 3:J:124:GLN:NE2 | 3:J:131:SER:OG | 2.38 | 0.52 |
| 3:V:174:SER:HB3 | 4:W:174:PHE:HZ | 1.73 | 0.52 |
| 4:K:33:THR:CG2 | 4:K:95:ASN:HD22 | 2.22 | 0.52 |
| 1:C:26:VAL:HG11 | 1:C:317:ALA:HB2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:244:ASN:ND2 | 1:S:221:PRO:HD3 | 2.23 | 0.52 |
| 3:X:124:GLN:HB2 | 4:T:122:TYR:CZ | 2.44 | 0.52 |
| 2:D:80:LEU:HD11 | 2:I:80:LEU:CD2 | 2.38 | 0.52 |
| 1:O:51:LEU:HD13 | 1:O:272:LEU:HB2 | 1.90 | 0.52 |
| 2:P:160:PRO:HA | 2:P:163:SER:HB2 | 1.92 | 0.52 |
| 3:L:193:THR:HG23 | 3:L:208:SER:HB3 | 1.90 | 0.52 |
| 3:E:193:THR:HG23 | 3:E:208:SER:HB3 | 1.91 | 0.52 |
| 3:J:174:SER:CB | 4:K:174:PHE:CE1 | 2.92 | 0.52 |
| 4:W:33:THR:CG2 | 4:W:95:ASN:HD22 | 2.22 | 0.52 |
| 3:E:193:THR:HG22 | 3:E:194:CYS:H | 1.74 | 0.52 |
| 4:T:157:TRP:HE1 | 4:T:189:SER:HG | 1.58 | 0.52 |
| 4:R:38:LYS:HB2 | 4:R:90:TYR:CE1 | 2.45 | 0.52 |
| 1:C:51:LEU:HD13 | 1:C:272:LEU:HB2 | 1.90 | 0.52 |
| 3:Q:147:LYS:HE3 | 3:Q:195:GLU:HB3 | 1.91 | 0.52 |
| 3:Q:193:THR:HG22 | 3:Q:194:CYS:H | 1.74 | 0.52 |
| 2:U:160:PRO:HA | 2:U:163:SER:HB2 | 1.92 | 0.52 |
| 4:W:38:LYS:HB2 | 4:W:90:TYR:CE1 | 2.45 | 0.52 |
| 2:B:160:PRO:HA | 2:B:163:SER:HB2 | 1.92 | 0.52 |
| 1:M:51:LEU:HD13 | 1:M:272:LEU:HB2 | 1.91 | 0.52 |
| 1:M:55(A):GLY:O | 3:X:50:ARG:NH2 | 2.42 | 0.52 |
| 3:X:118:PHE:CB | 4:T:124:LEU:HD22 | 2.40 | 0.52 |
| 3:V:147:LYS:HE3 | 3:V:195:GLU:HB3 | 1.91 | 0.52 |
| 4:H:33:THR:CG2 | 4:H:95:ASN:HD22 | 2.22 | 0.52 |
| 3:J:193:THR:HG23 | 3:J:208:SER:HB3 | 1.91 | 0.52 |
| 3:Q:141:PRO:HD2 | 3:Q:198:HIS:HE1 | 1.74 | 0.52 |
| 3:V:141:PRO:HD2 | 3:V:198:HIS:HE1 | 1.74 | 0.52 |
| 4:T:33:THR:CG2 | 4:T:95:ASN:HD22 | 2.23 | 0.52 |
| 4:T:38:LYS:HB2 | 4:T:90:TYR:CE1 | 2.45 | 0.52 |
| 1:S:16:GLY:HA3 | 2:U:14:TRP:CH2 | 2.44 | 0.52 |
| 4:F:38:LYS:HB2 | 4:F:90:TYR:CE1 | 2.45 | 0.52 |
| 2:D:160:PRO:HA | 2:D:163:SER:HB2 | 1.92 | 0.52 |
| 1:O:56:VAL:HG21 | 3:Q:30:LYS:HZ2 | 1.73 | 0.52 |
| 1:O:316:LEU:HD23 | 2:P:100:VAL:HG13 | 1.92 | 0.52 |
| 1:S:309:VAL:HG22 | 2:U:93:THR:HA | 1.92 | 0.52 |
| 4:K:38:LYS:HB2 | 4:K:90:TYR:CE1 | 2.45 | 0.52 |
| 2:B:124:LEU:HD13 | 2:I:9:PHE:HB2 | 1.91 | 0.51 |
| 3:J:193:THR:HG22 | 3:J:194:CYS:H | 1.74 | 0.51 |
| 3:V:193:THR:HG22 | 3:V:194:CYS:H | 1.74 | 0.51 |
| 2:D:32:SER:HB2 | 4:W:218:LYS:O | 2.11 | 0.51 |
| 1:O:16:GLY:N | 2:P:14:TRP:CZ3 | 2.79 | 0.51 |
| 4:H:38:LYS:HB2 | 4:H:90:TYR:CE1 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:W:37:MET:HE3 | 4:W:46:GLU:O | 2.10 | 0.51 |
| 1:A:13:ILE:HA | 2:B:26:HIS:HA | 1.91 | 0.51 |
| 1:C:56:VAL:CG2 | 3:E:50:ARG:NH1 | 2.74 | 0.51 |
| 3:E:120:PRO:O | 4:F:228:ARG:NH2 | 2.44 | 0.51 |
| 3:J:147:LYS:HE3 | 3:J:195:GLU:HB3 | 1.91 | 0.51 |
| 4:F:33:THR:CG2 | 4:F:95:ASN:HD22 | 2.22 | 0.51 |
| 1:S:106:GLU:HG2 | 2:U:70:PHE:CA | 2.41 | 0.51 |
| 3:V:13:VAL:HG11 | 3:V:78:VAL:HG21 | 1.93 | 0.51 |
| 1:A:56:VAL:CG2 | 3:L:30:LYS:NZ | 2.72 | 0.51 |
| 3:L:13:VAL:HG11 | 3:L:78:VAL:HG21 | 1.93 | 0.51 |
| 3:E:13:VAL:HG11 | 3:E:78:VAL:HG21 | 1.93 | 0.51 |
| 3:E:95:PRO:HA | 4:F:47:TRP:CZ3 | 2.46 | 0.51 |
| 4:T:12:VAL:HG23 | 4:T:111:VAL:HG22 | 1.93 | 0.51 |
| 1:A:83:PRO:HB3 | 3:L:49:TYR:CE2 | 2.45 | 0.51 |
| 1:G:11:ASP:HA | 2:I:27:SER:O | 2.11 | 0.51 |
| 2:N:168:LEU:CD1 | 2:N:169:ASN:N | 2.67 | 0.51 |
| 1:M:220:ARG:NE | 1:O:210:ASN:OD1 | 2.44 | 0.51 |
| 2:I:160:PRO:HA | 2:I:163:SER:HB2 | 1.92 | 0.51 |
| 3:J:174:SER:HB3 | 4:K:174:PHE:HZ | 1.76 | 0.51 |
| 4:W:12:VAL:HG23 | 4:W:111:VAL:HG22 | 1.93 | 0.51 |
| 3:Q:13:VAL:HG11 | 3:Q:78:VAL:HG21 | 1.93 | 0.50 |
| 4:R:190:SER:O | 4:R:190:SER:OG | 2.22 | 0.50 |
| 3:X:13:VAL:HG11 | 3:X:78:VAL:HG21 | 1.93 | 0.50 |
| 2:N:165:GLU:O | 2:N:168:LEU:HG | 2.12 | 0.50 |
| 3:E:96:ARG:HB2 | 4:F:47:TRP:CG | 2.47 | 0.50 |
| 3:E:148:TRP:CE3 | 3:E:179:LEU:HD13 | 2.47 | 0.50 |
| 1:O:221:PRO:HD3 | 1:S:244:ASN:ND2 | 2.27 | 0.50 |
| 3:E:121:SER:HB2 | 4:F:123:PRO:O | 2.12 | 0.50 |
| 3:J:13:VAL:HG11 | 3:J:78:VAL:HG21 | 1.93 | 0.50 |
| 4:F:19:LYS:HZ1 | 4:F:81:ASP:HB2 | 1.75 | 0.50 |
| 4:K:12:VAL:HG23 | 4:K:111:VAL:HG22 | 1.93 | 0.50 |
| 2:B:54:SER:OG | 1:G:32:LYS:NZ | 2.45 | 0.50 |
| 4:K:93:VAL:HG11 | 4:K:100(C):PHE:HB3 | 1.94 | 0.50 |
| 4:T:37:MET:HE3 | 4:T:46:GLU:O | 2.12 | 0.50 |
| 4:R:12:VAL:HG23 | 4:R:111:VAL:HG22 | 1.93 | 0.50 |
| 1:G:58:PRO:O | 4:K:96:TYR:OH | 2.27 | 0.50 |
| 1:O:274:TYR:OH | 4:R:97:GLY:C | 2.50 | 0.50 |
| 3:J:27(B):VAL:HG22 | 3:J:27(B):VAL:O | 2.12 | 0.50 |
| 3:J:148:TRP:CE3 | 3:J:179:LEU:HD13 | 2.47 | 0.50 |
| 3:X:148:TRP:CE3 | 3:X:179:LEU:HD13 | 2.47 | 0.50 |
| 3:X:166:GLN:HB2 | 3:X:173:TYR:CE1 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:160:PRO:HA | 2:N:163:SER:HB2 | 1.92 | 0.50 |
| 3:L:148:TRP:CE3 | 3:L:179:LEU:HD13 | 2.47 | 0.50 |
| 3:Q:27(B):VAL:O | 3:Q:27(B):VAL:HG22 | 2.12 | 0.50 |
| 1:M:107:GLU:OE2 | 2:U:76:ARG:NE | 2.45 | 0.49 |
| 1:S:106:GLU:OE1 | 2:U:71:ASN:ND2 | 2.34 | 0.49 |
| 3:J:164:THR:HG23 | 4:K:174:PHE:CE1 | 2.44 | 0.49 |
| 3:V:27(B):VAL:O | 3:V:27(B):VAL:HG22 | 2.12 | 0.49 |
| 3:V:166:GLN:HB2 | 3:V:173:TYR:CE1 | 2.48 | 0.49 |
| 4:R:93:VAL:HG11 | 4:R:100(C):PHE:HB3 | 1.94 | 0.49 |
| 2:B:51:LYS:HE3 | 1:G:30:MET:HE2 | 1.94 | 0.49 |
| 3:L:27(B):VAL:O | 3:L:27(B):VAL:HG22 | 2.12 | 0.49 |
| 3:Q:148:TRP:CE3 | 3:Q:179:LEU:HD13 | 2.47 | 0.49 |
| 3:V:148:TRP:CE3 | 3:V:179:LEU:HD13 | 2.47 | 0.49 |
| 4:W:93:VAL:HG11 | 4:W:100(C):PHE:HB3 | 1.94 | 0.49 |
| 1:C:17:TYR:O | 2:D:14:TRP:N | 2.36 | 0.49 |
| 1:G:98:TYR:CD1 | 1:G:230:MET:HG3 | 2.48 | 0.49 |
| 2:P:80:LEU:HD11 | 2:U:80:LEU:HD22 | 1.94 | 0.49 |
| 1:S:106:GLU:HG2 | 2:U:70:PHE:HA | 1.95 | 0.49 |
| 3:L:137:ASN:ND2 | 4:H:174:PHE:CZ | 2.73 | 0.49 |
| 4:F:12:VAL:HG23 | 4:F:111:VAL:HG22 | 1.93 | 0.49 |
| 1:M:98:TYR:CD1 | 1:M:230:MET:HG3 | 2.48 | 0.49 |
| 1:O:83:PRO:CB | 3:Q:49:TYR:CE2 | 2.95 | 0.49 |
| 1:S:98:TYR:CD1 | 1:S:230:MET:HG3 | 2.48 | 0.49 |
| 3:E:124:GLN:NE2 | 3:E:131:SER:OG | 2.38 | 0.49 |
| 4:T:190:SER:O | 4:T:190:SER:OG | 2.22 | 0.49 |
| 2:N:127:ARG:HH21 | 2:U:131:LYS:NZ | 2.10 | 0.49 |
| 3:X:174:SER:CB | 4:T:174:PHE:CE1 | 2.96 | 0.49 |
| 4:H:12:VAL:HG23 | 4:H:111:VAL:HG22 | 1.93 | 0.49 |
| 1:A:98:TYR:CD1 | 1:A:230:MET:HG3 | 2.48 | 0.49 |
| 1:C:307:LYS:HD3 | 2:D:59:MET:O | 2.13 | 0.49 |
| 1:M:147:PHE:CZ | 1:M:230:MET:HE1 | 2.48 | 0.49 |
| 3:E:27(B):VAL:HG22 | 3:E:27(B):VAL:O | 2.12 | 0.49 |
| 3:Q:124:GLN:NE2 | 3:Q:131:SER:OG | 2.38 | 0.49 |
| 3:V:119:PRO:HG2 | 4:W:228:ARG:HE | 1.78 | 0.49 |
| 4:F:93:VAL:HG11 | 4:F:100(C):PHE:HB3 | 1.94 | 0.49 |
| 3:J:135:PHE:CZ | 4:K:124:LEU:HD13 | 2.48 | 0.49 |
| 4:H:93:VAL:HG11 | 4:H:100(C):PHE:HB3 | 1.93 | 0.49 |
| 4:T:93:VAL:HG11 | 4:T:100(C):PHE:HB3 | 1.94 | 0.49 |
| 1:O:83(A):GLU:OE1 | 3:Q:53:ASN:ND2 | 2.46 | 0.49 |
| 1:O:316:LEU:CD2 | 2:P:100:VAL:HG22 | 2.41 | 0.49 |
| 3:J:166:GLN:HB2 | 3:J:173:TYR:CE1 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:244:ASN:HD22 | 1:G:221:PRO:HD3 | 1.76 | 0.48 |
| 1:O:98:TYR:CD1 | 1:O:230:MET:HG3 | 2.48 | 0.48 |
| 3:E:166:GLN:HB2 | 3:E:173:TYR:CE1 | 2.47 | 0.48 |
| 3:Q:166:GLN:HB2 | 3:Q:173:TYR:CE1 | 2.47 | 0.48 |
| 1:S:307:LYS:HZ2 | 2:U:59:MET:HB2 | 1.76 | 0.48 |
| 3:X:27(B):VAL:O | 3:X:27(B):VAL:HG22 | 2.12 | 0.48 |
| 1:C:98:TYR:CD1 | 1:C:230:MET:HG3 | 2.48 | 0.48 |
| 1:S:83:PRO:HG2 | 4:W:100(B):TYR:OH | 2.12 | 0.48 |
| 1:M:19:ALA:O | 2:N:15:GLN:HA | 2.14 | 0.48 |
| 3:L:166:GLN:HB2 | 3:L:173:TYR:CE1 | 2.47 | 0.48 |
| 2:B:51:LYS:HE3 | 1:G:30:MET:CE | 2.44 | 0.48 |
| 1:G:179:LEU:HD23 | 1:G:234:TRP:HB3 | 1.95 | 0.48 |
| 1:M:17:TYR:CZ | 2:N:12:GLY:O | 2.65 | 0.48 |
| 4:F:51:ILE:HD13 | 4:F:71:VAL:HG23 | 1.96 | 0.48 |
| 1:M:179:LEU:HD23 | 1:M:234:TRP:HB3 | 1.95 | 0.48 |
| 4:T:51:ILE:HD13 | 4:T:71:VAL:HG23 | 1.96 | 0.48 |
| 1:M:323:THR:HG21 | 2:N:13:GLY:H | 1.78 | 0.48 |
| 4:H:19:LYS:HZ3 | 4:H:81:ASP:HB2 | 1.77 | 0.48 |
| 1:A:56:VAL:HG21 | 3:L:30:LYS:HZ1 | 1.77 | 0.48 |
| 1:A:179:LEU:HD23 | 1:A:234:TRP:HB3 | 1.96 | 0.48 |
| 1:C:56:VAL:CG2 | 3:E:50:ARG:HH12 | 2.26 | 0.48 |
| 3:J:53:ASN:OD1 | 3:J:53:ASN:N | 2.47 | 0.48 |
| 3:J:119:PRO:HG2 | 4:K:228:ARG:HE | 1.79 | 0.48 |
| 3:X:118:PHE:HB3 | 4:T:124:LEU:HD22 | 1.95 | 0.48 |
| 3:Q:195:GLU:HG3 | 3:Q:206:VAL:HG22 | 1.96 | 0.48 |
| 1:A:134:GLY:HA3 | 1:A:153:TRP:HB3 | 1.96 | 0.48 |
| 1:C:56:VAL:HG22 | 3:E:50:ARG:NH1 | 2.28 | 0.48 |
| 1:C:134:GLY:HA3 | 1:C:153:TRP:HB3 | 1.96 | 0.48 |
| 1:G:134:GLY:HA3 | 1:G:153:TRP:HB3 | 1.96 | 0.48 |
| 3:E:33:MET:HB3 | 3:E:51:ALA:HB2 | 1.96 | 0.48 |
| 3:X:124:GLN:NE2 | 3:X:131:SER:OG | 2.38 | 0.48 |
| 1:C:14:CYS:C | 2:D:14:TRP:HH2 | 2.17 | 0.48 |
| 1:G:83(A):GLU:N | 3:J:49:TYR:OH | 2.29 | 0.48 |
| 2:N:47:GLY:O | 1:S:30:MET:HG2 | 2.14 | 0.48 |
| 1:O:106:GLU:OE1 | 2:P:71:ASN:ND2 | 2.28 | 0.48 |
| 1:O:134:GLY:HA3 | 1:O:153:TRP:HB3 | 1.96 | 0.48 |
| 1:O:179:LEU:HD23 | 1:O:234:TRP:HB3 | 1.95 | 0.47 |
| 3:L:33:MET:HB3 | 3:L:51:ALA:HB2 | 1.96 | 0.47 |
| 3:Q:33:MET:HB3 | 3:Q:51:ALA:HB2 | 1.96 | 0.47 |
| 4:H:51:ILE:HD13 | 4:H:71:VAL:HG23 | 1.96 | 0.47 |
| 4:K:51:ILE:HD13 | 4:K:71:VAL:HG23 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:106:GLU:OE1 | 2:I:71:ASN:ND2 | 2.24 | 0.47 |
| 3:J:195:GLU:HG3 | 3:J:206:VAL:HG22 | 1.96 | 0.47 |
| 3:V:33:MET:HB3 | 3:V:51:ALA:HB2 | 1.96 | 0.47 |
| 1:S:134:GLY:HA3 | 1:S:153:TRP:HB3 | 1.96 | 0.47 |
| 1:S:179:LEU:HD23 | 1:S:234:TRP:HB3 | 1.95 | 0.47 |
| 4:F:183:ASP:O | 4:F:184:LEU:HD23 | 2.15 | 0.47 |
| 4:W:51:ILE:HD13 | 4:W:71:VAL:HG23 | 1.96 | 0.47 |
| 1:A:276:ASN:ND2 | 4:H:52:PHE:CE1 | 2.82 | 0.47 |
| 1:C:147:PHE:CZ | 1:C:230:MET:HE1 | 2.49 | 0.47 |
| 1:C:147:PHE:HZ | 1:C:230:MET:HE1 | 1.80 | 0.47 |
| 1:M:134:GLY:HA3 | 1:M:153:TRP:HB3 | 1.96 | 0.47 |
| 3:L:174:SER:HB3 | 4:H:174:PHE:CE1 | 2.49 | 0.47 |
| 3:X:53:ASN:OD1 | 3:X:53:ASN:N | 2.47 | 0.47 |
| 4:R:183:ASP:O | 4:R:184:LEU:HD23 | 2.15 | 0.47 |
| 2:D:31:GLY:HA3 | 4:W:219:VAL:HG22 | 1.97 | 0.47 |
| 1:M:147:PHE:HZ | 1:M:230:MET:HE1 | 1.80 | 0.47 |
| 2:N:80:LEU:CD2 | 2:U:80:LEU:HD11 | 2.44 | 0.47 |
| 1:O:56:VAL:CG2 | 3:Q:30:LYS:HZ1 | 2.27 | 0.47 |
| 1:S:316:LEU:HD21 | 2:U:100:VAL:HG22 | 1.95 | 0.47 |
| 3:J:33:MET:HB3 | 3:J:51:ALA:HB2 | 1.96 | 0.47 |
| 3:Q:53:ASN:OD1 | 3:Q:53:ASN:N | 2.47 | 0.47 |
| 4:F:37:MET:HE3 | 4:F:46:GLU:O | 2.15 | 0.47 |
| 4:K:29:PHE:CD2 | 4:K:76:SER:HA | 2.50 | 0.47 |
| 4:T:183:ASP:O | 4:T:184:LEU:HD23 | 2.15 | 0.47 |
| 1:C:274:TYR:HD2 | 4:F:31:GLU:O | 1.97 | 0.47 |
| 1:M:17:TYR:CE2 | 2:N:13:GLY:HA2 | 2.47 | 0.47 |
| 3:V:53:ASN:OD1 | 3:V:53:ASN:N | 2.47 | 0.47 |
| 4:H:183:ASP:O | 4:H:184:LEU:HD23 | 2.15 | 0.47 |
| 4:F:48:ILE:HG12 | 4:F:63:PHE:CD2 | 2.50 | 0.47 |
| 4:K:183:ASP:O | 4:K:184:LEU:HD23 | 2.15 | 0.47 |
| 3:V:135:PHE:CZ | 4:W:124:LEU:CD1 | 2.98 | 0.47 |
| 4:R:29:PHE:CD2 | 4:R:76:SER:HA | 2.50 | 0.47 |
| 2:N:165:GLU:HA | 2:N:168:LEU:HD23 | 1.96 | 0.47 |
| 3:E:53:ASN:OD1 | 3:E:53:ASN:N | 2.47 | 0.47 |
| 4:F:29:PHE:CD2 | 4:F:76:SER:HA | 2.50 | 0.47 |
| 4:R:51:ILE:HD13 | 4:R:71:VAL:HG23 | 1.96 | 0.47 |
| 1:C:179:LEU:HD23 | 1:C:234:TRP:HB3 | 1.95 | 0.47 |
| 3:E:195:GLU:HG3 | 3:E:206:VAL:HG22 | 1.96 | 0.47 |
| 4:T:29:PHE:CD2 | 4:T:76:SER:HA | 2.50 | 0.47 |
| 4:W:19:LYS:HZ3 | 4:W:81:ASP:HB2 | 1.78 | 0.47 |
| 3:V:24:ARG:NH1 | 3:V:70:ASP:HB3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:V:195:GLU:HG3 | 3:V:206:VAL:HG22 | 1.96 | 0.46 |
| 4:K:48:ILE:HG12 | 4:K:63:PHE:CD2 | 2.50 | 0.46 |
| 4:T:48:ILE:HG12 | 4:T:63:PHE:CD2 | 2.50 | 0.46 |
| 1:O:147:PHE:CZ | 1:O:230:MET:HE1 | 2.50 | 0.46 |
| 3:L:195:GLU:HG3 | 3:L:206:VAL:HG22 | 1.96 | 0.46 |
| 3:X:195:GLU:HG3 | 3:X:206:VAL:HG22 | 1.96 | 0.46 |
| 3:Q:24:ARG:NH1 | 3:Q:70:ASP:HB3 | 2.31 | 0.46 |
| 4:W:29:PHE:CD2 | 4:W:76:SER:HA | 2.50 | 0.46 |
| 4:W:183:ASP:O | 4:W:184:LEU:HD23 | 2.15 | 0.46 |
| 3:E:24:ARG:NH1 | 3:E:70:ASP:HB3 | 2.31 | 0.46 |
| 3:X:33:MET:HB3 | 3:X:51:ALA:HB2 | 1.96 | 0.46 |
| 4:R:48:ILE:HG12 | 4:R:63:PHE:CD2 | 2.49 | 0.46 |
| 2:N:76:ARG:CZ | 1:O:110:HIS:HB2 | 2.46 | 0.46 |
| 3:X:131:SER:OG | 4:T:145:LYS:HE2 | 2.16 | 0.46 |
| 4:H:29:PHE:CD2 | 4:H:76:SER:HA | 2.50 | 0.46 |
| 1:G:147:PHE:HZ | 1:G:230:MET:HE1 | 1.80 | 0.46 |
| 1:S:147:PHE:HZ | 1:S:230:MET:HE1 | 1.81 | 0.46 |
| 3:E:135:PHE:CE2 | 4:F:190:SER:HB2 | 2.50 | 0.46 |
| 4:H:48:ILE:HG12 | 4:H:63:PHE:CD2 | 2.50 | 0.46 |
| 3:X:43:SER:HB3 | 4:T:91:TYR:CE1 | 2.51 | 0.46 |
| 4:W:48:ILE:HG12 | 4:W:63:PHE:CD2 | 2.50 | 0.46 |
| 1:S:141:TYR:CZ | 1:S:149:ARG:NH2 | 2.84 | 0.46 |
| 3:J:11:LEU:HD12 | 3:X:8:PRO:HG3 | 1.98 | 0.46 |
| 4:H:73:ARG:H | 4:H:73:ARG:HG2 | 1.49 | 0.46 |
| 1:A:12:GLN:N | 2:B:27:SER:O | 2.45 | 0.46 |
| 1:A:141:TYR:CZ | 1:A:149:ARG:NH2 | 2.84 | 0.46 |
| 1:G:141:TYR:CZ | 1:G:149:ARG:NH2 | 2.84 | 0.46 |
| 1:O:16:GLY:HA3 | 2:P:14:TRP:CZ3 | 2.51 | 0.46 |
| 3:L:24:ARG:NH1 | 3:L:70:ASP:HB3 | 2.31 | 0.46 |
| 3:V:174:SER:CB | 4:W:174:PHE:CZ | 2.99 | 0.46 |
| 4:F:60:ASN:OD1 | 4:F:61:GLN:N | 2.49 | 0.46 |
| 1:S:147:PHE:CZ | 1:S:230:MET:HE1 | 2.51 | 0.46 |
| 3:L:167:ASP:HB3 | 3:L:170:ASP:OD1 | 2.16 | 0.46 |
| 3:J:167:ASP:HB3 | 3:J:170:ASP:OD1 | 2.16 | 0.46 |
| 3:X:24:ARG:NH1 | 3:X:70:ASP:HB3 | 2.31 | 0.46 |
| 3:Q:167:ASP:HB3 | 3:Q:170:ASP:OD1 | 2.16 | 0.46 |
| 3:V:169:LYS:HD2 | 3:V:169:LYS:HA | 1.79 | 0.46 |
| 4:K:60:ASN:OD1 | 4:K:61:GLN:N | 2.49 | 0.46 |
| 4:K:66:ARG:H | 4:K:66:ARG:HG3 | 1.53 | 0.46 |
| 1:A:16:GLY:HA3 | 2:B:14:TRP:CH2 | 2.51 | 0.45 |
| 1:C:106:GLU:OE2 | 2:D:71:ASN:HB3 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:128:ASP:OD1 | 2:D:159:TYR:OH | 2.22 | 0.45 |
| 1:M:141:TYR:CZ | 1:M:149:ARG:NH2 | 2.84 | 0.45 |
| 3:X:167:ASP:HB3 | 3:X:170:ASP:OD1 | 2.16 | 0.45 |
| 1:C:16:GLY:HA3 | 2:D:14:TRP:CE2 | 2.51 | 0.45 |
| 1:G:15:ILE:O | 2:I:10:ILE:HD13 | 2.16 | 0.45 |
| 1:O:147:PHE:HZ | 1:O:230:MET:HE1 | 1.80 | 0.45 |
| 3:L:44:PRO:CG | 4:H:45:LEU:HD11 | 2.38 | 0.45 |
| 3:L:118:PHE:CE2 | 4:H:124:LEU:HB3 | 2.52 | 0.45 |
| 3:L:90:GLN:HE21 | 3:L:97:THR:HG22 | 1.82 | 0.45 |
| 3:E:50:ARG:HE | 3:E:50:ARG:HB2 | 1.53 | 0.45 |
| 3:J:24:ARG:NH1 | 3:J:70:ASP:HB3 | 2.31 | 0.45 |
| 1:A:14:CYS:O | 2:B:24:TYR:HA | 2.17 | 0.45 |
| 1:A:55(A):GLY:HA3 | 3:L:32:PHE:CZ | 2.51 | 0.45 |
| 1:G:147:PHE:CZ | 1:G:230:MET:HE1 | 2.50 | 0.45 |
| 3:L:174:SER:CB | 4:H:174:PHE:CE1 | 2.96 | 0.45 |
| 3:E:167:ASP:HB3 | 3:E:170:ASP:OD1 | 2.16 | 0.45 |
| 4:K:73:ARG:H | 4:K:73:ARG:HG2 | 1.49 | 0.45 |
| 2:D:163:SER:O | 2:D:167:ARG:HG3 | 2.17 | 0.45 |
| 3:Q:90:GLN:HE21 | 3:Q:97:THR:HG22 | 1.82 | 0.45 |
| 3:V:167:ASP:HB3 | 3:V:170:ASP:OD1 | 2.16 | 0.45 |
| 4:W:60:ASN:OD1 | 4:W:61:GLN:N | 2.49 | 0.45 |
| 1:C:11:ASP:HA | 2:D:27:SER:O | 2.17 | 0.45 |
| 1:M:244:ASN:HD22 | 1:S:221:PRO:HD3 | 1.82 | 0.45 |
| 1:O:14:CYS:C | 2:P:14:TRP:HH2 | 2.19 | 0.45 |
| 1:O:141:TYR:CZ | 1:O:149:ARG:NH2 | 2.84 | 0.45 |
| 4:H:60:ASN:OD1 | 4:H:61:GLN:N | 2.49 | 0.45 |
| 1:A:83:PRO:CB | 3:L:49:TYR:CE2 | 3.00 | 0.45 |
| 1:C:141:TYR:CZ | 1:C:149:ARG:NH2 | 2.84 | 0.45 |
| 3:V:34:HIS:O | 3:V:88:CYS:HA | 2.17 | 0.45 |
| 4:T:60:ASN:OD1 | 4:T:61:GLN:N | 2.49 | 0.45 |
| 4:R:30:THR:HB | 4:R:53:ASN:HB2 | 1.99 | 0.45 |
| 1:O:53:ASP:HA | 1:O:58:PRO:HD3 | 1.99 | 0.45 |
| 3:E:169:LYS:HD2 | 3:E:169:LYS:HA | 1.80 | 0.45 |
| 3:X:111:ALA:O | 3:X:200:THR:HG21 | 2.17 | 0.45 |
| 1:M:11:ASP:OD1 | 2:N:28:ASN:HA | 2.16 | 0.45 |
| 1:M:17:TYR:CD2 | 2:N:13:GLY:HA2 | 2.52 | 0.45 |
| 3:Q:111:ALA:O | 3:Q:200:THR:HG21 | 2.17 | 0.45 |
| 4:H:30:THR:HB | 4:H:53:ASN:HB2 | 1.99 | 0.45 |
| 4:R:19:LYS:HZ3 | 4:R:81:ASP:HB2 | 1.80 | 0.45 |
| 4:R:142:CYS:HB2 | 4:R:157:TRP:CH2 | 2.52 | 0.45 |
| 1:C:16:GLY:HA3 | 2:D:14:TRP:CH2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P:128:ASP:OD1 | 2:P:159:TYR:OH | 2.22 | 0.45 |
| 3:L:164:THR:HG22 | 4:H:175:PRO:HD3 | 1.98 | 0.45 |
| 2:N:128:ASP:OD1 | 2:N:159:TYR:OH | 2.22 | 0.44 |
| 3:E:111:ALA:O | 3:E:200:THR:HG21 | 2.17 | 0.44 |
| 3:X:90:GLN:HE21 | 3:X:97:THR:HG22 | 1.82 | 0.44 |
| 3:V:160:LEU:HD21 | 4:W:179:GLN:NE2 | 2.21 | 0.44 |
| 4:H:142:CYS:HB2 | 4:H:157:TRP:CH2 | 2.52 | 0.44 |
| 4:F:30:THR:HB | 4:F:53:ASN:HB2 | 1.99 | 0.44 |
| 4:F:142:CYS:HB2 | 4:F:157:TRP:CH2 | 2.52 | 0.44 |
| 4:K:30:THR:HB | 4:K:53:ASN:HB2 | 1.99 | 0.44 |
| 4:R:60:ASN:OD1 | 4:R:61:GLN:N | 2.49 | 0.44 |
| 3:Q:34:HIS:O | 3:Q:88:CYS:HA | 2.17 | 0.44 |
| 1:A:147:PHE:HZ | 1:A:230:MET:HE1 | 1.81 | 0.44 |
| 2:B:124:LEU:CD1 | 2:I:9:PHE:HB2 | 2.47 | 0.44 |
| 3:J:118:PHE:CE2 | 4:K:124:LEU:HB3 | 2.50 | 0.44 |
| 3:X:34:HIS:O | 3:X:88:CYS:HA | 2.17 | 0.44 |
| 4:T:142:CYS:HB2 | 4:T:157:TRP:CH2 | 2.52 | 0.44 |
| 2:D:19:ASP:OD1 | 2:D:19:ASP:N | 2.42 | 0.44 |
| 3:L:34:HIS:O | 3:L:88:CYS:HA | 2.17 | 0.44 |
| 3:J:34:HIS:O | 3:J:88:CYS:HA | 2.17 | 0.44 |
| 4:K:142:CYS:HB2 | 4:K:157:TRP:CH2 | 2.52 | 0.44 |
| 4:W:30:THR:HB | 4:W:53:ASN:HB2 | 1.99 | 0.44 |
| 1:S:62:ARG:CG | 1:S:63:ASP:H | 2.29 | 0.44 |
| 3:J:39:LYS:NZ | 3:J:39:LYS:HB3 | 2.33 | 0.44 |
| 3:X:124:GLN:HG3 | 4:T:122:TYR:CE2 | 2.53 | 0.44 |
| 2:U:128:ASP:OD1 | 2:U:159:TYR:OH | 2.22 | 0.44 |
| 4:T:30:THR:HB | 4:T:53:ASN:HB2 | 1.99 | 0.44 |
| 1:A:53:ASP:HA | 1:A:58:PRO:HD3 | 1.99 | 0.44 |
| 1:A:58:PRO:HG2 | 1:A:60:ILE:HD11 | 2.00 | 0.44 |
| 1:C:53:ASP:HA | 1:C:58:PRO:HD3 | 1.99 | 0.44 |
| 1:S:58:PRO:HG2 | 1:S:60:ILE:HD11 | 2.00 | 0.44 |
| 3:E:34:HIS:O | 3:E:88:CYS:HA | 2.17 | 0.44 |
| 3:E:90:GLN:HE21 | 3:E:97:THR:HG22 | 1.82 | 0.44 |
| 3:Q:148:TRP:CD2 | 3:Q:179:LEU:HD13 | 2.53 | 0.44 |
| 3:V:135:PHE:HZ | 4:W:124:LEU:CD1 | 2.31 | 0.44 |
| 4:W:142:CYS:HB2 | 4:W:157:TRP:CH2 | 2.52 | 0.44 |
| 1:O:16:GLY:HA3 | 2:P:14:TRP:CH2 | 2.53 | 0.44 |
| 3:L:148:TRP:CD2 | 3:L:179:LEU:HD13 | 2.53 | 0.44 |
| 3:X:124:GLN:HG3 | 4:T:122:TYR:CZ | 2.52 | 0.44 |
| 1:C:62:ARG:CG | 1:C:63:ASP:N | 2.73 | 0.44 |
| 1:G:53:ASP:HA | 1:G:58:PRO:HD3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:98:PHE:CE1 | 4:F:37:MET:CE | 3.00 | 0.44 |
| 3:J:148:TRP:CD2 | 3:J:179:LEU:HD13 | 2.53 | 0.44 |
| 3:Q:39:LYS:NZ | 3:Q:39:LYS:HB3 | 2.33 | 0.44 |
| 3:V:39:LYS:NZ | 3:V:39:LYS:HB3 | 2.33 | 0.44 |
| 3:E:150:ILE:HG12 | 3:E:192:TYR:CD1 | 2.53 | 0.44 |
| 3:V:111:ALA:O | 3:V:200:THR:HG21 | 2.17 | 0.44 |
| 4:F:52:PHE:CE2 | 4:F:53:ASN:HB3 | 2.53 | 0.44 |
| 4:T:52:PHE:CE2 | 4:T:53:ASN:HB3 | 2.53 | 0.44 |
| 1:M:53:ASP:HA | 1:M:58:PRO:HD3 | 1.99 | 0.43 |
| 1:O:58:PRO:HG2 | 1:O:60:ILE:HD11 | 2.00 | 0.43 |
| 3:L:150:ILE:HG12 | 3:L:192:TYR:CD1 | 2.53 | 0.43 |
| 3:J:111:ALA:O | 3:J:200:THR:HG21 | 2.17 | 0.43 |
| 3:J:164:THR:HG22 | 4:K:174:PHE:HA | 2.00 | 0.43 |
| 3:X:169:LYS:HD2 | 3:X:169:LYS:HA | 1.79 | 0.43 |
| 3:Q:150:ILE:HG12 | 3:Q:192:TYR:CD1 | 2.53 | 0.43 |
| 4:K:52:PHE:CE2 | 4:K:53:ASN:HB3 | 2.53 | 0.43 |
| 1:A:147:PHE:CZ | 1:A:230:MET:HE1 | 2.53 | 0.43 |
| 1:A:274:TYR:CZ | 4:H:97:GLY:HA2 | 2.53 | 0.43 |
| 3:X:39:LYS:HB3 | 3:X:39:LYS:NZ | 2.33 | 0.43 |
| 2:I:128:ASP:OD1 | 2:I:159:TYR:OH | 2.22 | 0.43 |
| 4:R:52:PHE:CE2 | 4:R:53:ASN:HB3 | 2.53 | 0.43 |
| 1:A:55(A):GLY:HA3 | 3:L:32:PHE:CE1 | 2.54 | 0.43 |
| 1:A:135:VAL:HG22 | 1:A:146:SER:HA | 2.00 | 0.43 |
| 2:N:76:ARG:HB2 | 1:O:107:GLU:OE2 | 2.17 | 0.43 |
| 1:S:53:ASP:HA | 1:S:58:PRO:HD3 | 1.99 | 0.43 |
| 3:J:118:PHE:HA | 3:J:119:PRO:HD3 | 1.87 | 0.43 |
| 3:X:148:TRP:CD2 | 3:X:179:LEU:HD13 | 2.53 | 0.43 |
| 3:L:111:ALA:O | 3:L:200:THR:HG21 | 2.17 | 0.43 |
| 3:V:148:TRP:CD2 | 3:V:179:LEU:HD13 | 2.53 | 0.43 |
| 4:R:48:ILE:HG12 | 4:R:63:PHE:CE2 | 2.54 | 0.43 |
| 4:W:48:ILE:HG12 | 4:W:63:PHE:CE2 | 2.54 | 0.43 |
| 1:C:55:ASN:O | 3:E:30:LYS:HE3 | 2.19 | 0.43 |
| 1:C:135:VAL:HG22 | 1:C:146:SER:HA | 2.00 | 0.43 |
| 1:M:276:ASN:ND2 | 4:T:31:GLU:O | 2.50 | 0.43 |
| 3:E:148:TRP:CD2 | 3:E:179:LEU:HD13 | 2.53 | 0.43 |
| 3:J:118:PHE:HE2 | 4:K:124:LEU:O | 2.01 | 0.43 |
| 3:J:169:LYS:HD2 | 3:J:169:LYS:HA | 1.80 | 0.43 |
| 3:X:162:SER:HB2 | 4:T:177:VAL:CG2 | 2.47 | 0.43 |
| 3:X:174:SER:HB3 | 4:T:174:PHE:CE1 | 2.53 | 0.43 |
| 5:Y:1:NAG:H61 | 5:Y:2:NAG:N2 | 2.33 | 0.43 |
| 1:G:58:PRO:HG2 | 1:G:60:ILE:HD11 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:135:VAL:HG22 | 1:G:146:SER:HA | 2.00 | 0.43 |
| 2:N:3:PHE:CE1 | 2:P:3:PHE:HE1 | 2.36 | 0.43 |
| 1:O:135:VAL:HG22 | 1:O:146:SER:HA | 2.00 | 0.43 |
| 3:L:39:LYS:NZ | 3:L:39:LYS:HB3 | 2.33 | 0.43 |
| 3:V:150:ILE:HG12 | 3:V:192:TYR:CD1 | 2.53 | 0.43 |
| 2:I:58:LYS:HA | 2:I:58:LYS:HD2 | 1.83 | 0.43 |
| 1:A:62:ARG:NH1 | 1:A:63:ASP:OD2 | 2.52 | 0.43 |
| 1:A:206:THR:HG23 | 1:A:241:ASP:OD2 | 2.19 | 0.43 |
| 1:C:16:GLY:HA3 | 2:D:14:TRP:CZ2 | 2.53 | 0.43 |
| 3:L:169:LYS:HD2 | 3:L:169:LYS:HA | 1.80 | 0.43 |
| 2:I:169:ASN:O | 2:I:172:GLU:OE1 | 2.37 | 0.43 |
| 4:R:66:ARG:H | 4:R:66:ARG:HG3 | 1.53 | 0.43 |
| 1:S:206:THR:HG23 | 1:S:241:ASP:OD2 | 2.19 | 0.43 |
| 3:E:203:SER:HA | 3:E:204:PRO:HD3 | 1.91 | 0.43 |
| 3:J:150:ILE:HG12 | 3:J:192:TYR:CD1 | 2.53 | 0.43 |
| 2:B:58:LYS:HA | 2:B:58:LYS:HD2 | 1.83 | 0.43 |
| 3:E:39:LYS:NZ | 3:E:39:LYS:HB3 | 2.33 | 0.43 |
| 4:H:48:ILE:HG12 | 4:H:63:PHE:CE2 | 2.54 | 0.43 |
| 4:H:137:MET:SD | 4:H:194:PRO:HA | 2.59 | 0.43 |
| 1:C:11:ASP:CA | 2:D:27:SER:O | 2.67 | 0.43 |
| 3:L:186:TYR:CE1 | 3:L:192:TYR:CE2 | 3.07 | 0.43 |
| 3:Q:186:TYR:CE1 | 3:Q:192:TYR:CE2 | 3.07 | 0.43 |
| 4:R:137:MET:SD | 4:R:194:PRO:HA | 2.59 | 0.43 |
| 1:C:316:LEU:HD23 | 2:D:100:VAL:HG13 | 2.01 | 0.42 |
| 3:J:8:PRO:CG | 3:X:11:LEU:HD12 | 2.49 | 0.42 |
| 3:J:135:PHE:CZ | 4:K:124:LEU:CD1 | 3.02 | 0.42 |
| 4:K:137:MET:SD | 4:K:194:PRO:HA | 2.59 | 0.42 |
| 4:W:137:MET:SD | 4:W:194:PRO:HA | 2.59 | 0.42 |
| 1:C:16:GLY:HA3 | 2:D:14:TRP:CZ3 | 2.55 | 0.42 |
| 1:C:16:GLY:CA | 2:D:14:TRP:CH2 | 3.01 | 0.42 |
| 1:C:109:LYS:NZ | 2:D:69:GLU:OE2 | 2.42 | 0.42 |
| 1:M:20:ASN:HA | 2:N:15:GLN:OE1 | 2.19 | 0.42 |
| 2:N:169:ASN:O | 2:N:172:GLU:OE1 | 2.37 | 0.42 |
| 2:P:22:TYR:HH | 2:P:111:HIS:HD1 | 1.64 | 0.42 |
| 2:P:76:ARG:CZ | 2:U:69:GLU:H | 2.32 | 0.42 |
| 3:L:4:LEU:HD23 | 3:L:4:LEU:HA | 1.73 | 0.42 |
| 3:E:59:PRO:HG2 | 3:E:62:PHE:CE2 | 2.55 | 0.42 |
| 3:E:186:TYR:CE1 | 3:E:192:TYR:CE2 | 3.07 | 0.42 |
| 3:J:193:THR:HG22 | 3:J:194:CYS:N | 2.34 | 0.42 |
| 3:X:4:LEU:HD23 | 3:X:4:LEU:HA | 1.73 | 0.42 |
| 3:Q:59:PRO:HG2 | 3:Q:62:PHE:CE2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:58:PRO:HG2 | 1:M:60:ILE:HD11 | 2.00 | 0.42 |
| 1:O:323:THR:HA | 1:O:324:PRO:HD3 | 1.77 | 0.42 |
| 3:L:133:VAL:HG21 | 4:H:143:LEU:HD13 | 2.00 | 0.42 |
| 3:J:62:PHE:CD1 | 3:J:75:ILE:HG12 | 2.55 | 0.42 |
| 3:X:150:ILE:HG12 | 3:X:192:TYR:CD1 | 2.53 | 0.42 |
| 3:Q:118:PHE:HA | 3:Q:119:PRO:HD3 | 1.87 | 0.42 |
| 4:H:52:PHE:CE2 | 4:H:53:ASN:HB3 | 2.53 | 0.42 |
| 4:K:48:ILE:HG12 | 4:K:63:PHE:CE2 | 2.54 | 0.42 |
| 4:T:48:ILE:HG12 | 4:T:63:PHE:CE2 | 2.54 | 0.42 |
| 1:C:14:CYS:O | 2:D:24:TYR:HA | 2.19 | 0.42 |
| 1:C:17:TYR:CE2 | 2:D:13:GLY:HA3 | 2.55 | 0.42 |
| 1:C:58:PRO:HG2 | 1:C:60:ILE:HD11 | 2.00 | 0.42 |
| 2:D:169:ASN:O | 2:D:172:GLU:OE1 | 2.37 | 0.42 |
| 1:G:28:THR:HA | 2:I:101:LEU:HD22 | 2.01 | 0.42 |
| 1:M:135:VAL:HG22 | 1:M:146:SER:HA | 2.00 | 0.42 |
| 3:J:119:PRO:HB3 | 3:J:209:PHE:CE2 | 2.55 | 0.42 |
| 3:X:119:PRO:HB3 | 3:X:209:PHE:CE2 | 2.55 | 0.42 |
| 4:T:19:LYS:NZ | 4:T:81:ASP:HB3 | 2.34 | 0.42 |
| 1:O:206:THR:HG23 | 1:O:241:ASP:OD2 | 2.19 | 0.42 |
| 3:X:186:TYR:CE1 | 3:X:192:TYR:CE2 | 3.07 | 0.42 |
| 3:Q:119:PRO:HB3 | 3:Q:209:PHE:CE2 | 2.55 | 0.42 |
| 3:V:59:PRO:HG2 | 3:V:62:PHE:CE2 | 2.55 | 0.42 |
| 4:R:19:LYS:HE2 | 4:R:81:ASP:OD1 | 2.20 | 0.42 |
| 1:A:280:LYS:HE3 | 1:A:304:GLU:CG | 2.50 | 0.42 |
| 1:C:206:THR:HG23 | 1:C:241:ASP:OD2 | 2.19 | 0.42 |
| 2:P:169:ASN:O | 2:P:172:GLU:OE1 | 2.37 | 0.42 |
| 3:E:62:PHE:CD1 | 3:E:75:ILE:HG12 | 2.55 | 0.42 |
| 3:J:186:TYR:CE1 | 3:J:192:TYR:CE2 | 3.07 | 0.42 |
| 3:Q:62:PHE:CD1 | 3:Q:75:ILE:HG12 | 2.55 | 0.42 |
| 3:V:186:TYR:CE1 | 3:V:192:TYR:CE2 | 3.07 | 0.42 |
| 4:K:19:LYS:HE2 | 4:K:81:ASP:OD1 | 2.20 | 0.42 |
| 1:C:280:LYS:HE3 | 1:C:304:GLU:CG | 2.50 | 0.42 |
| 2:D:3:PHE:CE2 | 2:D:113:SER:HB2 | 2.55 | 0.42 |
| 1:M:323:THR:HA | 1:M:324:PRO:HD3 | 1.77 | 0.42 |
| 3:E:44:PRO:HG2 | 4:F:45:LEU:HD11 | 2.02 | 0.42 |
| 3:E:119:PRO:HG3 | 3:E:209:PHE:CD2 | 2.55 | 0.42 |
| 3:V:119:PRO:HG3 | 3:V:209:PHE:CD2 | 2.55 | 0.42 |
| 4:F:19:LYS:HE2 | 4:F:81:ASP:OD1 | 2.20 | 0.42 |
| 4:T:93:VAL:CG1 | 4:T:100(C):PHE:HB3 | 2.50 | 0.42 |
| 4:T:137:MET:SD | 4:T:194:PRO:HA | 2.59 | 0.42 |
| 2:B:169:ASN:O | 2:B:172:GLU:OE1 | 2.37 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:16:GLY:CA | 2:D:14:TRP:CZ3 | 3.03 | 0.42 |
| 1:G:206:THR:HG23 | 1:G:241:ASP:OD2 | 2.19 | 0.42 |
| 2:P:76:ARG:NH1 | 2:U:69:GLU:H | 2.17 | 0.42 |
| 3:L:119:PRO:HB3 | 3:L:209:PHE:CE2 | 2.55 | 0.42 |
| 3:E:27(B):VAL:HG23 | 3:E:92:ASN:HB2 | 2.02 | 0.42 |
| 3:X:18:ARG:O | 3:X:18:ARG:HG3 | 2.20 | 0.42 |
| 3:X:62:PHE:CD1 | 3:X:75:ILE:HG12 | 2.55 | 0.42 |
| 3:V:27(B):VAL:HG23 | 3:V:92:ASN:HB2 | 2.02 | 0.42 |
| 4:T:125:ALA:HA | 4:T:126:PRO:HD3 | 1.85 | 0.42 |
| 4:W:33:THR:HG1 | 4:W:35:HIS:HE2 | 1.66 | 0.42 |
| 1:M:280:LYS:HE3 | 1:M:304:GLU:CG | 2.50 | 0.42 |
| 2:N:3:PHE:CE2 | 2:N:113:SER:HB2 | 2.55 | 0.42 |
| 1:O:280:LYS:HE3 | 1:O:304:GLU:CG | 2.50 | 0.42 |
| 1:S:14:CYS:O | 2:U:24:TYR:HA | 2.20 | 0.42 |
| 1:S:18:HIS:HB2 | 2:U:20:GLY:O | 2.20 | 0.42 |
| 1:S:135:VAL:HG22 | 1:S:146:SER:HA | 2.00 | 0.42 |
| 3:L:59:PRO:HG2 | 3:L:62:PHE:CE2 | 2.55 | 0.42 |
| 3:E:119:PRO:HB3 | 3:E:209:PHE:CE2 | 2.55 | 0.42 |
| 3:J:174:SER:CB | 4:K:174:PHE:HE1 | 2.28 | 0.42 |
| 3:V:119:PRO:HB3 | 3:V:209:PHE:CE2 | 2.55 | 0.42 |
| 4:F:48:ILE:HG12 | 4:F:63:PHE:CE2 | 2.54 | 0.42 |
| 4:K:33:THR:HG1 | 4:K:35:HIS:HE2 | 1.67 | 0.42 |
| 1:G:280:LYS:HE3 | 1:G:304:GLU:CG | 2.50 | 0.42 |
| 1:M:11:ASP:CG | 2:N:28:ASN:CA | 2.85 | 0.42 |
| 1:M:17:TYR:OH | 2:N:13:GLY:N | 2.52 | 0.42 |
| 1:M:206:THR:HG23 | 1:M:241:ASP:OD2 | 2.19 | 0.42 |
| 2:N:168:LEU:HD12 | 2:N:169:ASN:CA | 2.48 | 0.42 |
| 1:O:62:ARG:CG | 1:O:63:ASP:H | 2.29 | 0.42 |
| 3:L:62:PHE:CD1 | 3:L:75:ILE:HG12 | 2.55 | 0.42 |
| 3:L:174:SER:HB2 | 4:H:174:PHE:CE1 | 2.54 | 0.42 |
| 3:X:59:PRO:HG2 | 3:X:62:PHE:CE2 | 2.55 | 0.42 |
| 3:X:124:GLN:CB | 4:T:122:TYR:CZ | 3.03 | 0.42 |
| 3:V:62:PHE:CD1 | 3:V:75:ILE:HG12 | 2.55 | 0.42 |
| 3:V:98:PHE:CZ | 4:W:45:LEU:HB3 | 2.55 | 0.42 |
| 2:U:73:LEU:HD23 | 2:U:73:LEU:HA | 1.91 | 0.42 |
| 4:H:199:THR:O | 4:H:204:GLU:N | 2.50 | 0.42 |
| 4:W:19:LYS:HE2 | 4:W:81:ASP:OD1 | 2.20 | 0.42 |
| 2:N:62:GLN:HG3 | 2:N:92:TRP:CD2 | 2.55 | 0.41 |
| 2:N:74:GLU:CD | 2:U:76:ARG:HH12 | 2.23 | 0.41 |
| 1:S:323:THR:HG21 | 2:U:13:GLY:H | 1.85 | 0.41 |
| 3:E:193:THR:HG22 | 3:E:194:CYS:N | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:J:4:LEU:HA | 3:J:4:LEU:HD23 | 1.73 | 0.41 |
| 3:J:119:PRO:CG | 4:K:228:ARG:HH21 | 2.33 | 0.41 |
| 3:V:18:ARG:O | 3:V:18:ARG:HG3 | 2.20 | 0.41 |
| 4:H:19:LYS:HE2 | 4:H:81:ASP:OD1 | 2.20 | 0.41 |
| 4:F:137:MET:SD | 4:F:194:PRO:HA | 2.59 | 0.41 |
| 4:T:95:ASN:HA | 4:T:100(C):PHE:HA | 2.02 | 0.41 |
| 1:C:164:ILE:O | 1:C:246:GLU:HA | 2.20 | 0.41 |
| 2:D:73:LEU:HD23 | 2:D:73:LEU:HA | 1.91 | 0.41 |
| 1:O:16:GLY:CA | 2:P:14:TRP:CZ3 | 3.03 | 0.41 |
| 2:P:3:PHE:CE2 | 2:P:113:SER:HB2 | 2.55 | 0.41 |
| 3:J:119:PRO:HG3 | 3:J:209:PHE:CD2 | 2.55 | 0.41 |
| 3:Q:18:ARG:O | 3:Q:18:ARG:HG3 | 2.20 | 0.41 |
| 3:Q:87:PHE:CE1 | 3:Q:101:GLY:HA3 | 2.56 | 0.41 |
| 3:V:135:PHE:CE2 | 4:W:124:LEU:HD13 | 2.55 | 0.41 |
| 2:U:169:ASN:O | 2:U:172:GLU:OE1 | 2.37 | 0.41 |
| 4:F:95:ASN:HA | 4:F:100(C):PHE:HA | 2.02 | 0.41 |
| 4:W:66:ARG:H | 4:W:66:ARG:HG3 | 1.53 | 0.41 |
| 1:C:16:GLY:HA3 | 2:D:14:TRP:CD2 | 2.55 | 0.41 |
| 1:S:307:LYS:HB3 | 2:U:62:GLN:NE2 | 2.36 | 0.41 |
| 3:E:18:ARG:O | 3:E:18:ARG:HG3 | 2.20 | 0.41 |
| 3:J:90:GLN:HE21 | 3:J:97:THR:HG22 | 1.82 | 0.41 |
| 3:X:87:PHE:CE1 | 3:X:101:GLY:HA3 | 2.56 | 0.41 |
| 2:U:3:PHE:CE2 | 2:U:113:SER:HB2 | 2.55 | 0.41 |
| 4:H:66:ARG:H | 4:H:66:ARG:HG3 | 1.53 | 0.41 |
| 2:B:3:PHE:CE2 | 2:B:113:SER:HB2 | 2.55 | 0.41 |
| 1:G:238:LYS:HA | 1:G:239:PRO:HD3 | 1.94 | 0.41 |
| 3:L:27(B):VAL:HG23 | 3:L:92:ASN:HB2 | 2.02 | 0.41 |
| 3:E:124:GLN:HG3 | 4:F:122:TYR:CE2 | 2.54 | 0.41 |
| 3:J:59:PRO:HG2 | 3:J:62:PHE:CE2 | 2.54 | 0.41 |
| 3:V:4:LEU:HA | 3:V:4:LEU:HD23 | 1.73 | 0.41 |
| 4:H:11:LEU:HA | 4:H:110:THR:O | 2.21 | 0.41 |
| 4:W:93:VAL:CG1 | 4:W:100(C):PHE:HB3 | 2.50 | 0.41 |
| 1:A:265:SER:OG | 1:A:266:ALA:N | 2.53 | 0.41 |
| 3:L:18:ARG:O | 3:L:18:ARG:HG3 | 2.20 | 0.41 |
| 3:E:24:ARG:HH11 | 3:E:70:ASP:HB3 | 1.86 | 0.41 |
| 3:J:18:ARG:O | 3:J:18:ARG:HG3 | 2.20 | 0.41 |
| 3:J:27(B):VAL:HG23 | 3:J:92:ASN:HB2 | 2.02 | 0.41 |
| 2:I:62:GLN:HG3 | 2:I:92:TRP:CD2 | 2.55 | 0.41 |
| 4:H:148:PHE:HA | 4:H:149:PRO:HA | 1.85 | 0.41 |
| 4:F:93:VAL:CG1 | 4:F:100(C):PHE:HB3 | 2.50 | 0.41 |
| 4:W:19:LYS:HZ1 | 4:W:81:ASP:HB2 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:17:TYR:CE2 | 2:D:13:GLY:CA | 3.04 | 0.41 |
| 1:G:13:ILE:O | 2:I:137:CYS:HA | 2.21 | 0.41 |
| 4:K:95:ASN:HA | 4:K:100(C):PHE:HA | 2.03 | 0.41 |
| 2:D:58:LYS:HD2 | 2:D:58:LYS:HA | 1.83 | 0.41 |
| 1:G:164:ILE:O | 1:G:246:GLU:HA | 2.20 | 0.41 |
| 2:N:11:GLU:O | 2:N:11:GLU:HG3 | 2.21 | 0.41 |
| 2:N:55:ILE:HG23 | 2:N:99:LEU:HD23 | 2.03 | 0.41 |
| 1:S:18:HIS:HB2 | 2:U:21:TRP:HA | 2.01 | 0.41 |
| 3:X:95:PRO:O | 3:X:97:THR:HG22 | 2.21 | 0.41 |
| 3:V:193:THR:HG22 | 3:V:194:CYS:N | 2.34 | 0.41 |
| 4:F:176:ALA:HA | 4:F:187:LEU:HB3 | 2.03 | 0.41 |
| 4:K:33:THR:HG23 | 4:K:95:ASN:HD22 | 1.86 | 0.41 |
| 4:T:11:LEU:HA | 4:T:110:THR:O | 2.21 | 0.41 |
| 4:W:199:THR:O | 4:W:204:GLU:N | 2.51 | 0.41 |
| 2:B:62:GLN:HG3 | 2:B:92:TRP:CD2 | 2.55 | 0.41 |
| 1:O:164:ILE:O | 1:O:246:GLU:HA | 2.20 | 0.41 |
| 1:O:265:SER:OG | 1:O:266:ALA:N | 2.53 | 0.41 |
| 2:P:11:GLU:O | 2:P:11:GLU:HG3 | 2.21 | 0.41 |
| 2:P:62:GLN:HG3 | 2:P:92:TRP:CD2 | 2.55 | 0.41 |
| 1:S:164:ILE:O | 1:S:246:GLU:HA | 2.21 | 0.41 |
| 1:S:280:LYS:HE3 | 1:S:304:GLU:CG | 2.50 | 0.41 |
| 3:L:87:PHE:CE1 | 3:L:101:GLY:HA3 | 2.56 | 0.41 |
| 3:E:139:PHE:HD2 | 3:E:198:HIS:HE2 | 1.69 | 0.41 |
| 2:I:3:PHE:CE2 | 2:I:113:SER:HB2 | 2.55 | 0.41 |
| 4:H:157:TRP:CZ2 | 4:H:191:VAL:HG12 | 2.56 | 0.41 |
| 4:F:140:LEU:HD23 | 4:F:140:LEU:HA | 1.90 | 0.41 |
| 4:K:11:LEU:HA | 4:K:110:THR:O | 2.21 | 0.41 |
| 4:W:11:LEU:HA | 4:W:110:THR:O | 2.21 | 0.41 |
| 4:W:157:TRP:CZ2 | 4:W:191:VAL:HG12 | 2.56 | 0.41 |
| 1:A:218:ALA:CB | 1:C:203:SER:HB2 | 2.46 | 0.41 |
| 1:C:62:ARG:NH1 | 1:C:63:ASP:OD2 | 2.53 | 0.41 |
| 2:D:83:GLN:NE2 | 2:I:63:PHE:CZ | 2.89 | 0.41 |
| 1:G:265:SER:OG | 1:G:266:ALA:N | 2.53 | 0.41 |
| 1:M:52:CYS:HB2 | 1:M:279:THR:HG22 | 2.03 | 0.41 |
| 2:P:55:ILE:HG23 | 2:P:99:LEU:HD23 | 2.03 | 0.41 |
| 2:P:150:GLU:CB | 10:P:2001:NAG:H62 | 2.47 | 0.41 |
| 1:S:52:CYS:HB2 | 1:S:279:THR:HG22 | 2.03 | 0.41 |
| 3:L:119:PRO:HG3 | 3:L:209:PHE:CD2 | 2.55 | 0.41 |
| 3:J:87:PHE:CE1 | 3:J:101:GLY:HA3 | 2.56 | 0.41 |
| 3:X:24:ARG:HH11 | 3:X:70:ASP:HB3 | 1.86 | 0.41 |
| 3:X:119:PRO:HG3 | 3:X:209:PHE:CD2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:193:THR:HG22 | 3:X:194:CYS:N | 2.34 | 0.41 |
| 3:Q:193:THR:HG22 | 3:Q:194:CYS:N | 2.35 | 0.41 |
| 3:V:87:PHE:CE1 | 3:V:101:GLY:HA3 | 2.56 | 0.41 |
| 3:V:95:PRO:O | 3:V:97:THR:HG22 | 2.21 | 0.41 |
| 2:I:11:GLU:HG3 | 2:I:11:GLU:O | 2.21 | 0.41 |
| 2:U:11:GLU:HG3 | 2:U:11:GLU:O | 2.21 | 0.41 |
| 2:U:55:ILE:HG23 | 2:U:99:LEU:HD23 | 2.03 | 0.41 |
| 2:U:62:GLN:HG3 | 2:U:92:TRP:CD2 | 2.55 | 0.41 |
| 4:H:36:TRP:CZ3 | 4:H:92:CYS:HB2 | 2.56 | 0.41 |
| 4:H:176:ALA:HA | 4:H:187:LEU:HB3 | 2.03 | 0.41 |
| 4:F:33:THR:HG23 | 4:F:95:ASN:HD22 | 1.86 | 0.41 |
| 4:K:36:TRP:CZ3 | 4:K:92:CYS:HB2 | 2.56 | 0.41 |
| 4:T:176:ALA:HA | 4:T:187:LEU:HB3 | 2.03 | 0.41 |
| 2:B:11:GLU:HG3 | 2:B:11:GLU:O | 2.21 | 0.41 |
| 1:C:211:GLN:NE2 | 1:C:213:LEU:HD11 | 2.36 | 0.41 |
| 1:G:62:ARG:NH1 | 1:G:63:ASP:OD2 | 2.53 | 0.41 |
| 1:M:106:GLU:HG2 | 2:N:70:PHE:HA | 2.03 | 0.41 |
| 1:M:164:ILE:O | 1:M:246:GLU:HA | 2.20 | 0.41 |
| 2:P:168:LEU:HD23 | 2:P:168:LEU:HA | 1.96 | 0.41 |
| 3:Q:119:PRO:HG3 | 3:Q:209:PHE:CD2 | 2.55 | 0.41 |
| 3:Q:124:GLN:HB2 | 4:R:122:TYR:CG | 2.56 | 0.41 |
| 4:H:33:THR:HG23 | 4:H:95:ASN:HD22 | 1.86 | 0.41 |
| 4:H:93:VAL:CG1 | 4:H:100(C):PHE:HB3 | 2.50 | 0.41 |
| 4:F:36:TRP:CZ3 | 4:F:92:CYS:HB2 | 2.56 | 0.41 |
| 4:R:11:LEU:HA | 4:R:110:THR:O | 2.21 | 0.41 |
| 4:R:33:THR:HG23 | 4:R:95:ASN:HD22 | 1.86 | 0.41 |
| 4:R:93:VAL:CG1 | 4:R:100(C):PHE:HB3 | 2.50 | 0.41 |
| 4:R:157:TRP:CZ2 | 4:R:191:VAL:HG12 | 2.56 | 0.41 |
| 1:A:211:GLN:NE2 | 1:A:213:LEU:HD11 | 2.36 | 0.40 |
| 1:C:52:CYS:HB2 | 1:C:279:THR:HG22 | 2.03 | 0.40 |
| 1:G:28:THR:CA | 2:I:101:LEU:HD22 | 2.52 | 0.40 |
| 1:G:211:GLN:NE2 | 1:G:213:LEU:HD11 | 2.36 | 0.40 |
| 1:M:62:ARG:NH1 | 1:M:63:ASP:OD2 | 2.53 | 0.40 |
| 1:S:53:ASP:OD1 | 1:S:56:VAL:C | 2.60 | 0.40 |
| 3:L:24:ARG:HH11 | 3:L:70:ASP:HB3 | 1.86 | 0.40 |
| 2:I:22:TYR:OH | 2:I:111:HIS:ND1 | 2.40 | 0.40 |
| 2:I:55:ILE:HG23 | 2:I:99:LEU:HD23 | 2.03 | 0.40 |
| 2:U:22:TYR:OH | 2:U:111:HIS:ND1 | 2.40 | 0.40 |
| 4:K:93:VAL:CG1 | 4:K:100(C):PHE:HB3 | 2.50 | 0.40 |
| 4:W:95:ASN:HA | 4:W:100(C):PHE:HA | 2.02 | 0.40 |
| 1:G:15:ILE:HG13 | 2:I:119:TYR:HA | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:62:ARG:CG | 1:G:63:ASP:H | 2.29 | 0.40 |
| 1:M:323:THR:HG21 | 2:N:12:GLY:HA2 | 2.02 | 0.40 |
| 1:O:211:GLN:NE2 | 1:O:213:LEU:HD11 | 2.36 | 0.40 |
| 3:L:95:PRO:O | 3:L:97:THR:HG22 | 2.21 | 0.40 |
| 3:L:193:THR:HG22 | 3:L:194:CYS:N | 2.34 | 0.40 |
| 3:X:27(B):VAL:HG23 | 3:X:92:ASN:HB2 | 2.02 | 0.40 |
| 3:X:162:SER:HB2 | 4:T:177:VAL:HG21 | 2.04 | 0.40 |
| 3:Q:139:PHE:HD2 | 3:Q:198:HIS:HE2 | 1.69 | 0.40 |
| 4:H:24:THR:HG22 | 4:H:76:SER:OG | 2.21 | 0.40 |
| 4:F:157:TRP:CZ2 | 4:F:191:VAL:HG12 | 2.56 | 0.40 |
| 4:T:36:TRP:CH2 | 4:T:92:CYS:HB2 | 2.56 | 0.40 |
| 1:C:62:ARG:CG | 1:C:63:ASP:H | 2.29 | 0.40 |
| 2:D:11:GLU:O | 2:D:11:GLU:HG3 | 2.21 | 0.40 |
| 2:D:55:ILE:HG23 | 2:D:99:LEU:HD23 | 2.03 | 0.40 |
| 1:G:53:ASP:OD1 | 1:G:56:VAL:C | 2.60 | 0.40 |
| 1:M:131:ASP:OD2 | 1:M:133(A):SER:OG | 2.37 | 0.40 |
| 1:O:62:ARG:NH1 | 1:O:63:ASP:OD2 | 2.53 | 0.40 |
| 3:L:118:PHE:HA | 3:L:119:PRO:HD3 | 1.87 | 0.40 |
| 3:Q:24:ARG:HH11 | 3:Q:70:ASP:HB3 | 1.86 | 0.40 |
| 3:Q:27(B):VAL:HG23 | 3:Q:92:ASN:HB2 | 2.02 | 0.40 |
| 3:Q:95:PRO:O | 3:Q:97:THR:HG22 | 2.21 | 0.40 |
| 3:V:24:ARG:HH11 | 3:V:70:ASP:HB3 | 1.86 | 0.40 |
| 4:T:66:ARG:H | 4:T:66:ARG:HG3 | 1.53 | 0.40 |
| 4:R:19:LYS:HZ1 | 4:R:81:ASP:HB2 | 1.85 | 0.40 |
| 4:W:36:TRP:CH2 | 4:W:92:CYS:HB2 | 2.57 | 0.40 |
| 1:A:164:ILE:O | 1:A:246:GLU:HA | 2.21 | 0.40 |
| 2:D:62:GLN:HG3 | 2:D:92:TRP:CD2 | 2.55 | 0.40 |
| 3:J:24:ARG:HH11 | 3:J:70:ASP:HB3 | 1.86 | 0.40 |
| 3:J:139:PHE:HD2 | 3:J:198:HIS:HE2 | 1.69 | 0.40 |
| 4:F:36:TRP:CH2 | 4:F:92:CYS:HB2 | 2.56 | 0.40 |
| 4:K:176:ALA:HA | 4:K:187:LEU:HB3 | 2.03 | 0.40 |
| 4:R:36:TRP:CZ3 | 4:R:92:CYS:HB2 | 2.56 | 0.40 |
| 4:W:36:TRP:CZ3 | 4:W:92:CYS:HB2 | 2.56 | 0.40 |
| 1:A:53:ASP:OD1 | 1:A:56:VAL:C | 2.60 | 0.40 |
| 1:C:53:ASP:OD1 | 1:C:56:VAL:C | 2.60 | 0.40 |
| 1:M:53:ASP:OD1 | 1:M:56:VAL:C | 2.60 | 0.40 |
| 1:S:62:ARG:NH1 | 1:S:63:ASP:OD2 | 2.53 | 0.40 |
| 4:K:24:THR:HG22 | 4:K:76:SER:OG | 2.21 | 0.40 |
| 4:K:82(A):ARG:NH1 | 4:K:82(A):ARG:HB3 | 2.37 | 0.40 |
| 4:K:222:LYS:H | 4:K:222:LYS:HG2 | 1.69 | 0.40 |
| 4:T:24:THR:HG22 | 4:T:76:SER:OG | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:W:33:THR:HG23 | 4:W:95:ASN:HD22 | 1.86 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 318/334 (95%) | 309 (97%) | 9 (3%) | 0 | 100 | 100 |
| 1 | C | 315/334 (94%) | 305 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | G | 315/334 (94%) | 306 (97%) | 9 (3%) | 0 | 100 | 100 |
| 1 | M | 318/334 (95%) | 309 (97%) | 9 (3%) | 0 | 100 | 100 |
| 1 | O | 314/334 (94%) | 305 (97%) | 9 (3%) | 0 | 100 | 100 |
| 1 | S | 318/334 (95%) | 308 (97%) | 10 (3%) | 0 | 100 | 100 |
| 2 | B | 168/182 (92%) | 164 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | D | 168/182 (92%) | 164 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | I | 171/182 (94%) | 167 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | N | 163/182 (90%) | 160 (98%) | 3 (2%) | 0 | 100 | 100 |
| 2 | P | 168/182 (92%) | 164 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | U | 171/182 (94%) | 167 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | E | 212/218 (97%) | 194 (92%) | 18 (8%) | 0 | 100 | 100 |
| 3 | J | 203/218 (93%) | 185 (91%) | 18 (9%) | 0 | 100 | 100 |
| 3 | L | 209/218 (96%) | 191 (91%) | 18 (9%) | 0 | 100 | 100 |
| 3 | Q | 209/218 (96%) | 191 (91%) | 18 (9%) | 0 | 100 | 100 |
| 3 | V | 206/218 (94%) | 189 (92%) | 17 (8%) | 0 | 100 | 100 |
| 3 | X | 212/218 (97%) | 194 (92%) | 18 (8%) | 0 | 100 | 100 |
| 4 | F | 217/222 (98%) | 187 (86%) | 26 (12%) | 4 (2%) | 8 | 40 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 4 | H | 217/222 (98%) | 189 (87%) | 24 (11%) | 4 (2%) | 8 40 |
| 4 | K | 217/222 (98%) | 188 (87%) | 25 (12%) | 4 (2%) | 8 40 |
| 4 | R | 217/222 (98%) | 189 (87%) | 24 (11%) | 4 (2%) | 8 40 |
| 4 | T | 216/222 (97%) | 188 (87%) | 25 (12%) | 3 (1%) | 11 46 |
| 4 | W | 217/222 (98%) | 188 (87%) | 25 (12%) | 4 (2%) | 8 40 |
| All | All | 5459/5736 (95%) | 5101 (93%) | 335 (6%) | 23 (0%) | 34 72 |

All (23) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | H | 135 | ASN |
| 4 | F | 135 | ASN |
| 4 | K | 135 | ASN |
| 4 | R | 135 | ASN |
| 4 | W | 135 | ASN |
| 4 | H | 229 | ASP |
| 4 | F | 229 | ASP |
| 4 | K | 229 | ASP |
| 4 | T | 229 | ASP |
| 4 | R | 229 | ASP |
| 4 | W | 229 | ASP |
| 4 | H | 96 | TYR |
| 4 | F | 96 | TYR |
| 4 | K | 96 | TYR |
| 4 | T | 96 | TYR |
| 4 | R | 96 | TYR |
| 4 | W | 96 | TYR |
| 4 | H | 41 | HIS |
| 4 | F | 41 | HIS |
| 4 | K | 41 | HIS |
| 4 | T | 41 | HIS |
| 4 | R | 41 | HIS |
| 4 | W | 41 | HIS |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 286/297 (96%) | 276 (96%) | 10 (4%) | 36 | 59 |
| 1 | C | 285/297 (96%) | 274 (96%) | 11 (4%) | 32 | 56 |
| 1 | G | 285/297 (96%) | 275 (96%) | 10 (4%) | 36 | 59 |
| 1 | M | 286/297 (96%) | 276 (96%) | 10 (4%) | 36 | 59 |
| 1 | O | 283/297 (95%) | 273 (96%) | 10 (4%) | 36 | 59 |
| 1 | S | 286/297 (96%) | 276 (96%) | 10 (4%) | 36 | 59 |
| 2 | B | 147/155 (95%) | 146 (99%) | 1 (1%) | 84 | 90 |
| 2 | D | 147/155 (95%) | 146 (99%) | 1 (1%) | 84 | 90 |
| 2 | I | 148/155 (96%) | 147 (99%) | 1 (1%) | 84 | 90 |
| 2 | N | 144/155 (93%) | 144 (100%) | 0 | 100 | 100 |
| 2 | P | 147/155 (95%) | 146 (99%) | 1 (1%) | 84 | 90 |
| 2 | U | 148/155 (96%) | 146 (99%) | 2 (1%) | 67 | 80 |
| 3 | E | 189/191 (99%) | 172 (91%) | 17 (9%) | 9 | 30 |
| 3 | J | 185/191 (97%) | 169 (91%) | 16 (9%) | 10 | 32 |
| 3 | L | 188/191 (98%) | 171 (91%) | 17 (9%) | 9 | 30 |
| 3 | Q | 188/191 (98%) | 172 (92%) | 16 (8%) | 10 | 33 |
| 3 | V | 187/191 (98%) | 170 (91%) | 17 (9%) | 9 | 29 |
| 3 | X | 189/191 (99%) | 172 (91%) | 17 (9%) | 9 | 30 |
| 4 | F | 192/193 (100%) | 176 (92%) | 16 (8%) | 11 | 34 |
| 4 | H | 192/193 (100%) | 176 (92%) | 16 (8%) | 11 | 34 |
| 4 | K | 192/193 (100%) | 176 (92%) | 16 (8%) | 11 | 34 |
| 4 | R | 192/193 (100%) | 176 (92%) | 16 (8%) | 11 | 34 |
| 4 | T | 191/193 (99%) | 174 (91%) | 17 (9%) | 9 | 30 |
| 4 | W | 192/193 (100%) | 175 (91%) | 17 (9%) | 9 | 30 |
| All | All | 4869/5016 (97%) | 4604 (95%) | 265 (5%) | 22 | 47 |

All (265) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 26 | VAL |
| 1 | A | 29 | ILE |
| 1 | A | 36 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 82 | VAL |
| 1 | A | 111 | LEU |
| 1 | A | 125(A) | LYS |
| 1 | A | 135 | VAL |
| 1 | A | 151 | VAL |
| 1 | A | 195 | TYR |
| 1 | A | 197 | ASN |
| 2 | B | 69 | GLU |
| 1 | C | 26 | VAL |
| 1 | C | 29 | ILE |
| 1 | C | 36 | VAL |
| 1 | C | 82 | VAL |
| 1 | C | 111 | LEU |
| 1 | C | 125(A) | LYS |
| 1 | C | 135 | VAL |
| 1 | C | 151 | VAL |
| 1 | C | 195 | TYR |
| 1 | C | 197 | ASN |
| 1 | C | 210 | ASN |
| 2 | D | 69 | GLU |
| 1 | G | 26 | VAL |
| 1 | G | 29 | ILE |
| 1 | G | 36 | VAL |
| 1 | G | 82 | VAL |
| 1 | G | 111 | LEU |
| 1 | G | 125(A) | LYS |
| 1 | G | 135 | VAL |
| 1 | G | 151 | VAL |
| 1 | G | 195 | TYR |
| 1 | G | 197 | ASN |
| 1 | M | 26 | VAL |
| 1 | M | 29 | ILE |
| 1 | M | 36 | VAL |
| 1 | M | 82 | VAL |
| 1 | M | 111 | LEU |
| 1 | M | 125(A) | LYS |
| 1 | M | 135 | VAL |
| 1 | M | 151 | VAL |
| 1 | M | 195 | TYR |
| 1 | M | 197 | ASN |
| 1 | O | 26 | VAL |
| 1 | O | 29 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 36 | VAL |
| 1 | O | 82 | VAL |
| 1 | O | 111 | LEU |
| 1 | O | 125(A) | LYS |
| 1 | O | 135 | VAL |
| 1 | O | 151 | VAL |
| 1 | O | 195 | TYR |
| 1 | O | 197 | ASN |
| 2 | P | 69 | GLU |
| 1 | S | 26 | VAL |
| 1 | S | 29 | ILE |
| 1 | S | 36 | VAL |
| 1 | S | 82 | VAL |
| 1 | S | 111 | LEU |
| 1 | S | 125(A) | LYS |
| 1 | S | 135 | VAL |
| 1 | S | 151 | VAL |
| 1 | S | 195 | TYR |
| 1 | S | 197 | ASN |
| 3 | L | 14 | SER |
| 3 | L | 24 | ARG |
| 3 | L | 30 | LYS |
| 3 | L | 39 | LYS |
| 3 | L | 42 | GLN |
| 3 | L | 43 | SER |
| 3 | L | 53 | ASN |
| 3 | L | 69 | THR |
| 3 | L | 70 | ASP |
| 3 | L | 83 | VAL |
| 3 | L | 97 | THR |
| 3 | L | 116 | SER |
| 3 | L | 142 | LYS |
| 3 | L | 157 | ASN |
| 3 | L | 184 | ASP |
| 3 | L | 197 | THR |
| 3 | L | 202 | THR |
| 3 | E | 14 | SER |
| 3 | E | 24 | ARG |
| 3 | E | 30 | LYS |
| 3 | E | 39 | LYS |
| 3 | E | 42 | GLN |
| 3 | E | 43 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | E | 53 | ASN |
| 3 | E | 69 | THR |
| 3 | E | 70 | ASP |
| 3 | E | 83 | VAL |
| 3 | E | 97 | THR |
| 3 | E | 116 | SER |
| 3 | E | 142 | LYS |
| 3 | E | 157 | ASN |
| 3 | E | 184 | ASP |
| 3 | E | 197 | THR |
| 3 | E | 202 | THR |
| 3 | J | 14 | SER |
| 3 | J | 24 | ARG |
| 3 | J | 30 | LYS |
| 3 | J | 39 | LYS |
| 3 | J | 42 | GLN |
| 3 | J | 43 | SER |
| 3 | J | 53 | ASN |
| 3 | J | 69 | THR |
| 3 | J | 70 | ASP |
| 3 | J | 83 | VAL |
| 3 | J | 97 | THR |
| 3 | J | 116 | SER |
| 3 | J | 142 | LYS |
| 3 | J | 184 | ASP |
| 3 | J | 197 | THR |
| 3 | J | 202 | THR |
| 3 | X | 14 | SER |
| 3 | X | 24 | ARG |
| 3 | X | 30 | LYS |
| 3 | X | 39 | LYS |
| 3 | X | 42 | GLN |
| 3 | X | 43 | SER |
| 3 | X | 53 | ASN |
| 3 | X | 69 | THR |
| 3 | X | 70 | ASP |
| 3 | X | 83 | VAL |
| 3 | X | 97 | THR |
| 3 | X | 116 | SER |
| 3 | X | 142 | LYS |
| 3 | X | 157 | ASN |
| 3 | X | 184 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | X | 197 | THR |
| 3 | X | 202 | THR |
| 3 | Q | 14 | SER |
| 3 | Q | 24 | ARG |
| 3 | Q | 30 | LYS |
| 3 | Q | 39 | LYS |
| 3 | Q | 42 | GLN |
| 3 | Q | 43 | SER |
| 3 | Q | 53 | ASN |
| 3 | Q | 69 | THR |
| 3 | Q | 70 | ASP |
| 3 | Q | 83 | VAL |
| 3 | Q | 97 | THR |
| 3 | Q | 116 | SER |
| 3 | Q | 142 | LYS |
| 3 | Q | 157 | ASN |
| 3 | Q | 184 | ASP |
| 3 | Q | 197 | THR |
| 3 | V | 14 | SER |
| 3 | V | 24 | ARG |
| 3 | V | 30 | LYS |
| 3 | V | 39 | LYS |
| 3 | V | 42 | GLN |
| 3 | V | 43 | SER |
| 3 | V | 53 | ASN |
| 3 | V | 69 | THR |
| 3 | V | 70 | ASP |
| 3 | V | 83 | VAL |
| 3 | V | 97 | THR |
| 3 | V | 116 | SER |
| 3 | V | 142 | LYS |
| 3 | V | 157 | ASN |
| 3 | V | 184 | ASP |
| 3 | V | 197 | THR |
| 3 | V | 202 | THR |
| 2 | I | 69 | GLU |
| 2 | U | 69 | GLU |
| 2 | U | 97 | GLU |
| 4 | H | 1 | GLU |
| 4 | H | 2 | VAL |
| 4 | H | 11 | LEU |
| 4 | H | 12 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | H | 18 | VAL |
| 4 | H | 24 | THR |
| 4 | H | 30 | THR |
| 4 | H | 33 | THR |
| 4 | H | 58 | THR |
| 4 | H | 73 | ARG |
| 4 | H | 75 | SER |
| 4 | H | 190 | SER |
| 4 | H | 204 | GLU |
| 4 | H | 209 | ASN |
| 4 | H | 222 | LYS |
| 4 | H | 229 | ASP |
| 4 | F | 1 | GLU |
| 4 | F | 2 | VAL |
| 4 | F | 11 | LEU |
| 4 | F | 12 | VAL |
| 4 | F | 18 | VAL |
| 4 | F | 24 | THR |
| 4 | F | 30 | THR |
| 4 | F | 33 | THR |
| 4 | F | 58 | THR |
| 4 | F | 73 | ARG |
| 4 | F | 75 | SER |
| 4 | F | 190 | SER |
| 4 | F | 204 | GLU |
| 4 | F | 209 | ASN |
| 4 | F | 222 | LYS |
| 4 | F | 229 | ASP |
| 4 | K | 1 | GLU |
| 4 | K | 2 | VAL |
| 4 | K | 11 | LEU |
| 4 | K | 12 | VAL |
| 4 | K | 18 | VAL |
| 4 | K | 24 | THR |
| 4 | K | 30 | THR |
| 4 | K | 33 | THR |
| 4 | K | 58 | THR |
| 4 | K | 73 | ARG |
| 4 | K | 75 | SER |
| 4 | K | 190 | SER |
| 4 | K | 204 | GLU |
| 4 | K | 209 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | K | 222 | LYS |
| 4 | K | 229 | ASP |
| 4 | T | 1 | GLU |
| 4 | T | 2 | VAL |
| 4 | T | 11 | LEU |
| 4 | T | 12 | VAL |
| 4 | T | 18 | VAL |
| 4 | T | 24 | THR |
| 4 | T | 30 | THR |
| 4 | T | 33 | THR |
| 4 | T | 58 | THR |
| 4 | T | 73 | ARG |
| 4 | T | 75 | SER |
| 4 | T | 81 | ASP |
| 4 | T | 190 | SER |
| 4 | T | 204 | GLU |
| 4 | T | 209 | ASN |
| 4 | T | 222 | LYS |
| 4 | T | 229 | ASP |
| 4 | R | 1 | GLU |
| 4 | R | 2 | VAL |
| 4 | R | 11 | LEU |
| 4 | R | 12 | VAL |
| 4 | R | 18 | VAL |
| 4 | R | 24 | THR |
| 4 | R | 30 | THR |
| 4 | R | 33 | THR |
| 4 | R | 58 | THR |
| 4 | R | 73 | ARG |
| 4 | R | 75 | SER |
| 4 | R | 190 | SER |
| 4 | R | 204 | GLU |
| 4 | R | 209 | ASN |
| 4 | R | 222 | LYS |
| 4 | R | 229 | ASP |
| 4 | W | 1 | GLU |
| 4 | W | 2 | VAL |
| 4 | W | 11 | LEU |
| 4 | W | 12 | VAL |
| 4 | W | 18 | VAL |
| 4 | W | 24 | THR |
| 4 | W | 30 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | W | 33 | THR |
| 4 | W | 58 | THR |
| 4 | W | 73 | ARG |
| 4 | W | 75 | SER |
| 4 | W | 179 | GLN |
| 4 | W | 190 | SER |
| 4 | W | 204 | GLU |
| 4 | W | 209 | ASN |
| 4 | W | 222 | LYS |
| 4 | W | 229 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 211 | GLN |
| 1 | C | 211 | GLN |
| 1 | C | 276 | ASN |
| 1 | G | 211 | GLN |
| 1 | M | 211 | GLN |
| 1 | M | 276 | ASN |
| 1 | O | 211 | GLN |
| 1 | S | 211 | GLN |
| 3 | V | 38 | GLN |
| 4 | H | 95 | ASN |
| 4 | F | 95 | ASN |
| 4 | K | 95 | ASN |
| 4 | K | 172 | HIS |
| 4 | T | 95 | ASN |
| 4 | R | 95 | ASN |
| 4 | W | 39 | GLN |
| 4 | W | 95 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

28 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 | $\#\|Z\| > 2$ |
| 5 | NAG | Y | 1 | 5,1 | 14,14,15 | 1.31 | 2 (14%) | 17,19,21 | 2.07 | 5 (29%) |
| 5 | NAG | Y | 2 | 5 | 14,14,15 | 1.85 | 4 (28%) | 17,19,21 | 1.57 | 3 (17%) |
| 5 | MAN | Y | 3 | 5 | 11,11,12 | 1.97 | 4 (36%) | 15,15,17 | 2.01 | 5 (33%) |
| 6 | NAG | Z | 1 | 6,1 | 14,14,15 | 0.49 | 0 | 17,19,21 | 2.23 | 3 (17%) |
| 6 | NAG | Z | 2 | 6 | 14,14,15 | 0.51 | 0 | 17,19,21 | 1.39 | 3 (17%) |
| 6 | BMA | Z | 3 | 6 | 11,11,12 | 0.64 | 0 | 15,15,17 | 1.47 | 3 (20%) |
| 6 | MAN | Z | 4 | 6 | 11,11,12 | 0.61 | 0 | 15,15,17 | 2.54 | 4 (26%) |
| 6 | MAN | Z | 5 | 6 | 11,11,12 | 0.59 | 0 | 15,15,17 | 2.03 | 6 (40%) |
| 6 | MAN | Z | 6 | 6 | 11,11,12 | 0.60 | 0 | 15,15,17 | 2.02 | 6 (40%) |
| 6 | MAN | Z | 7 | 6 | 11,11,12 | 0.60 | 0 | 15,15,17 | 2.43 | 7 (46%) |
| 6 | MAN | Z | 8 | 6 | 11,11,12 | 0.62 | 0 | 15,15,17 | 2.42 | 6 (40%) |
| 7 | NAG | a | 1 | 1,7 | 14,14,15 | 1.39 | 3 (21%) | 17,19,21 | 2.00 | 4 (23%) |
| 7 | NAG | a | 2 | 7 | 14,14,15 | 1.72 | 4 (28%) | 17,19,21 | 1.79 | 6 (35%) |
| 8 | NAG | b | 1 | 1,8 | 14,14,15 | 0.55 | 0 | 17,19,21 | 1.29 | 3 (17%) |
| 8 | NAG | b | 2 | 8 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.70 | 0 |
| 8 | BMA | b | 3 | 8 | 11,11,12 | 0.63 | 0 | 15,15,17 | 0.68 | 0 |
| 7 | NAG | c | 1 | 1,7 | 14,14,15 | 1.30 | 2 (14%) | 17,19,21 | 2.07 | 5 (29%) |
| 7 | NAG | c | 2 | 7 | 14,14,15 | 1.84 | 4 (28%) | 17,19,21 | 1.57 | 2 (11%) |
| 5 | NAG | d | 1 | 5,1 | 14,14,15 | 1.27 | 2 (14%) | 17,19,21 | 1.84 | 4 (23%) |
| 5 | NAG | d | 2 | 5 | 14,14,15 | 1.81 | 4 (28%) | 17,19,21 | 1.76 | 6 (35%) |
| 5 | MAN | d | 3 | 5 | 11,11,12 | 1.86 | 3 (27%) | 15,15,17 | 2.03 | 4 (26%) |
| 9 | NAG | e | 1 | 9,1 | 14,14,15 | 0.59 | 0 | 17,19,21 | 1.25 | 2 (11%) |
| 9 | NAG | e | 2 | 9 | 14,14,15 | 0.48 | 0 | 17,19,21 | 1.14 | 1 (5%) |
| 9 | BMA | e | 3 | 9 | 11,11,12 | 0.75 | 0 | 15,15,17 | 0.65 | 0 |
| 9 | MAN | e | 4 | 9 | 11,11,12 | 0.61 | 0 | 15,15,17 | 1.06 | 1 (6%) |
| 5 | NAG | f | 1 | 5,1 | 14,14,15 | 1.39 | 3 (21%) | 17,19,21 | 2.01 | 4 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 5 | NAG | f | 2 | 5 | 14,14,15 | 1.73 | 4 (28%) | 17,19,21 | 1.80 | 6 (35%) |
| 5 | MAN | f | 3 | 5 | 11,11,12 | 1.83 | 3 (27%) | 15,15,17 | 2.08 | 5 (33%) |

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 |
|---|---|---|---|---|---|---|---|
| 5 | NAG | Y | 1 | 5,1 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | NAG | Y | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | MAN | Y | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 6 | NAG | Z | 1 | 6,1 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | Z | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | Z | 3 | 6 | - | 2/2/19/22 | 0/1/1/1 |
| 6 | MAN | Z | 4 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | MAN | Z | 5 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | MAN | Z | 6 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | MAN | Z | 7 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | MAN | Z | 8 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | NAG | a | 1 | 1,7 | - | 1/6/23/26 | 0/1/1/1 |
| 7 | NAG | a | 2 | 7 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | NAG | b | 1 | 1,8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | NAG | b | 2 | 8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | BMA | b | 3 | 8 | - | 1/2/19/22 | 0/1/1/1 |
| 7 | NAG | c | 1 | 1,7 | - | 1/6/23/26 | 0/1/1/1 |
| 7 | NAG | c | 2 | 7 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | d | 1 | 5,1 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | NAG | d | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | MAN | d | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 9 | NAG | e | 1 | 9,1 | - | 0/6/23/26 | 0/1/1/1 |
| 9 | NAG | e | 2 | 9 | - | 0/6/23/26 | 0/1/1/1 |
| 9 | BMA | e | 3 | 9 | - | 0/2/19/22 | 0/1/1/1 |
| 9 | MAN | e | 4 | 9 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | f | 1 | 5,1 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | NAG | f | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | MAN | f | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | Y | 2 | NAG | C1-C2 | 3.53 | 1.57 | 1.52 |
| 7 | c | 2 | NAG | C1-C2 | 3.44 | 1.57 | 1.52 |
| 7 | a | 2 | NAG | C1-C2 | 3.42 | 1.57 | 1.52 |
| 5 | f | 2 | NAG | C1-C2 | 3.38 | 1.57 | 1.52 |
| 5 | d | 2 | NAG | O4-C4 | 3.12 | 1.50 | 1.43 |
| 5 | f | 3 | MAN | C2-C3 | 3.09 | 1.57 | 1.52 |
| 5 | Y | 3 | MAN | C4-C3 | 3.06 | 1.60 | 1.52 |
| 5 | Y | 2 | NAG | C4-C3 | 3.02 | 1.60 | 1.52 |
| 7 | c | 2 | NAG | C4-C3 | 3.02 | 1.60 | 1.52 |
| 5 | d | 2 | NAG | C1-C2 | 2.95 | 1.56 | 1.52 |
| 5 | Y | 3 | MAN | C2-C3 | 2.94 | 1.56 | 1.52 |
| 5 | d | 3 | MAN | C2-C3 | 2.94 | 1.56 | 1.52 |
| 5 | d | 3 | MAN | C1-C2 | 2.91 | 1.58 | 1.52 |
| 5 | Y | 2 | NAG | O4-C4 | 2.82 | 1.49 | 1.43 |
| 7 | c | 2 | NAG | O4-C4 | 2.80 | 1.49 | 1.43 |
| 5 | f | 2 | NAG | C4-C3 | 2.76 | 1.59 | 1.52 |
| 7 | a | 2 | NAG | C4-C3 | 2.72 | 1.59 | 1.52 |
| 5 | d | 1 | NAG | C1-C2 | 2.61 | 1.56 | 1.52 |
| 5 | f | 2 | NAG | C3-C2 | 2.53 | 1.57 | 1.52 |
| 7 | a | 2 | NAG | C3-C2 | 2.49 | 1.57 | 1.52 |
| 5 | d | 2 | NAG | C4-C5 | 2.48 | 1.58 | 1.53 |
| 7 | c | 1 | NAG | O3-C3 | 2.46 | 1.48 | 1.43 |
| 5 | Y | 1 | NAG | O3-C3 | 2.40 | 1.48 | 1.43 |
| 5 | f | 3 | MAN | C1-C2 | 2.39 | 1.57 | 1.52 |
| 5 | d | 2 | NAG | C4-C3 | 2.35 | 1.58 | 1.52 |
| 5 | f | 3 | MAN | C4-C3 | 2.30 | 1.58 | 1.52 |
| 5 | d | 3 | MAN | C4-C3 | 2.30 | 1.58 | 1.52 |
| 7 | c | 2 | NAG | C4-C5 | 2.29 | 1.57 | 1.53 |
| 5 | Y | 2 | NAG | C4-C5 | 2.29 | 1.57 | 1.53 |
| 5 | Y | 3 | MAN | C1-C2 | 2.28 | 1.57 | 1.52 |
| 5 | f | 2 | NAG | O4-C4 | 2.21 | 1.48 | 1.43 |
| 5 | f | 1 | NAG | C3-C2 | 2.21 | 1.57 | 1.52 |
| 5 | Y | 1 | NAG | C3-C2 | 2.21 | 1.57 | 1.52 |
| 7 | a | 2 | NAG | O4-C4 | 2.20 | 1.48 | 1.43 |
| 5 | f | 1 | NAG | C1-C2 | 2.19 | 1.55 | 1.52 |
| 7 | a | 1 | NAG | C3-C2 | 2.19 | 1.57 | 1.52 |
| 7 | c | 1 | NAG | C3-C2 | 2.18 | 1.57 | 1.52 |
| 7 | a | 1 | NAG | C1-C2 | 2.13 | 1.55 | 1.52 |
| 7 | a | 1 | NAG | C4-C5 | 2.10 | 1.57 | 1.53 |
| 5 | f | 1 | NAG | C4-C5 | 2.10 | 1.57 | 1.53 |
| 5 | Y | 3 | MAN | O5-C1 | 2.02 | 1.46 | 1.43 |
| 5 | d | 1 | NAG | C3-C2 | 2.02 | 1.56 | 1.52 |

All (104) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 1 | NAG | O5-C1-C2 | -7.36 | 99.67 | 111.29 |
| 6 | Z | 4 | MAN | C1-C2-C3 | 6.99 | 118.25 | 109.67 |
| 6 | Z | 8 | MAN | C1-O5-C5 | 5.78 | 120.02 | 112.19 |
| 7 | c | 1 | NAG | C1-O5-C5 | 5.10 | 119.10 | 112.19 |
| 5 | Y | 1 | NAG | C1-O5-C5 | 5.08 | 119.07 | 112.19 |
| 6 | Z | 7 | MAN | C6-C5-C4 | -5.05 | 101.18 | 113.00 |
| 5 | f | 3 | MAN | C1-O5-C5 | 4.89 | 118.82 | 112.19 |
| 5 | f | 1 | NAG | C1-O5-C5 | 4.59 | 118.41 | 112.19 |
| 7 | a | 1 | NAG | C1-O5-C5 | 4.58 | 118.39 | 112.19 |
| 5 | d | 1 | NAG | C1-O5-C5 | 4.40 | 118.15 | 112.19 |
| 5 | d | 3 | MAN | O2-C2-C1 | 4.19 | 117.73 | 109.15 |
| 5 | Y | 3 | MAN | C1-O5-C5 | 4.15 | 117.82 | 112.19 |
| 6 | Z | 4 | MAN | C2-C3-C4 | -4.10 | 103.80 | 110.89 |
| 5 | f | 1 | NAG | C8-C7-N2 | -4.00 | 109.32 | 116.10 |
| 7 | a | 1 | NAG | C8-C7-N2 | -3.93 | 109.44 | 116.10 |
| 6 | Z | 5 | MAN | O4-C4-C3 | -3.93 | 101.27 | 110.35 |
| 5 | Y | 3 | MAN | O5-C5-C6 | 3.81 | 113.17 | 107.20 |
| 5 | d | 3 | MAN | C1-O5-C5 | 3.62 | 117.09 | 112.19 |
| 6 | Z | 7 | MAN | O4-C4-C3 | -3.58 | 102.07 | 110.35 |
| 5 | d | 2 | NAG | O3-C3-C4 | 3.55 | 118.57 | 110.35 |
| 6 | Z | 2 | NAG | O5-C5-C6 | -3.55 | 101.64 | 107.20 |
| 6 | Z | 4 | MAN | O5-C1-C2 | -3.47 | 105.41 | 110.77 |
| 5 | Y | 3 | MAN | O2-C2-C1 | 3.46 | 116.24 | 109.15 |
| 6 | Z | 7 | MAN | O5-C5-C6 | 3.45 | 112.61 | 107.20 |
| 6 | Z | 6 | MAN | O4-C4-C3 | -3.41 | 102.46 | 110.35 |
| 6 | Z | 8 | MAN | C3-C4-C5 | 3.40 | 116.30 | 110.24 |
| 5 | d | 3 | MAN | O5-C5-C6 | 3.33 | 112.42 | 107.20 |
| 5 | f | 3 | MAN | C2-C3-C4 | 3.27 | 116.55 | 110.89 |
| 7 | c | 1 | NAG | C2-N2-C7 | 3.26 | 127.54 | 122.90 |
| 9 | e | 4 | MAN | C1-O5-C5 | 3.25 | 116.60 | 112.19 |
| 5 | Y | 1 | NAG | C2-N2-C7 | 3.24 | 127.52 | 122.90 |
| 6 | Z | 6 | MAN | C2-C3-C4 | 3.24 | 116.51 | 110.89 |
| 6 | Z | 5 | MAN | O4-C4-C5 | 3.23 | 117.31 | 109.30 |
| 6 | Z | 7 | MAN | C3-C4-C5 | -3.14 | 104.64 | 110.24 |
| 5 | d | 3 | MAN | C2-C3-C4 | 3.11 | 116.28 | 110.89 |
| 5 | f | 3 | MAN | O5-C5-C6 | 3.11 | 112.08 | 107.20 |
| 9 | e | 1 | NAG | C1-O5-C5 | 3.10 | 116.39 | 112.19 |
| 5 | f | 2 | NAG | C1-O5-C5 | 3.10 | 116.39 | 112.19 |
| 5 | f | 2 | NAG | C3-C4-C5 | -3.09 | 104.72 | 110.24 |
| 7 | a | 2 | NAG | C3-C4-C5 | -3.09 | 104.73 | 110.24 |
| 6 | Z | 6 | MAN | O5-C5-C6 | -3.05 | 102.43 | 107.20 |
| 7 | a | 2 | NAG | C1-O5-C5 | 3.03 | 116.30 | 112.19 |
| 8 | b | 1 | NAG | C2-N2-C7 | -3.02 | 118.60 | 122.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | a | 2 | NAG | O3-C3-C4 | 3.02 | 117.33 | 110.35 |
| 5 | f | 2 | NAG | O3-C3-C4 | 3.00 | 117.28 | 110.35 |
| 5 | Y | 2 | NAG | O3-C3-C4 | 3.00 | 117.28 | 110.35 |
| 5 | d | 2 | NAG | C4-C3-C2 | 2.97 | 115.37 | 111.02 |
| 5 | f | 3 | MAN | O2-C2-C1 | 2.97 | 115.23 | 109.15 |
| 7 | c | 2 | NAG | O3-C3-C4 | 2.97 | 117.21 | 110.35 |
| 6 | Z | 7 | MAN | O2-C2-C3 | -2.97 | 104.19 | 110.14 |
| 6 | Z | 3 | BMA | O2-C2-C3 | 2.97 | 116.08 | 110.14 |
| 5 | Y | 1 | NAG | C8-C7-N2 | -2.96 | 111.09 | 116.10 |
| 6 | Z | 8 | MAN | O2-C2-C1 | 2.95 | 115.19 | 109.15 |
| 7 | c | 1 | NAG | C8-C7-N2 | -2.92 | 111.15 | 116.10 |
| 5 | d | 1 | NAG | C8-C7-N2 | -2.88 | 111.23 | 116.10 |
| 7 | c | 2 | NAG | C3-C4-C5 | -2.80 | 105.24 | 110.24 |
| 6 | Z | 8 | MAN | O4-C4-C5 | 2.79 | 116.22 | 109.30 |
| 6 | Z | 5 | MAN | O5-C5-C6 | -2.78 | 102.85 | 107.20 |
| 5 | Y | 2 | NAG | C3-C4-C5 | -2.75 | 105.33 | 110.24 |
| 6 | Z | 1 | NAG | O7-C7-C8 | -2.73 | 116.98 | 122.06 |
| 5 | d | 2 | NAG | C2-N2-C7 | 2.69 | 126.73 | 122.90 |
| 6 | Z | 1 | NAG | C4-C3-C2 | -2.68 | 107.09 | 111.02 |
| 5 | Y | 3 | MAN | C2-C3-C4 | 2.66 | 115.51 | 110.89 |
| 6 | Z | 3 | BMA | O4-C4-C5 | -2.62 | 102.79 | 109.30 |
| 6 | Z | 6 | MAN | O5-C1-C2 | 2.61 | 114.81 | 110.77 |
| 6 | Z | 8 | MAN | O5-C5-C6 | -2.60 | 103.12 | 107.20 |
| 5 | f | 1 | NAG | O3-C3-C2 | 2.60 | 114.84 | 109.47 |
| 7 | a | 1 | NAG | O3-C3-C2 | 2.56 | 114.76 | 109.47 |
| 9 | e | 1 | NAG | C1-C2-N2 | 2.56 | 114.86 | 110.49 |
| 5 | Y | 1 | NAG | O3-C3-C2 | 2.53 | 114.70 | 109.47 |
| 5 | d | 2 | NAG | C8-C7-N2 | -2.50 | 111.87 | 116.10 |
| 6 | Z | 6 | MAN | O3-C3-C2 | 2.50 | 114.77 | 109.99 |
| 8 | b | 1 | NAG | O3-C3-C2 | -2.47 | 104.35 | 109.47 |
| 7 | c | 1 | NAG | O3-C3-C2 | 2.46 | 114.56 | 109.47 |
| 6 | Z | 7 | MAN | O2-C2-C1 | 2.42 | 114.11 | 109.15 |
| 6 | Z | 3 | BMA | C6-C5-C4 | -2.42 | 107.34 | 113.00 |
| 8 | b | 1 | NAG | O5-C1-C2 | -2.36 | 107.55 | 111.29 |
| 7 | c | 1 | NAG | O5-C5-C6 | 2.35 | 110.88 | 107.20 |
| 7 | a | 2 | NAG | C1-C2-N2 | 2.31 | 114.43 | 110.49 |
| 5 | f | 2 | NAG | C1-C2-N2 | 2.29 | 114.41 | 110.49 |
| 6 | Z | 5 | MAN | C1-O5-C5 | 2.28 | 115.28 | 112.19 |
| 5 | Y | 1 | NAG | O5-C5-C6 | 2.27 | 110.77 | 107.20 |
| 5 | f | 2 | NAG | O4-C4-C3 | 2.27 | 115.59 | 110.35 |
| 6 | Z | 2 | NAG | O5-C1-C2 | -2.27 | 107.71 | 111.29 |
| 7 | a | 2 | NAG | O4-C4-C3 | 2.24 | 115.52 | 110.35 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 5 | MAN | O3-C3-C2 | -2.23 | 105.72 | 109.99 |
| 5 | f | 3 | MAN | C3-C4-C5 | 2.23 | 114.22 | 110.24 |
| 6 | Z | 8 | MAN | C1-C2-C3 | -2.22 | 106.94 | 109.67 |
| 6 | Z | 2 | NAG | C4-C3-C2 | -2.20 | 107.80 | 111.02 |
| 5 | d | 1 | NAG | O3-C3-C2 | 2.19 | 114.00 | 109.47 |
| 6 | Z | 6 | MAN | C1-O5-C5 | 2.18 | 115.14 | 112.19 |
| 5 | d | 1 | NAG | C2-N2-C7 | 2.17 | 126.00 | 122.90 |
| 6 | Z | 7 | MAN | C2-C3-C4 | 2.10 | 114.52 | 110.89 |
| 5 | d | 2 | NAG | O4-C4-C3 | 2.09 | 115.17 | 110.35 |
| 5 | f | 2 | NAG | C8-C7-N2 | -2.08 | 112.57 | 116.10 |
| 5 | f | 1 | NAG | O7-C7-N2 | 2.08 | 125.77 | 121.95 |
| 7 | a | 1 | NAG | O7-C7-N2 | 2.06 | 125.73 | 121.95 |
| 6 | Z | 4 | MAN | O5-C5-C6 | -2.05 | 103.99 | 107.20 |
| 9 | e | 2 | NAG | C1-O5-C5 | 2.04 | 114.96 | 112.19 |
| 5 | Y | 3 | MAN | C3-C4-C5 | 2.04 | 113.88 | 110.24 |
| 7 | a | 2 | NAG | C8-C7-N2 | -2.03 | 112.67 | 116.10 |
| 5 | Y | 2 | NAG | O5-C5-C6 | 2.01 | 110.36 | 107.20 |
| 5 | d | 2 | NAG | C3-C4-C5 | -2.00 | 106.67 | 110.24 |
| 6 | Z | 5 | MAN | O5-C1-C2 | 2.00 | 113.86 | 110.77 |

There are no chirality outliers.

All (15) torsion outliers are listed below:

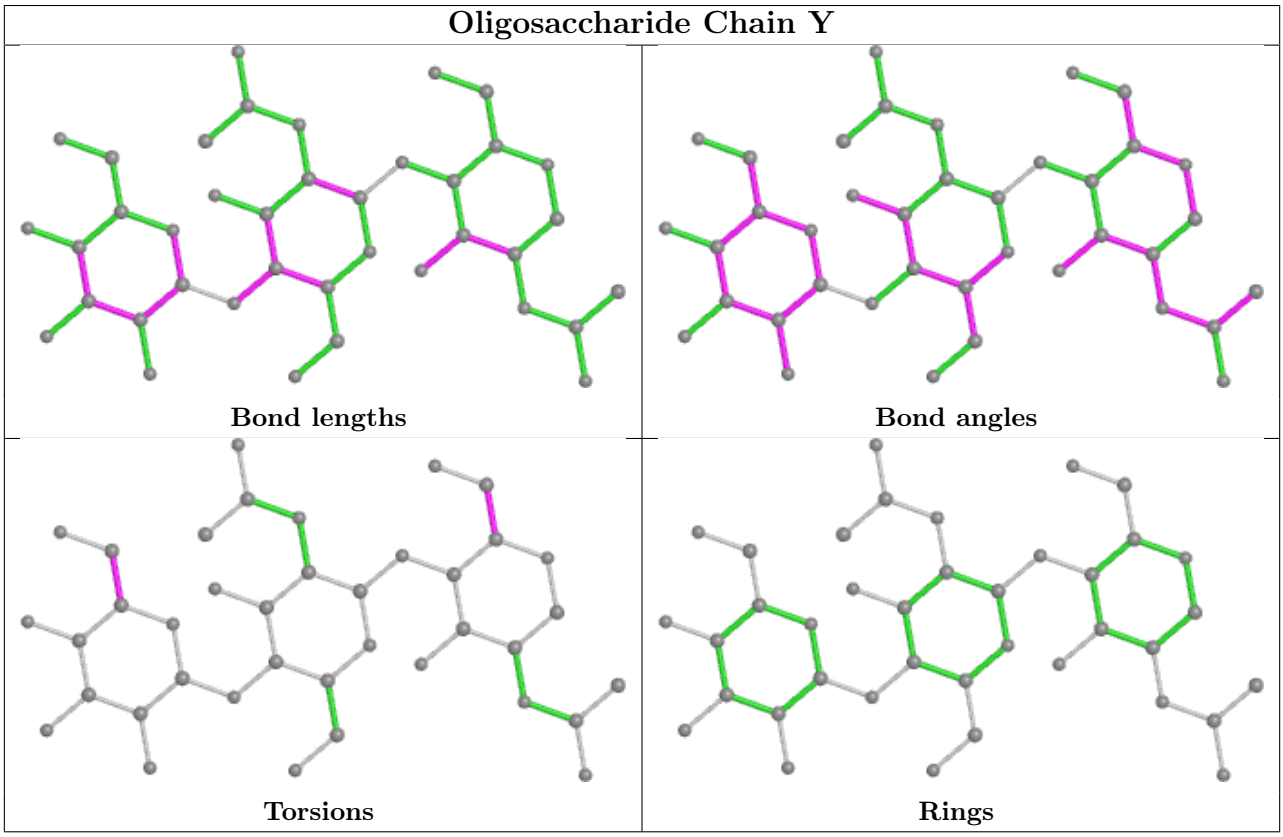
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | d | 3 | MAN | C4-C5-C6-O6 |
| 5 | Y | 3 | MAN | C4-C5-C6-O6 |
| 5 | f | 3 | MAN | C4-C5-C6-O6 |
| 5 | d | 3 | MAN | O5-C5-C6-O6 |
| 5 | f | 3 | MAN | O5-C5-C6-O6 |
| 7 | a | 1 | NAG | C4-C5-C6-O6 |
| 5 | f | 1 | NAG | C4-C5-C6-O6 |
| 5 | Y | 3 | MAN | O5-C5-C6-O6 |
| 5 | Y | 1 | NAG | C4-C5-C6-O6 |
| 7 | c | 1 | NAG | C4-C5-C6-O6 |
| 5 | d | 1 | NAG | C4-C5-C6-O6 |
| 8 | b | 3 | BMA | O5-C5-C6-O6 |
| 6 | Z | 3 | BMA | C4-C5-C6-O6 |
| 6 | Z | 3 | BMA | O5-C5-C6-O6 |
| 6 | Z | 1 | NAG | O7-C7-N2-C2 |

There are no ring outliers.

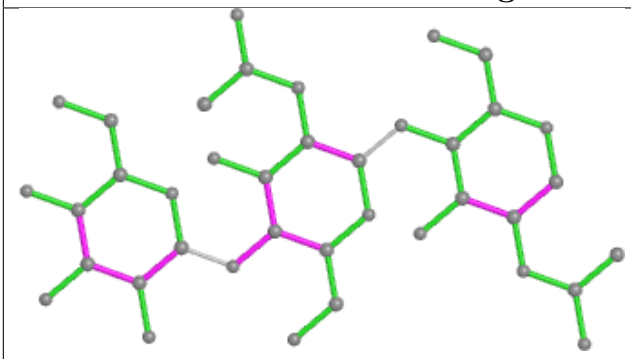
2 monomers are involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | Y | 2 | NAG | 1 | 0 |
| 5 | Y | 1 | NAG | 1 | 0 |

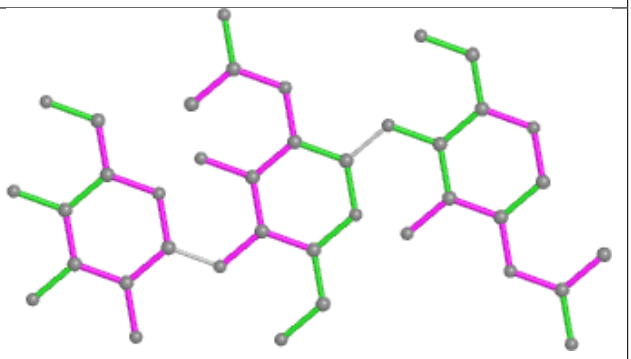
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



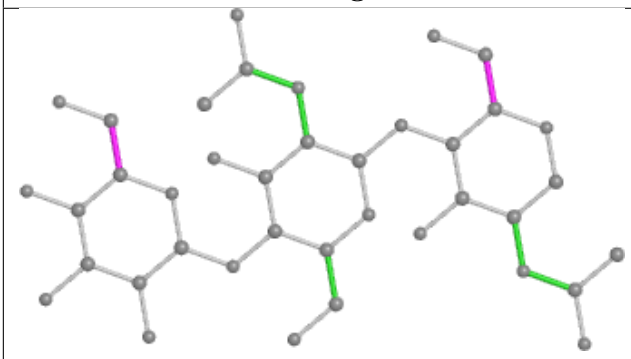
## Oligosaccharide Chain d



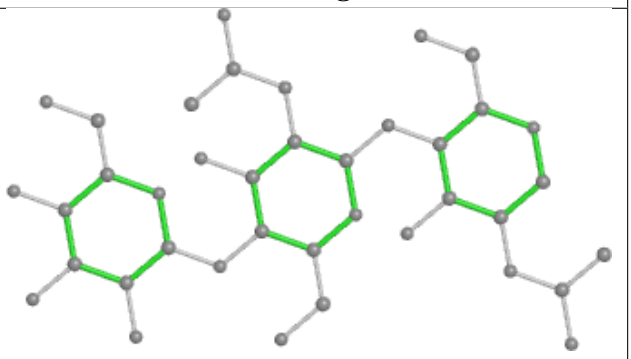
Bond lengths



Bond angles

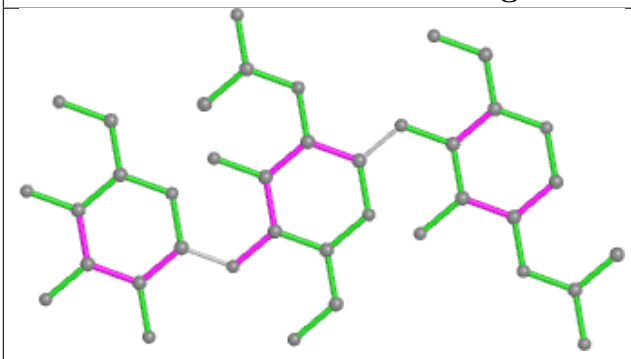


Torsions

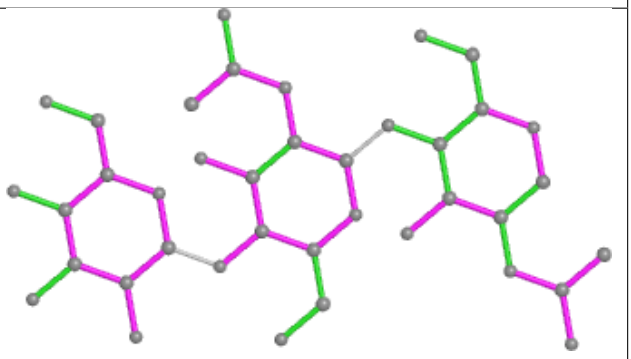


Rings

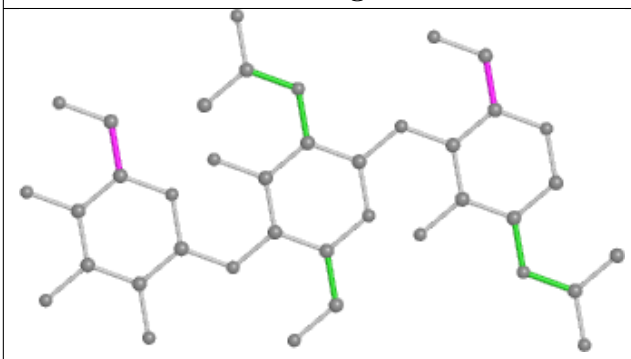
## Oligosaccharide Chain f



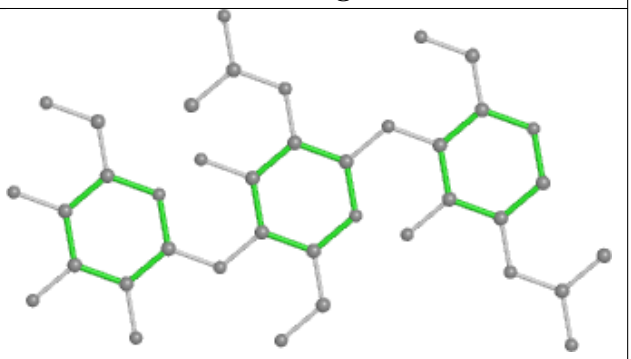
Bond lengths



Bond angles

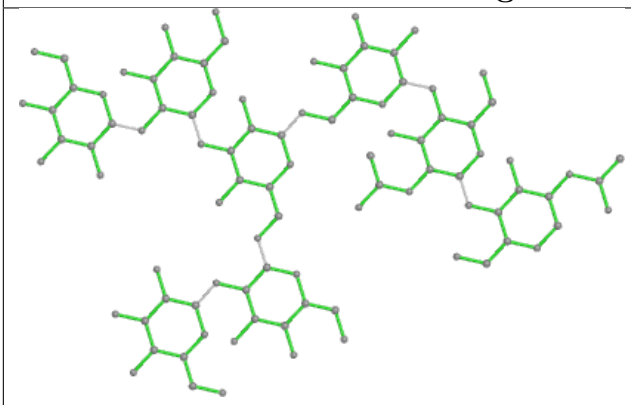


Torsions

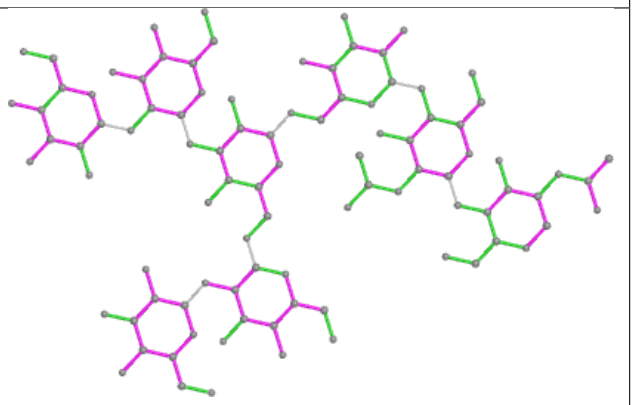


Rings

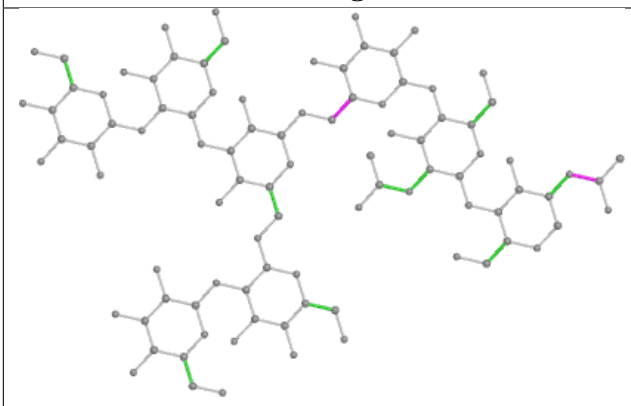
**Oligosaccharide Chain Z**



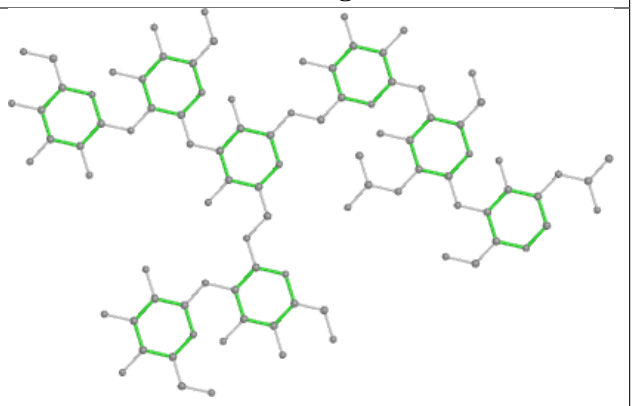
**Bond lengths**



**Bond angles**

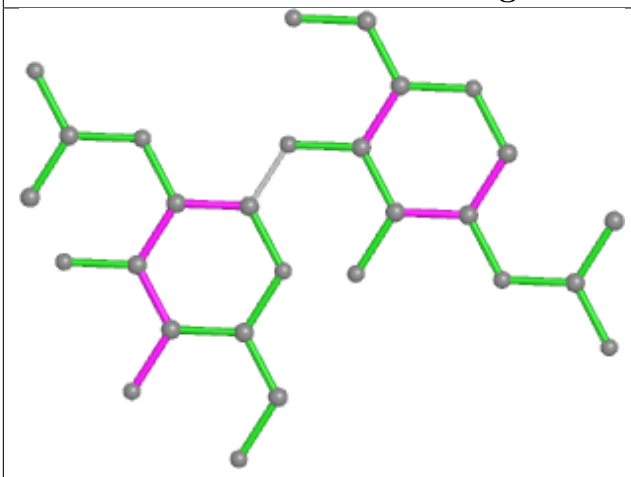


**Torsions**

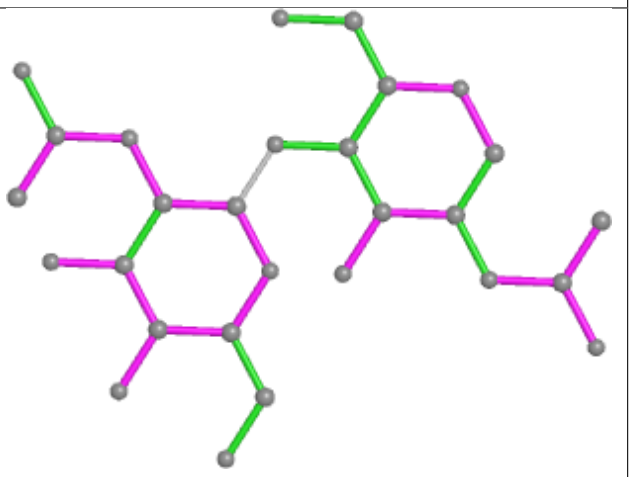


**Rings**

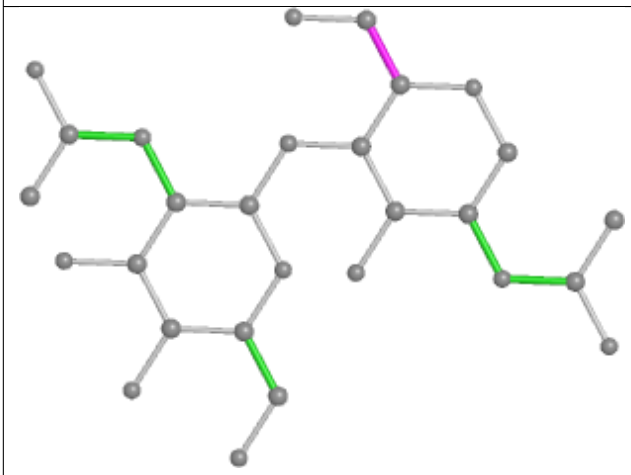
**Oligosaccharide Chain a**



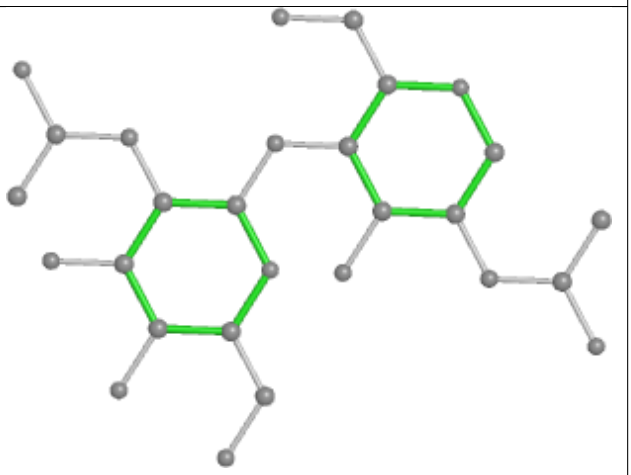
**Bond lengths**



**Bond angles**

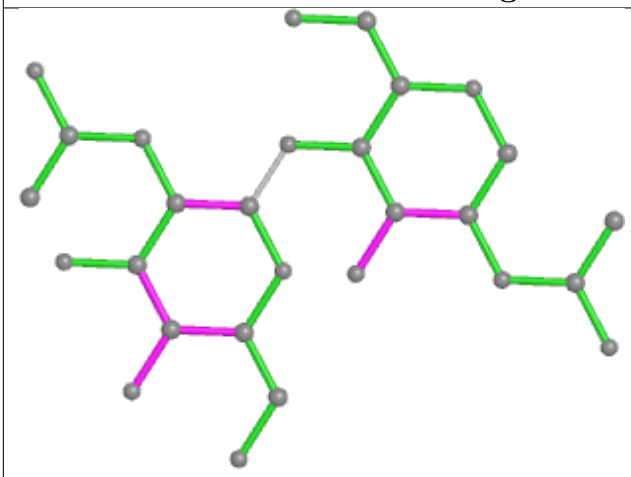


**Torsions**

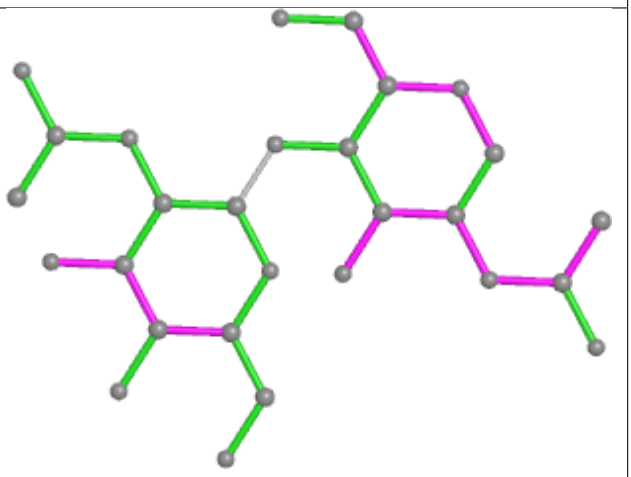


**Rings**

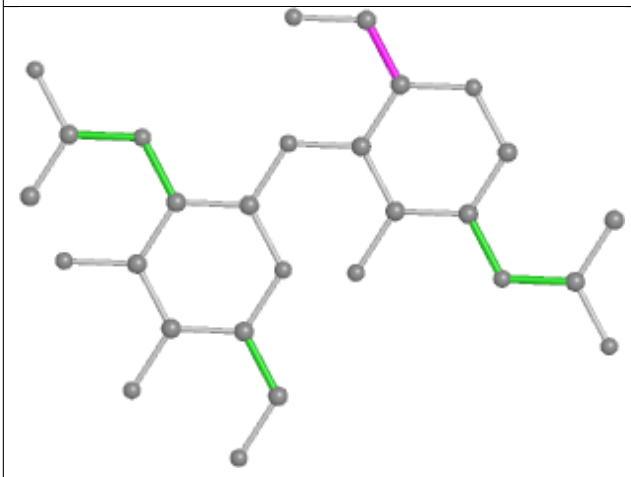
**Oligosaccharide Chain c**



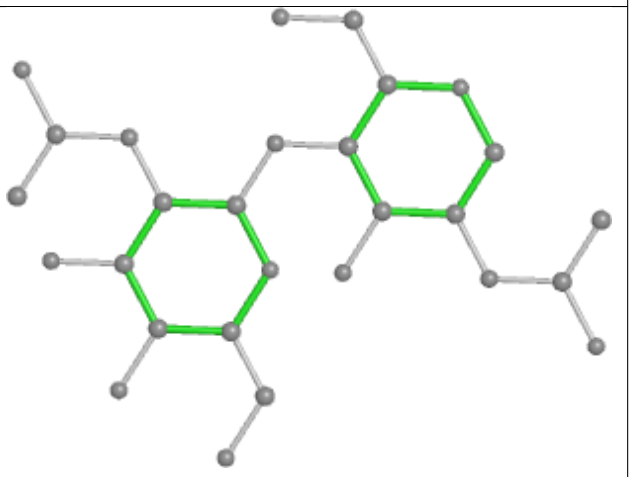
**Bond lengths**



**Bond angles**

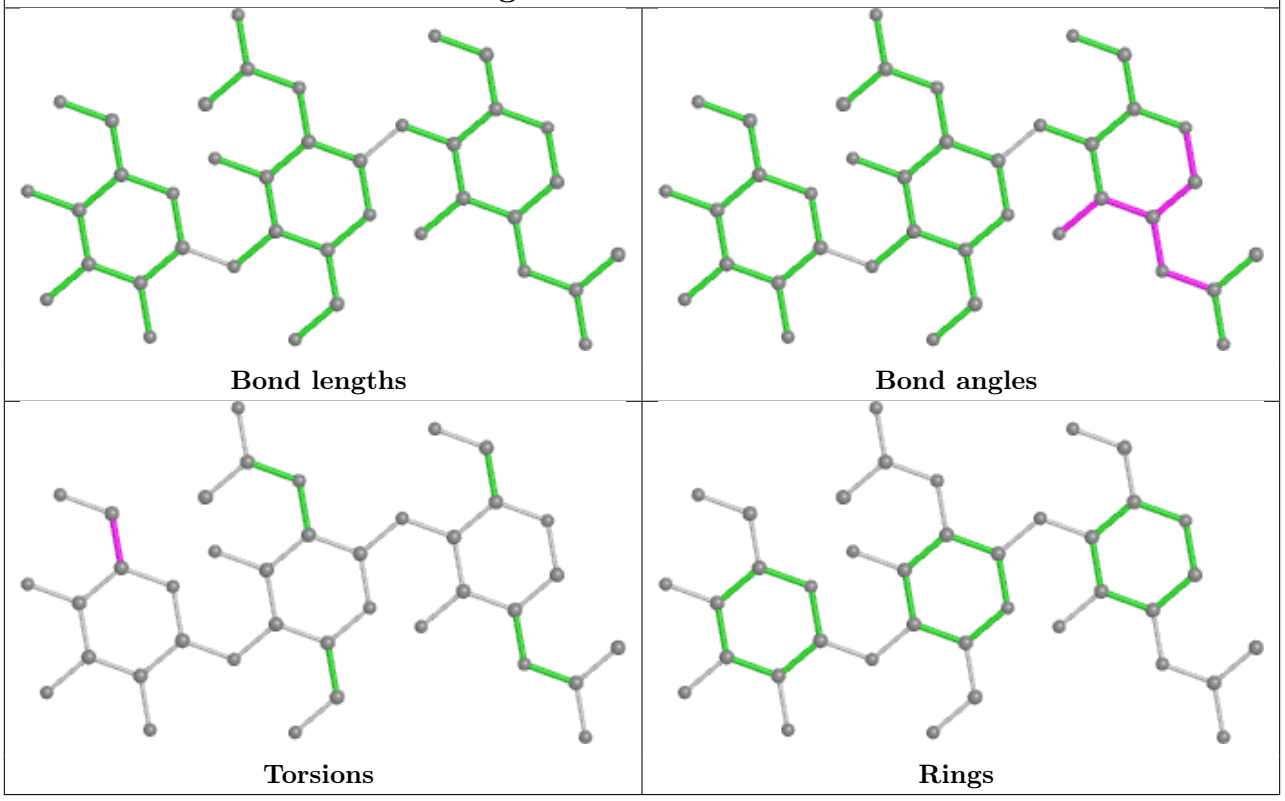


**Torsions**

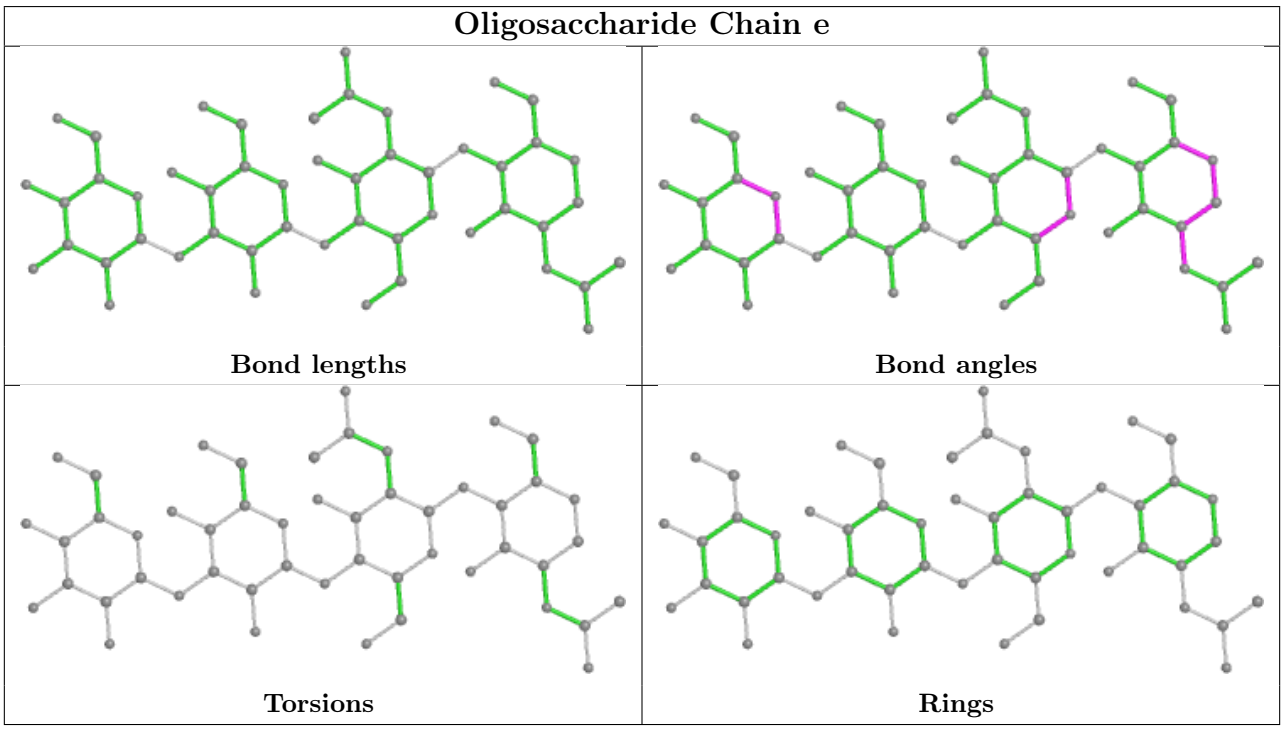


**Rings**

**Oligosaccharide Chain b**




**Oligosaccharide Chain e**




## 5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 10 | NAG | S | 2004 | 1 | 14,14,15 | 1.85 | 4 (28%) | 17,19,21 | 2.62 | 8 (47%) |
| 10 | NAG | M | 2003 | 1 | 14,14,15 | 1.93 | 4 (28%) | 17,19,21 | 2.57 | 9 (52%) |
| 10 | NAG | C | 2001 | 1 | 14,14,15 | 1.28 | 2 (14%) | 17,19,21 | 1.84 | 4 (23%) |
| 10 | NAG | P | 2001 | 2 | 14,14,15 | 2.18 | 5 (35%) | 17,19,21 | 2.69 | 8 (47%) |
| 10 | NAG | A | 2004 | 1 | 14,14,15 | 1.94 | 4 (28%) | 17,19,21 | 2.58 | 9 (52%) |
| 10 | NAG | O | 2004 | 1 | 14,14,15 | 1.88 | 4 (28%) | 17,19,21 | 2.60 | 8 (47%) |

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 |
|---|---|---|---|---|---|---|---|
| 10 | NAG | S | 2004 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 10 | NAG | M | 2003 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 10 | NAG | C | 2001 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 10 | NAG | P | 2001 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NAG | A | 2004 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 10 | NAG | O | 2004 | 1 | - | 1/6/23/26 | 0/1/1/1 |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | P | 2001 | NAG | C1-C2 | 4.32 | 1.58 | 1.52 |
| 10 | A | 2004 | NAG | C1-C2 | 3.56 | 1.57 | 1.52 |
| 10 | O | 2004 | NAG | C1-C2 | 3.55 | 1.57 | 1.52 |
| 10 | M | 2003 | NAG | C1-C2 | 3.53 | 1.57 | 1.52 |
| 10 | P | 2001 | NAG | C2-N2 | 3.30 | 1.51 | 1.46 |
| 10 | S | 2004 | NAG | O4-C4 | 3.30 | 1.50 | 1.43 |
| 10 | P | 2001 | NAG | C4-C5 | 3.14 | 1.59 | 1.53 |
| 10 | A | 2004 | NAG | C4-C3 | 3.08 | 1.60 | 1.52 |
| 10 | M | 2003 | NAG | C4-C3 | 3.05 | 1.60 | 1.52 |
| 10 | M | 2003 | NAG | O3-C3 | 3.03 | 1.50 | 1.43 |
| 10 | A | 2004 | NAG | O3-C3 | 3.00 | 1.50 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | S | 2004 | NAG | C4-C3 | 2.96 | 1.59 | 1.52 |
| 10 | M | 2003 | NAG | O4-C4 | 2.95 | 1.49 | 1.43 |
| 10 | A | 2004 | NAG | O4-C4 | 2.94 | 1.49 | 1.43 |
| 10 | O | 2004 | NAG | C4-C3 | 2.92 | 1.59 | 1.52 |
| 10 | S | 2004 | NAG | C1-C2 | 2.80 | 1.56 | 1.52 |
| 10 | O | 2004 | NAG | O4-C4 | 2.73 | 1.49 | 1.43 |
| 10 | C | 2001 | NAG | C1-C2 | 2.70 | 1.56 | 1.52 |
| 10 | O | 2004 | NAG | O3-C3 | 2.55 | 1.49 | 1.43 |
| 10 | P | 2001 | NAG | C3-C2 | 2.41 | 1.57 | 1.52 |
| 10 | S | 2004 | NAG | C2-N2 | 2.32 | 1.50 | 1.46 |
| 10 | P | 2001 | NAG | C4-C3 | 2.10 | 1.57 | 1.52 |
| 10 | C | 2001 | NAG | C3-C2 | 2.02 | 1.56 | 1.52 |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | P | 2001 | NAG | C2-N2-C7 | 8.06 | 134.38 | 122.90 |
| 10 | O | 2004 | NAG | C1-C2-N2 | 5.69 | 120.21 | 110.49 |
| 10 | S | 2004 | NAG | C4-C3-C2 | 5.62 | 119.26 | 111.02 |
| 10 | A | 2004 | NAG | C1-C2-N2 | 5.08 | 119.16 | 110.49 |
| 10 | M | 2003 | NAG | C1-C2-N2 | 5.04 | 119.11 | 110.49 |
| 10 | S | 2004 | NAG | O5-C5-C6 | 4.98 | 115.00 | 107.20 |
| 10 | A | 2004 | NAG | C4-C3-C2 | 4.94 | 118.26 | 111.02 |
| 10 | M | 2003 | NAG | C4-C3-C2 | 4.91 | 118.22 | 111.02 |
| 10 | C | 2001 | NAG | C1-O5-C5 | 4.42 | 118.18 | 112.19 |
| 10 | O | 2004 | NAG | O5-C5-C6 | 3.86 | 113.26 | 107.20 |
| 10 | O | 2004 | NAG | C4-C3-C2 | 3.84 | 116.65 | 111.02 |
| 10 | M | 2003 | NAG | O5-C5-C6 | 3.82 | 113.20 | 107.20 |
| 10 | S | 2004 | NAG | C1-C2-N2 | 3.82 | 117.01 | 110.49 |
| 10 | A | 2004 | NAG | O5-C5-C6 | 3.79 | 113.14 | 107.20 |
| 10 | S | 2004 | NAG | O3-C3-C4 | 3.28 | 117.92 | 110.35 |
| 10 | O | 2004 | NAG | C1-O5-C5 | 3.22 | 116.55 | 112.19 |
| 10 | A | 2004 | NAG | O3-C3-C4 | 3.17 | 117.67 | 110.35 |
| 10 | P | 2001 | NAG | O5-C1-C2 | 3.15 | 116.26 | 111.29 |
| 10 | M | 2003 | NAG | O3-C3-C4 | 3.13 | 117.60 | 110.35 |
| 10 | A | 2004 | NAG | C3-C4-C5 | 2.93 | 115.47 | 110.24 |
| 10 | M | 2003 | NAG | C3-C4-C5 | 2.91 | 115.43 | 110.24 |
| 10 | C | 2001 | NAG | C8-C7-N2 | -2.87 | 111.23 | 116.10 |
| 10 | P | 2001 | NAG | O7-C7-N2 | 2.84 | 127.18 | 121.95 |
| 10 | P | 2001 | NAG | C1-O5-C5 | 2.82 | 116.02 | 112.19 |
| 10 | O | 2004 | NAG | O4-C4-C5 | -2.75 | 102.47 | 109.30 |
| 10 | O | 2004 | NAG | C3-C4-C5 | 2.71 | 115.08 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | S | 2004 | NAG | C2-N2-C7 | 2.67 | 126.71 | 122.90 |
| 10 | O | 2004 | NAG | O5-C5-C4 | 2.60 | 117.16 | 110.83 |
| 10 | P | 2001 | NAG | O3-C3-C2 | 2.52 | 114.68 | 109.47 |
| 10 | S | 2004 | NAG | C3-C4-C5 | 2.39 | 114.50 | 110.24 |
| 10 | S | 2004 | NAG | O5-C5-C4 | 2.35 | 116.54 | 110.83 |
| 10 | M | 2003 | NAG | O5-C5-C4 | 2.30 | 116.42 | 110.83 |
| 10 | A | 2004 | NAG | O5-C5-C4 | 2.25 | 116.31 | 110.83 |
| 10 | C | 2001 | NAG | O3-C3-C2 | 2.19 | 113.99 | 109.47 |
| 10 | P | 2001 | NAG | O4-C4-C5 | 2.17 | 114.70 | 109.30 |
| 10 | C | 2001 | NAG | C2-N2-C7 | 2.16 | 125.98 | 122.90 |
| 10 | O | 2004 | NAG | O3-C3-C4 | 2.11 | 115.23 | 110.35 |
| 10 | P | 2001 | NAG | C4-C3-C2 | 2.08 | 114.06 | 111.02 |
| 10 | A | 2004 | NAG | C8-C7-N2 | -2.07 | 112.60 | 116.10 |
| 10 | S | 2004 | NAG | O4-C4-C5 | -2.06 | 104.19 | 109.30 |
| 10 | P | 2001 | NAG | C8-C7-N2 | -2.05 | 112.63 | 116.10 |
| 10 | M | 2003 | NAG | C8-C7-N2 | -2.05 | 112.64 | 116.10 |
| 10 | A | 2004 | NAG | O4-C4-C3 | 2.03 | 115.04 | 110.35 |
| 10 | M | 2003 | NAG | O4-C4-C3 | 2.02 | 115.02 | 110.35 |
| 10 | A | 2004 | NAG | O4-C4-C5 | -2.01 | 104.30 | 109.30 |
| 10 | M | 2003 | NAG | O4-C4-C5 | -2.00 | 104.32 | 109.30 |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 10 | S | 2004 | NAG | O5-C5-C6-O6 |
| 10 | O | 2004 | NAG | O5-C5-C6-O6 |
| 10 | A | 2004 | NAG | O5-C5-C6-O6 |
| 10 | M | 2003 | NAG | O5-C5-C6-O6 |
| 10 | C | 2001 | NAG | C4-C5-C6-O6 |
| 10 | P | 2001 | NAG | O5-C5-C6-O6 |
| 10 | P | 2001 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 10 | P | 2001 | NAG | 2 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 322/334 (96%) | 0.71 | 30 (9%) 8 11 | 60, 90, 90, 90 | 0 |
| 1 | C | 321/334 (96%) | 0.84 | 44 (13%) 3 6 | 60, 90, 90, 90 | 0 |
| 1 | G | 321/334 (96%) | 0.80 | 38 (11%) 4 8 | 60, 90, 90, 90 | 0 |
| 1 | M | 322/334 (96%) | 0.71 | 32 (9%) 7 10 | 60, 90, 90, 90 | 0 |
| 1 | O | 318/334 (95%) | 0.90 | 47 (14%) 2 5 | 90, 90, 90, 90 | 0 |
| 1 | S | 322/334 (96%) | 0.69 | 37 (11%) 4 9 | 60, 90, 90, 90 | 0 |
| 2 | B | 172/182 (94%) | 0.36 | 10 (5%) 23 23 | 90, 90, 90, 90 | 0 |
| 2 | D | 172/182 (94%) | 0.49 | 13 (7%) 13 15 | 90, 90, 90, 90 | 0 |
| 2 | I | 173/182 (95%) | 0.97 | 21 (12%) 4 8 | 90, 90, 90, 90 | 0 |
| 2 | N | 169/182 (92%) | 0.57 | 14 (8%) 11 13 | 90, 90, 90, 90 | 0 |
| 2 | P | 172/182 (94%) | 0.49 | 7 (4%) 37 34 | 90, 90, 90, 90 | 0 |
| 2 | U | 173/182 (95%) | 0.29 | 5 (2%) 51 44 | 90, 90, 90, 90 | 0 |
| 3 | E | 216/218 (99%) | 1.17 | 44 (20%) 1 3 | 90, 90, 90, 90 | 0 |
| 3 | J | 211/218 (96%) | 1.02 | 32 (15%) 2 5 | 90, 90, 90, 90 | 0 |
| 3 | L | 215/218 (98%) | 0.68 | 23 (10%) 6 9 | 90, 90, 90, 90 | 0 |
| 3 | Q | 215/218 (98%) | 0.80 | 27 (12%) 3 8 | 90, 90, 90, 90 | 0 |
| 3 | V | 214/218 (98%) | 1.22 | 54 (25%) 0 2 | 90, 90, 90, 90 | 0 |
| 3 | X | 216/218 (99%) | 0.62 | 13 (6%) 21 21 | 90, 90, 90, 90 | 0 |
| 4 | F | 221/222 (99%) | 0.95 | 43 (19%) 1 3 | 90, 90, 90, 90 | 1 (0%) |
| 4 | H | 221/222 (99%) | 1.36 | 61 (27%) 0 2 | 90, 90, 90, 90 | 1 (0%) |
| 4 | K | 221/222 (99%) | 1.17 | 43 (19%) 1 3 | 90, 90, 90, 90 | 1 (0%) |
| 4 | R | 221/222 (99%) | 1.00 | 41 (18%) 1 4 | 90, 90, 90, 90 | 1 (0%) |
| 4 | T | 220/222 (99%) | 0.99 | 37 (16%) 1 4 | 90, 90, 90, 90 | 1 (0%) |
| 4 | W | 221/222 (99%) | 1.37 | 54 (24%) 0 2 | 90, 90, 90, 90 | 1 (0%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|
| All | All | 5569/5736 (97%) | 0.85 | 770 (13%) | 2 6 | 60, 90, 90, 90 | 6 (0%) |

All (770) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | W | 130 | ALA | 14.6 |
| 3 | E | 157 | ASN | 10.0 |
| 1 | C | 273 | GLU | 8.7 |
| 4 | W | 129 | ALA | 8.2 |
| 4 | W | 123 | PRO | 8.2 |
| 3 | J | 120 | PRO | 7.8 |
| 3 | E | 155 | ARG | 7.7 |
| 3 | E | 146 | VAL | 7.4 |
| 3 | V | 181 | LEU | 7.4 |
| 4 | K | 123 | PRO | 7.2 |
| 3 | V | 115 | VAL | 7.1 |
| 3 | E | 156 | GLN | 7.1 |
| 4 | W | 128 | SER | 6.8 |
| 1 | C | 60 | ILE | 6.6 |
| 4 | W | 223 | ILE | 6.5 |
| 3 | E | 145 | ASN | 6.4 |
| 4 | W | 227 | PRO | 6.4 |
| 4 | K | 227 | PRO | 6.4 |
| 3 | V | 116 | SER | 6.2 |
| 4 | H | 11 | LEU | 6.0 |
| 3 | V | 130 | ALA | 6.0 |
| 4 | K | 124 | LEU | 5.9 |
| 4 | T | 140 | LEU | 5.9 |
| 1 | C | 272 | LEU | 5.9 |
| 4 | W | 202 | PRO | 5.8 |
| 4 | K | 206 | VAL | 5.8 |
| 1 | S | 273 | GLU | 5.8 |
| 3 | V | 180 | THR | 5.8 |
| 1 | A | 273 | GLU | 5.7 |
| 4 | W | 121 | VAL | 5.7 |
| 1 | O | 60 | ILE | 5.7 |
| 3 | L | 200 | THR | 5.7 |
| 4 | H | 139 | THR | 5.5 |
| 4 | K | 205 | THR | 5.5 |
| 3 | J | 1 | ASP | 5.5 |
| 4 | K | 125 | ALA | 5.4 |
| 4 | W | 124 | LEU | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | W | 140 | LEU | 5.4 |
| 3 | E | 200 | THR | 5.4 |
| 4 | T | 206 | VAL | 5.3 |
| 1 | M | 317 | ALA | 5.3 |
| 3 | V | 135 | PHE | 5.1 |
| 3 | E | 113 | PRO | 5.1 |
| 1 | M | 273 | GLU | 5.1 |
| 2 | P | 62 | GLN | 5.0 |
| 3 | J | 119 | PRO | 5.0 |
| 1 | S | 60 | ILE | 5.0 |
| 4 | W | 203 | SER | 5.0 |
| 4 | T | 69 | LEU | 5.0 |
| 1 | C | 274 | TYR | 4.9 |
| 4 | W | 122 | TYR | 4.9 |
| 1 | O | 133(A) | SER | 4.9 |
| 4 | H | 130 | ALA | 4.9 |
| 4 | R | 69 | LEU | 4.8 |
| 1 | O | 98 | TYR | 4.8 |
| 1 | O | 103 | ASN | 4.8 |
| 4 | H | 168 | SER | 4.8 |
| 4 | W | 141 | GLY | 4.8 |
| 4 | H | 123 | PRO | 4.8 |
| 4 | H | 120 | SER | 4.7 |
| 1 | A | 317 | ALA | 4.7 |
| 2 | N | 62 | GLN | 4.7 |
| 4 | H | 227 | PRO | 4.7 |
| 4 | H | 121 | VAL | 4.7 |
| 1 | G | 273 | GLU | 4.6 |
| 4 | R | 71 | VAL | 4.6 |
| 1 | G | 312 | ASN | 4.6 |
| 1 | G | 289 | ASN | 4.6 |
| 3 | E | 115 | VAL | 4.5 |
| 4 | K | 226 | VAL | 4.5 |
| 1 | O | 311 | SER | 4.5 |
| 2 | N | 32 | SER | 4.5 |
| 4 | W | 126 | PRO | 4.5 |
| 3 | E | 27 | GLU | 4.5 |
| 4 | H | 124 | LEU | 4.5 |
| 4 | K | 202 | PRO | 4.5 |
| 4 | F | 30 | THR | 4.5 |
| 4 | T | 126 | PRO | 4.4 |
| 3 | Q | 79 | GLU | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | J | 27 | GLU | 4.4 |
| 4 | T | 139 | THR | 4.4 |
| 3 | V | 157 | ASN | 4.4 |
| 3 | E | 207 | LYS | 4.4 |
| 3 | Q | 110 | ASP | 4.3 |
| 3 | V | 182 | THR | 4.3 |
| 4 | H | 206 | VAL | 4.3 |
| 4 | R | 78 | ALA | 4.3 |
| 4 | H | 12 | VAL | 4.3 |
| 4 | H | 125 | ALA | 4.2 |
| 4 | W | 200 | TRP | 4.2 |
| 4 | T | 229 | ASP | 4.2 |
| 4 | T | 223 | ILE | 4.2 |
| 4 | W | 226 | VAL | 4.2 |
| 4 | T | 219 | VAL | 4.2 |
| 4 | R | 142 | CYS | 4.1 |
| 4 | T | 227 | PRO | 4.1 |
| 4 | K | 223 | ILE | 4.1 |
| 3 | V | 129 | GLY | 4.1 |
| 1 | O | 312 | ASN | 4.1 |
| 3 | V | 146 | VAL | 4.1 |
| 4 | R | 20 | MET | 4.1 |
| 3 | V | 15 | LEU | 4.1 |
| 4 | K | 228 | ARG | 4.1 |
| 4 | H | 226 | VAL | 4.0 |
| 4 | W | 204 | GLU | 4.0 |
| 1 | M | 153 | TRP | 4.0 |
| 4 | W | 125 | ALA | 4.0 |
| 4 | W | 127 | GLY | 4.0 |
| 1 | S | 98 | TYR | 4.0 |
| 1 | O | 318 | THR | 4.0 |
| 1 | O | 45 | LYS | 4.0 |
| 4 | H | 126 | PRO | 4.0 |
| 3 | Q | 19 | ALA | 4.0 |
| 2 | B | 32 | SER | 4.0 |
| 3 | V | 205 | ILE | 3.9 |
| 2 | N | 72 | ASN | 3.9 |
| 4 | K | 8 | GLY | 3.9 |
| 4 | F | 53 | ASN | 3.9 |
| 4 | F | 134 | THR | 3.9 |
| 4 | K | 141 | GLY | 3.9 |
| 4 | K | 142 | CYS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | W | 115 | LYS | 3.9 |
| 4 | H | 189 | SER | 3.9 |
| 4 | K | 126 | PRO | 3.9 |
| 4 | F | 114 | ALA | 3.9 |
| 4 | F | 126 | PRO | 3.9 |
| 4 | R | 140 | LEU | 3.9 |
| 4 | H | 223 | ILE | 3.8 |
| 1 | M | 210 | ASN | 3.8 |
| 4 | T | 67 | ALA | 3.8 |
| 4 | W | 139 | THR | 3.8 |
| 3 | V | 114 | THR | 3.8 |
| 4 | H | 166 | LEU | 3.8 |
| 4 | H | 112 | SER | 3.8 |
| 4 | H | 167 | SER | 3.8 |
| 1 | C | 61 | LEU | 3.8 |
| 3 | V | 16 | GLY | 3.8 |
| 3 | L | 201 | SER | 3.8 |
| 4 | K | 119 | PRO | 3.8 |
| 3 | Q | 2 | ILE | 3.8 |
| 4 | W | 221 | LYS | 3.8 |
| 4 | R | 70 | THR | 3.8 |
| 3 | E | 112 | ALA | 3.7 |
| 4 | T | 220 | ASP | 3.7 |
| 4 | T | 68 | THR | 3.7 |
| 2 | I | 23 | GLY | 3.7 |
| 3 | V | 131 | SER | 3.7 |
| 1 | C | 216 | GLU | 3.7 |
| 3 | Q | 131 | SER | 3.7 |
| 1 | O | 123 | ILE | 3.7 |
| 3 | E | 27(A) | SER | 3.7 |
| 4 | H | 141 | GLY | 3.7 |
| 3 | J | 132 | VAL | 3.7 |
| 2 | N | 19 | ASP | 3.7 |
| 4 | H | 71 | VAL | 3.7 |
| 2 | D | 68 | ARG | 3.6 |
| 1 | C | 276 | ASN | 3.6 |
| 4 | K | 188 | SER | 3.6 |
| 3 | V | 108 | ARG | 3.6 |
| 4 | R | 116 | THR | 3.6 |
| 3 | J | 207 | LYS | 3.6 |
| 3 | V | 107 | LYS | 3.6 |
| 1 | C | 51 | LEU | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | G | 103 | ASN | 3.6 |
| 4 | F | 135 | ASN | 3.6 |
| 1 | G | 15 | ILE | 3.6 |
| 4 | F | 11 | LEU | 3.6 |
| 1 | M | 318 | THR | 3.6 |
| 1 | M | 12 | GLN | 3.6 |
| 4 | T | 45 | LEU | 3.6 |
| 4 | T | 207 | THR | 3.6 |
| 4 | H | 114 | ALA | 3.6 |
| 1 | S | 9 | PRO | 3.5 |
| 2 | I | 72 | ASN | 3.5 |
| 1 | C | 88 | VAL | 3.5 |
| 4 | W | 230 | CYS | 3.5 |
| 1 | G | 290 | SER | 3.5 |
| 4 | W | 222 | LYS | 3.5 |
| 1 | O | 317 | ALA | 3.5 |
| 3 | E | 148 | TRP | 3.5 |
| 1 | G | 250 | ASN | 3.5 |
| 3 | E | 197 | THR | 3.5 |
| 4 | F | 127 | GLY | 3.5 |
| 3 | L | 202 | THR | 3.5 |
| 3 | J | 208 | SER | 3.5 |
| 3 | L | 113 | PRO | 3.4 |
| 1 | G | 51 | LEU | 3.4 |
| 2 | B | 33 | GLY | 3.4 |
| 4 | T | 44 | SER | 3.4 |
| 3 | E | 159 | VAL | 3.4 |
| 1 | M | 272 | LEU | 3.4 |
| 2 | I | 62 | GLN | 3.4 |
| 4 | R | 210 | VAL | 3.4 |
| 4 | W | 18 | VAL | 3.4 |
| 4 | W | 191 | VAL | 3.4 |
| 1 | O | 268 | MET | 3.4 |
| 1 | O | 61 | LEU | 3.4 |
| 1 | O | 159 | SER | 3.4 |
| 1 | M | 60 | ILE | 3.4 |
| 4 | F | 230 | CYS | 3.4 |
| 3 | Q | 78 | VAL | 3.4 |
| 4 | W | 45 | LEU | 3.4 |
| 1 | A | 147 | PHE | 3.4 |
| 4 | F | 133 | GLN | 3.4 |
| 2 | D | 67 | GLY | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | H | 113 | SER | 3.3 |
| 2 | I | 126 | LEU | 3.3 |
| 3 | V | 158 | GLY | 3.3 |
| 3 | E | 144 | ILE | 3.3 |
| 1 | O | 154 | LEU | 3.3 |
| 4 | T | 169 | GLY | 3.3 |
| 4 | H | 205 | THR | 3.3 |
| 4 | R | 114 | ALA | 3.3 |
| 3 | Q | 82 | ASP | 3.3 |
| 3 | V | 14 | SER | 3.3 |
| 4 | F | 124 | LEU | 3.3 |
| 3 | E | 158 | GLY | 3.3 |
| 3 | V | 134 | CYS | 3.3 |
| 3 | V | 159 | VAL | 3.3 |
| 1 | C | 62 | ARG | 3.3 |
| 2 | D | 62 | GLN | 3.3 |
| 2 | I | 158 | ASP | 3.3 |
| 4 | H | 119 | PRO | 3.3 |
| 3 | V | 109 | ALA | 3.3 |
| 3 | J | 27(A) | SER | 3.3 |
| 1 | C | 13 | ILE | 3.3 |
| 1 | M | 25 | GLN | 3.3 |
| 3 | V | 156 | GLN | 3.3 |
| 4 | H | 140 | LEU | 3.3 |
| 4 | W | 114 | ALA | 3.3 |
| 3 | Q | 11 | LEU | 3.3 |
| 4 | W | 143 | LEU | 3.3 |
| 2 | N | 65 | ALA | 3.3 |
| 4 | W | 219 | VAL | 3.3 |
| 4 | R | 143 | LEU | 3.3 |
| 4 | F | 223 | ILE | 3.3 |
| 4 | R | 139 | THR | 3.3 |
| 2 | B | 22 | TYR | 3.2 |
| 2 | D | 65 | ALA | 3.2 |
| 4 | T | 230 | CYS | 3.2 |
| 4 | T | 200 | TRP | 3.2 |
| 3 | J | 93 | GLU | 3.2 |
| 2 | N | 71 | ASN | 3.2 |
| 3 | Q | 50 | ARG | 3.2 |
| 4 | F | 20 | MET | 3.2 |
| 2 | P | 65 | ALA | 3.2 |
| 1 | G | 210 | ASN | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | G | 288 | ILE | 3.2 |
| 1 | S | 55 | ASN | 3.2 |
| 2 | B | 21 | TRP | 3.2 |
| 2 | P | 63 | PHE | 3.2 |
| 4 | F | 123 | PRO | 3.2 |
| 4 | W | 142 | CYS | 3.2 |
| 2 | I | 122 | VAL | 3.2 |
| 3 | E | 199 | LYS | 3.2 |
| 3 | V | 21 | ILE | 3.2 |
| 1 | O | 101 | ASP | 3.2 |
| 4 | T | 226 | VAL | 3.2 |
| 1 | C | 311 | SER | 3.2 |
| 4 | F | 52(A) | PRO | 3.2 |
| 3 | E | 196 | ALA | 3.2 |
| 1 | O | 153 | TRP | 3.2 |
| 4 | K | 113 | SER | 3.2 |
| 1 | O | 273 | GLU | 3.2 |
| 4 | W | 205 | THR | 3.2 |
| 4 | H | 142 | CYS | 3.2 |
| 3 | Q | 20 | THR | 3.2 |
| 4 | K | 222 | LYS | 3.2 |
| 4 | F | 71 | VAL | 3.1 |
| 4 | T | 191 | VAL | 3.1 |
| 3 | V | 47 | LEU | 3.1 |
| 1 | O | 127 | TRP | 3.1 |
| 4 | R | 218 | LYS | 3.1 |
| 1 | O | 158 | ASN | 3.1 |
| 1 | G | 60 | ILE | 3.1 |
| 1 | M | 39 | ALA | 3.1 |
| 4 | H | 222 | LYS | 3.1 |
| 4 | H | 202 | PRO | 3.1 |
| 1 | C | 267 | ILE | 3.1 |
| 3 | L | 2 | ILE | 3.1 |
| 3 | E | 111 | ALA | 3.1 |
| 3 | Q | 132 | VAL | 3.1 |
| 4 | H | 144 | VAL | 3.1 |
| 2 | I | 1 | GLY | 3.1 |
| 3 | Q | 33 | MET | 3.1 |
| 1 | O | 230 | MET | 3.1 |
| 4 | R | 34 | ILE | 3.1 |
| 3 | J | 146 | VAL | 3.1 |
| 4 | H | 191 | VAL | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | K | 229 | ASP | 3.1 |
| 1 | S | 86 | TYR | 3.1 |
| 4 | F | 73 | ARG | 3.1 |
| 4 | W | 100(B) | TYR | 3.1 |
| 1 | M | 51 | LEU | 3.1 |
| 4 | H | 133 | GLN | 3.1 |
| 4 | K | 134 | THR | 3.1 |
| 4 | H | 134 | THR | 3.0 |
| 1 | G | 9 | PRO | 3.0 |
| 3 | V | 120 | PRO | 3.0 |
| 4 | W | 133 | GLN | 3.0 |
| 3 | E | 25 | ALA | 3.0 |
| 1 | A | 313 | ARG | 3.0 |
| 4 | T | 152 | VAL | 3.0 |
| 3 | E | 194 | CYS | 3.0 |
| 1 | C | 178 | VAL | 3.0 |
| 3 | V | 204 | PRO | 3.0 |
| 1 | M | 211 | GLN | 3.0 |
| 1 | C | 214 | VAL | 3.0 |
| 3 | L | 104 | LEU | 3.0 |
| 3 | V | 128 | GLY | 3.0 |
| 1 | C | 89 | GLU | 3.0 |
| 2 | I | 71 | ASN | 3.0 |
| 3 | X | 212 | ASN | 3.0 |
| 2 | I | 157 | TYR | 2.9 |
| 2 | D | 122 | VAL | 2.9 |
| 4 | R | 113 | SER | 2.9 |
| 4 | F | 80 | MET | 2.9 |
| 1 | O | 55(A) | GLY | 2.9 |
| 1 | C | 297 | ILE | 2.9 |
| 1 | G | 254 | PRO | 2.9 |
| 3 | E | 57 | GLY | 2.9 |
| 4 | F | 206 | VAL | 2.9 |
| 4 | H | 188 | SER | 2.9 |
| 4 | H | 43 | LYS | 2.9 |
| 1 | C | 164 | ILE | 2.9 |
| 3 | V | 155 | ARG | 2.9 |
| 3 | V | 132 | VAL | 2.9 |
| 4 | R | 141 | GLY | 2.9 |
| 1 | A | 39 | ALA | 2.9 |
| 1 | C | 179 | LEU | 2.9 |
| 1 | O | 314 | LEU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | L | 21 | ILE | 2.9 |
| 3 | Q | 21 | ILE | 2.9 |
| 1 | A | 55(A) | GLY | 2.9 |
| 3 | J | 186 | TYR | 2.9 |
| 3 | J | 131 | SER | 2.9 |
| 1 | G | 101 | ASP | 2.9 |
| 3 | V | 1 | ASP | 2.9 |
| 4 | R | 126 | PRO | 2.9 |
| 1 | C | 312 | ASN | 2.9 |
| 1 | A | 10 | GLY | 2.9 |
| 2 | I | 35 | ALA | 2.9 |
| 3 | J | 148 | TRP | 2.9 |
| 4 | W | 217 | THR | 2.9 |
| 2 | D | 66 | VAL | 2.9 |
| 1 | S | 97 | CYS | 2.9 |
| 1 | A | 210 | ASN | 2.9 |
| 1 | C | 82 | VAL | 2.8 |
| 2 | I | 140 | PHE | 2.8 |
| 3 | E | 120 | PRO | 2.8 |
| 1 | S | 103 | ASN | 2.8 |
| 2 | B | 111 | HIS | 2.8 |
| 4 | H | 154 | VAL | 2.8 |
| 4 | R | 211 | ALA | 2.8 |
| 1 | O | 297 | ILE | 2.8 |
| 4 | H | 190 | SER | 2.8 |
| 4 | K | 191 | VAL | 2.8 |
| 4 | R | 51 | ILE | 2.8 |
| 3 | J | 154 | GLU | 2.8 |
| 1 | M | 315 | VAL | 2.8 |
| 1 | A | 316 | LEU | 2.8 |
| 2 | I | 63 | PHE | 2.8 |
| 2 | P | 71 | ASN | 2.8 |
| 3 | V | 179 | LEU | 2.8 |
| 4 | R | 154 | VAL | 2.8 |
| 4 | T | 78 | ALA | 2.8 |
| 4 | W | 82 | LEU | 2.8 |
| 4 | K | 196 | SER | 2.8 |
| 4 | H | 20 | MET | 2.8 |
| 1 | M | 313 | ARG | 2.8 |
| 3 | V | 178 | THR | 2.8 |
| 3 | J | 115 | VAL | 2.8 |
| 4 | F | 67 | ALA | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | U | 126 | LEU | 2.8 |
| 4 | T | 205 | THR | 2.8 |
| 3 | J | 206 | VAL | 2.8 |
| 4 | K | 152 | VAL | 2.8 |
| 4 | H | 179 | GLN | 2.8 |
| 1 | O | 59 | LEU | 2.8 |
| 2 | N | 16 | GLY | 2.8 |
| 2 | D | 136 | GLY | 2.7 |
| 4 | W | 109 | VAL | 2.7 |
| 2 | U | 64 | GLU | 2.7 |
| 4 | W | 192 | THR | 2.7 |
| 1 | M | 103 | ASN | 2.7 |
| 1 | G | 232 | PHE | 2.7 |
| 1 | O | 102 | PHE | 2.7 |
| 1 | O | 270 | SER | 2.7 |
| 4 | F | 34 | ILE | 2.7 |
| 4 | R | 112 | SER | 2.7 |
| 4 | R | 188 | SER | 2.7 |
| 4 | T | 188 | SER | 2.7 |
| 1 | A | 274 | TYR | 2.7 |
| 1 | O | 46 | THR | 2.7 |
| 4 | F | 183 | ASP | 2.7 |
| 1 | C | 58 | PRO | 2.7 |
| 1 | S | 78 | GLU | 2.7 |
| 3 | E | 192 | TYR | 2.7 |
| 4 | H | 110 | THR | 2.7 |
| 4 | H | 116 | THR | 2.7 |
| 2 | U | 62 | GLN | 2.7 |
| 3 | Q | 204 | PRO | 2.7 |
| 1 | G | 120 | LYS | 2.7 |
| 2 | N | 75 | ARG | 2.7 |
| 3 | E | 119 | PRO | 2.7 |
| 1 | C | 275 | GLY | 2.7 |
| 1 | M | 88 | VAL | 2.7 |
| 1 | M | 59 | LEU | 2.7 |
| 1 | S | 92 | SER | 2.6 |
| 2 | D | 132 | GLU | 2.6 |
| 3 | J | 118 | PHE | 2.6 |
| 4 | H | 152 | VAL | 2.6 |
| 3 | X | 100 | GLY | 2.6 |
| 4 | K | 200 | TRP | 2.6 |
| 1 | S | 176 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | L | 112 | ALA | 2.6 |
| 1 | S | 314 | LEU | 2.6 |
| 2 | N | 33 | GLY | 2.6 |
| 4 | R | 115 | LYS | 2.6 |
| 4 | W | 152 | VAL | 2.6 |
| 1 | A | 9 | PRO | 2.6 |
| 1 | A | 60 | ILE | 2.6 |
| 1 | C | 59 | LEU | 2.6 |
| 1 | G | 317 | ALA | 2.6 |
| 3 | V | 206 | VAL | 2.6 |
| 3 | L | 88 | CYS | 2.6 |
| 3 | J | 92 | ASN | 2.6 |
| 3 | J | 133 | VAL | 2.6 |
| 4 | T | 40 | SER | 2.6 |
| 1 | G | 251 | PHE | 2.6 |
| 3 | Q | 27(B) | VAL | 2.6 |
| 4 | F | 180 | SER | 2.6 |
| 1 | O | 77 | ASP | 2.6 |
| 2 | B | 62 | GLN | 2.6 |
| 1 | O | 313 | ARG | 2.6 |
| 3 | E | 121 | SER | 2.6 |
| 1 | A | 267 | ILE | 2.6 |
| 1 | C | 79 | PHE | 2.6 |
| 1 | S | 324 | PRO | 2.6 |
| 2 | I | 21 | TRP | 2.6 |
| 1 | O | 88 | VAL | 2.6 |
| 3 | L | 41 | GLY | 2.6 |
| 4 | F | 18 | VAL | 2.6 |
| 4 | R | 166 | LEU | 2.6 |
| 4 | K | 166 | LEU | 2.6 |
| 3 | X | 82 | ASP | 2.6 |
| 4 | H | 200 | TRP | 2.6 |
| 3 | E | 117 | ILE | 2.6 |
| 4 | K | 162 | ASN | 2.6 |
| 2 | P | 158 | ASP | 2.6 |
| 4 | H | 40 | SER | 2.6 |
| 1 | G | 212 | ARG | 2.6 |
| 1 | G | 282 | GLN | 2.6 |
| 1 | S | 61 | LEU | 2.6 |
| 3 | X | 202 | THR | 2.6 |
| 3 | V | 177 | SER | 2.6 |
| 1 | A | 289 | ASN | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | S | 138 | ALA | 2.6 |
| 3 | V | 89 | GLN | 2.6 |
| 2 | N | 58 | LYS | 2.6 |
| 4 | T | 192 | THR | 2.6 |
| 4 | W | 168 | SER | 2.6 |
| 2 | P | 7 | ALA | 2.5 |
| 1 | M | 168 | TYR | 2.5 |
| 3 | L | 44 | PRO | 2.5 |
| 3 | J | 181 | LEU | 2.5 |
| 3 | E | 41 | GLY | 2.5 |
| 3 | Q | 16 | GLY | 2.5 |
| 1 | A | 230 | MET | 2.5 |
| 1 | M | 101 | ASP | 2.5 |
| 3 | L | 115 | VAL | 2.5 |
| 3 | V | 154 | GLU | 2.5 |
| 1 | O | 39 | ALA | 2.5 |
| 3 | V | 117 | ILE | 2.5 |
| 4 | W | 110 | THR | 2.5 |
| 4 | R | 18 | VAL | 2.5 |
| 4 | T | 70 | THR | 2.5 |
| 4 | H | 115 | LYS | 2.5 |
| 1 | A | 148 | PHE | 2.5 |
| 4 | F | 125 | ALA | 2.5 |
| 1 | C | 301 | THR | 2.5 |
| 3 | Q | 197 | THR | 2.5 |
| 1 | M | 243 | ILE | 2.5 |
| 3 | V | 136 | LEU | 2.5 |
| 3 | V | 207 | LYS | 2.5 |
| 1 | C | 167 | SER | 2.5 |
| 2 | I | 152 | VAL | 2.5 |
| 3 | V | 149 | LYS | 2.5 |
| 1 | C | 45 | LYS | 2.5 |
| 3 | Q | 13 | VAL | 2.5 |
| 3 | J | 116 | SER | 2.5 |
| 3 | J | 27(B) | VAL | 2.5 |
| 1 | C | 254 | PRO | 2.5 |
| 1 | S | 58 | PRO | 2.5 |
| 1 | S | 210 | ASN | 2.5 |
| 4 | W | 113 | SER | 2.5 |
| 1 | G | 52 | CYS | 2.5 |
| 1 | A | 288 | ILE | 2.5 |
| 3 | X | 27(A) | SER | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 272 | LEU | 2.5 |
| 3 | V | 44 | PRO | 2.4 |
| 4 | K | 183 | ASP | 2.4 |
| 1 | C | 268 | MET | 2.4 |
| 2 | D | 134 | GLY | 2.4 |
| 1 | C | 210 | ASN | 2.4 |
| 3 | E | 147 | LYS | 2.4 |
| 1 | S | 312 | ASN | 2.4 |
| 1 | M | 154 | LEU | 2.4 |
| 1 | S | 137 | SER | 2.4 |
| 4 | K | 57 | THR | 2.4 |
| 4 | H | 127 | GLY | 2.4 |
| 1 | C | 180 | TRP | 2.4 |
| 1 | A | 66 | VAL | 2.4 |
| 1 | C | 9 | PRO | 2.4 |
| 4 | K | 9 | PRO | 2.4 |
| 4 | T | 141 | GLY | 2.4 |
| 1 | O | 104 | ASP | 2.4 |
| 3 | J | 196 | ALA | 2.4 |
| 4 | K | 143 | LEU | 2.4 |
| 1 | G | 268 | MET | 2.4 |
| 4 | H | 192 | THR | 2.4 |
| 4 | F | 122 | TYR | 2.4 |
| 4 | R | 196 | SER | 2.4 |
| 1 | C | 284 | PRO | 2.4 |
| 4 | T | 179 | GLN | 2.4 |
| 2 | N | 140 | PHE | 2.4 |
| 3 | J | 193 | THR | 2.4 |
| 1 | A | 55 | ASN | 2.4 |
| 1 | O | 263 | GLY | 2.4 |
| 1 | A | 314 | LEU | 2.4 |
| 1 | A | 153 | TRP | 2.4 |
| 1 | G | 306 | PRO | 2.4 |
| 4 | T | 228 | ARG | 2.4 |
| 4 | F | 210 | VAL | 2.4 |
| 3 | Q | 115 | VAL | 2.4 |
| 2 | N | 59 | MET | 2.4 |
| 3 | E | 179 | LEU | 2.3 |
| 3 | E | 181 | LEU | 2.3 |
| 4 | H | 143 | LEU | 2.3 |
| 4 | T | 114 | ALA | 2.3 |
| 3 | V | 194 | CYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | H | 13 | LYS | 2.3 |
| 1 | M | 26 | VAL | 2.3 |
| 3 | E | 198 | HIS | 2.3 |
| 2 | N | 55 | ILE | 2.3 |
| 4 | R | 111 | VAL | 2.3 |
| 1 | O | 293 | PRO | 2.3 |
| 1 | S | 254 | PRO | 2.3 |
| 4 | F | 110 | THR | 2.3 |
| 1 | O | 232 | PHE | 2.3 |
| 3 | V | 133 | VAL | 2.3 |
| 4 | W | 206 | VAL | 2.3 |
| 4 | F | 14 | PRO | 2.3 |
| 4 | K | 127 | GLY | 2.3 |
| 4 | F | 150 | GLU | 2.3 |
| 3 | E | 26 | SER | 2.3 |
| 4 | R | 128 | SER | 2.3 |
| 4 | T | 43 | LYS | 2.3 |
| 1 | C | 87 | ILE | 2.3 |
| 1 | C | 102 | PHE | 2.3 |
| 4 | F | 130 | ALA | 2.3 |
| 2 | D | 71 | ASN | 2.3 |
| 4 | F | 62 | LYS | 2.3 |
| 4 | F | 86 | ASP | 2.3 |
| 4 | W | 86 | ASP | 2.3 |
| 3 | X | 62 | PHE | 2.3 |
| 2 | D | 59 | MET | 2.3 |
| 3 | Q | 15 | LEU | 2.3 |
| 3 | V | 104 | LEU | 2.3 |
| 2 | I | 153 | LYS | 2.3 |
| 3 | X | 47 | LEU | 2.3 |
| 4 | R | 167 | SER | 2.3 |
| 2 | B | 72 | ASN | 2.3 |
| 4 | F | 112 | SER | 2.3 |
| 1 | O | 44 | GLU | 2.3 |
| 2 | P | 69 | GLU | 2.3 |
| 1 | S | 59 | LEU | 2.3 |
| 3 | L | 73 | LEU | 2.3 |
| 3 | J | 41 | GLY | 2.3 |
| 3 | Q | 66 | GLY | 2.3 |
| 4 | R | 127 | GLY | 2.3 |
| 1 | G | 150 | ASN | 2.3 |
| 1 | S | 153 | TRP | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | L | 42 | GLN | 2.3 |
| 3 | L | 86 | TYR | 2.3 |
| 2 | I | 68 | ARG | 2.3 |
| 3 | E | 78 | VAL | 2.3 |
| 1 | O | 264 | ASP | 2.3 |
| 4 | F | 69 | LEU | 2.3 |
| 1 | A | 178 | VAL | 2.3 |
| 1 | M | 245 | PHE | 2.3 |
| 3 | L | 40 | PRO | 2.3 |
| 1 | O | 179 | LEU | 2.2 |
| 4 | K | 140 | LEU | 2.2 |
| 4 | R | 67 | ALA | 2.2 |
| 3 | X | 157 | ASN | 2.2 |
| 4 | H | 44 | SER | 2.2 |
| 4 | H | 173 | THR | 2.2 |
| 1 | S | 96(A) | LEU | 2.2 |
| 4 | F | 143 | LEU | 2.2 |
| 4 | K | 221 | LYS | 2.2 |
| 3 | E | 186 | TYR | 2.2 |
| 4 | F | 82 | LEU | 2.2 |
| 1 | A | 96(A) | LEU | 2.2 |
| 1 | M | 268 | MET | 2.2 |
| 4 | R | 129 | ALA | 2.2 |
| 3 | E | 105 | GLU | 2.2 |
| 1 | G | 83 | PRO | 2.2 |
| 1 | O | 254 | PRO | 2.2 |
| 4 | W | 229 | ASP | 2.2 |
| 3 | Q | 31 | SER | 2.2 |
| 4 | H | 204 | GLU | 2.2 |
| 2 | B | 96 | ALA | 2.2 |
| 3 | E | 201 | SER | 2.2 |
| 3 | V | 106 | ILE | 2.2 |
| 4 | W | 96 | TYR | 2.2 |
| 3 | Q | 180 | THR | 2.2 |
| 1 | O | 178 | VAL | 2.2 |
| 1 | O | 294 | PHE | 2.2 |
| 1 | G | 88 | VAL | 2.2 |
| 1 | O | 99 | PRO | 2.2 |
| 1 | S | 178 | VAL | 2.2 |
| 4 | T | 11 | LEU | 2.2 |
| 1 | O | 310 | LYS | 2.2 |
| 1 | S | 271 | GLU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 275 | GLY | 2.2 |
| 1 | M | 13 | ILE | 2.2 |
| 4 | R | 133 | GLN | 2.2 |
| 4 | R | 124 | LEU | 2.2 |
| 1 | C | 66 | VAL | 2.2 |
| 4 | H | 103 | TRP | 2.2 |
| 1 | M | 98 | TYR | 2.2 |
| 2 | D | 96 | ALA | 2.2 |
| 2 | U | 71 | ASN | 2.2 |
| 3 | E | 55 | GLU | 2.2 |
| 4 | W | 8 | GLY | 2.2 |
| 3 | L | 15 | LEU | 2.2 |
| 1 | G | 211 | GLN | 2.2 |
| 2 | N | 20 | GLY | 2.2 |
| 3 | X | 16 | GLY | 2.2 |
| 4 | R | 1 | GLU | 2.2 |
| 1 | G | 230 | MET | 2.2 |
| 1 | G | 106 | GLU | 2.2 |
| 4 | K | 192 | THR | 2.2 |
| 4 | R | 45 | LEU | 2.2 |
| 3 | X | 119 | PRO | 2.2 |
| 1 | G | 172 | ASN | 2.2 |
| 4 | K | 207 | THR | 2.2 |
| 1 | G | 102 | PHE | 2.2 |
| 1 | S | 235 | THR | 2.2 |
| 3 | L | 16 | GLY | 2.2 |
| 4 | T | 42 | GLY | 2.2 |
| 1 | C | 200 | THR | 2.2 |
| 2 | D | 69 | GLU | 2.2 |
| 3 | X | 144 | ILE | 2.2 |
| 4 | R | 109 | VAL | 2.2 |
| 4 | R | 144 | VAL | 2.2 |
| 1 | S | 62 | ARG | 2.2 |
| 1 | C | 235 | THR | 2.2 |
| 1 | G | 267 | ILE | 2.2 |
| 1 | O | 131 | ASP | 2.2 |
| 3 | E | 132 | VAL | 2.2 |
| 4 | W | 134 | THR | 2.2 |
| 1 | A | 152 | VAL | 2.2 |
| 3 | E | 205 | ILE | 2.2 |
| 2 | I | 22 | TYR | 2.2 |
| 1 | S | 123 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | F | 128 | SER | 2.2 |
| 4 | T | 157 | TRP | 2.1 |
| 1 | S | 55(A) | GLY | 2.1 |
| 3 | X | 132 | VAL | 2.1 |
| 4 | H | 149 | PRO | 2.1 |
| 1 | C | 15 | ILE | 2.1 |
| 1 | M | 314 | LEU | 2.1 |
| 1 | O | 319 | GLY | 2.1 |
| 4 | W | 9 | PRO | 2.1 |
| 4 | W | 10 | GLU | 2.1 |
| 3 | L | 20 | THR | 2.1 |
| 4 | R | 217 | THR | 2.1 |
| 4 | K | 40 | SER | 2.1 |
| 2 | I | 96 | ALA | 2.1 |
| 3 | Q | 106 | ILE | 2.1 |
| 3 | L | 35 | TRP | 2.1 |
| 1 | G | 311 | SER | 2.1 |
| 1 | M | 167 | SER | 2.1 |
| 4 | H | 80 | MET | 2.1 |
| 1 | O | 135 | VAL | 2.1 |
| 1 | S | 237 | LEU | 2.1 |
| 3 | Q | 104 | LEU | 2.1 |
| 3 | L | 199 | LYS | 2.1 |
| 1 | S | 101 | ASP | 2.1 |
| 3 | V | 22 | SER | 2.1 |
| 1 | G | 215 | PRO | 2.1 |
| 4 | W | 144 | VAL | 2.1 |
| 1 | A | 211 | GLN | 2.1 |
| 3 | L | 102 | THR | 2.1 |
| 4 | H | 135 | ASN | 2.1 |
| 2 | I | 130 | ALA | 2.1 |
| 3 | J | 104 | LEU | 2.1 |
| 3 | J | 55 | GLU | 2.1 |
| 1 | O | 290 | SER | 2.1 |
| 1 | S | 88 | VAL | 2.1 |
| 3 | E | 122 | SER | 2.1 |
| 4 | H | 118 | PRO | 2.1 |
| 1 | M | 316 | LEU | 2.1 |
| 3 | V | 2 | ILE | 2.1 |
| 4 | H | 162 | ASN | 2.1 |
| 1 | M | 274 | TYR | 2.1 |
| 3 | V | 195 | GLU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 232 | PHE | 2.1 |
| 4 | K | 217 | THR | 2.1 |
| 4 | W | 112 | SER | 2.1 |
| 3 | J | 152 | GLY | 2.1 |
| 3 | J | 192 | TYR | 2.1 |
| 3 | J | 2 | ILE | 2.1 |
| 4 | F | 221 | LYS | 2.1 |
| 1 | S | 69 | TRP | 2.1 |
| 1 | G | 123 | ILE | 2.1 |
| 1 | S | 311 | SER | 2.1 |
| 3 | E | 104 | LEU | 2.1 |
| 4 | T | 71 | VAL | 2.1 |
| 1 | S | 102 | PHE | 2.1 |
| 2 | U | 72 | ASN | 2.1 |
| 3 | V | 90 | GLN | 2.1 |
| 4 | K | 208 | CYS | 2.1 |
| 3 | Q | 71 | PHE | 2.1 |
| 4 | F | 145 | LYS | 2.1 |
| 1 | M | 40 | GLN | 2.1 |
| 2 | B | 115 | VAL | 2.1 |
| 3 | V | 145 | ASN | 2.1 |
| 4 | K | 71 | VAL | 2.1 |
| 3 | V | 93 | GLU | 2.1 |
| 4 | K | 157 | TRP | 2.1 |
| 1 | C | 288 | ILE | 2.1 |
| 1 | G | 16 | GLY | 2.1 |
| 4 | H | 42 | GLY | 2.1 |
| 4 | F | 113 | SER | 2.1 |
| 1 | C | 215 | PRO | 2.0 |
| 4 | K | 117 | THR | 2.0 |
| 4 | F | 187 | LEU | 2.0 |
| 1 | S | 136 | SER | 2.0 |
| 2 | I | 24 | TYR | 2.0 |
| 1 | A | 112 | LEU | 2.0 |
| 3 | X | 143 | ASP | 2.0 |
| 4 | R | 110 | THR | 2.0 |
| 4 | H | 150 | GLU | 2.0 |
| 2 | B | 6 | ILE | 2.0 |
| 3 | L | 180 | THR | 2.0 |
| 4 | F | 188 | SER | 2.0 |
| 1 | M | 24 | GLU | 2.0 |
| 3 | Q | 113 | PRO | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | K | 139 | THR | 2.0 |
| 4 | W | 169 | GLY | 2.0 |
| 4 | W | 210 | VAL | 2.0 |
| 2 | I | 36 | ALA | 2.0 |
| 4 | H | 122 | TYR | 2.0 |
| 4 | T | 124 | LEU | 2.0 |
| 1 | G | 291 | SER | 2.0 |
| 1 | A | 179 | LEU | 2.0 |
| 1 | G | 151 | VAL | 2.0 |
| 1 | S | 291 | SER | 2.0 |
| 3 | V | 196 | ALA | 2.0 |
| 1 | A | 315 | VAL | 2.0 |
| 3 | J | 150 | ILE | 2.0 |
| 4 | K | 24 | THR | 2.0 |
| 3 | E | 73 | LEU | 2.0 |
| 3 | J | 125 | LEU | 2.0 |
| 3 | V | 110 | ASP | 2.0 |
| 4 | R | 7 | SER | 2.0 |
| 1 | C | 317 | ALA | 2.0 |

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

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

## 6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 5 | MAN | Y | 3 | 11/12 | 0.49 | 0.51 | 90,90,90,90 | 0 |
| 9 | MAN | e | 4 | 11/12 | 0.56 | 0.41 | 47,49,50,52 | 0 |
| 8 | BMA | b | 3 | 11/12 | 0.57 | 0.40 | 102,115,122,126 | 0 |
| 9 | NAG | e | 1 | 14/15 | 0.57 | 0.45 | 32,37,44,45 | 0 |
| 5 | MAN | d | 3 | 11/12 | 0.57 | 0.41 | 90,90,90,90 | 0 |
| 6 | MAN | Z | 6 | 11/12 | 0.59 | 0.28 | 90,90,90,90 | 0 |
| 5 | MAN | f | 3 | 11/12 | 0.66 | 0.23 | 90,90,90,90 | 0 |
| 6 | NAG | Z | 1 | 14/15 | 0.66 | 0.38 | 90,90,90,90 | 0 |
| 5 | NAG | Y | 2 | 14/15 | 0.66 | 0.51 | 90,90,90,90 | 0 |

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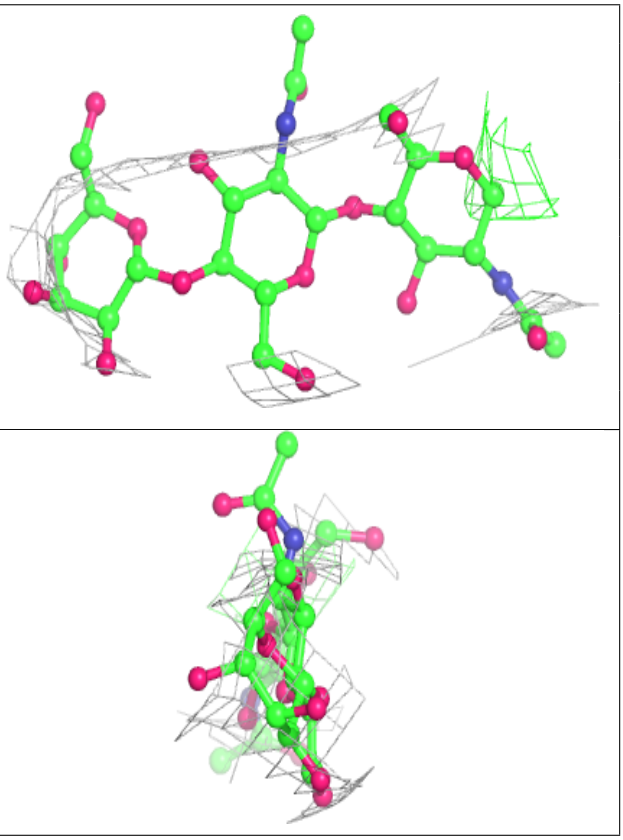
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 5 | NAG | f | 1 | 14/15 | 0.68 | 0.33 | 90,90,90,90 | 0 |
| 7 | NAG | a | 2 | 14/15 | 0.69 | 0.31 | 90,90,90,90 | 0 |
| 5 | NAG | d | 2 | 14/15 | 0.69 | 0.40 | 90,90,90,90 | 0 |
| 8 | NAG | b | 2 | 14/15 | 0.70 | 0.40 | 48,62,76,87 | 0 |
| 9 | BMA | e | 3 | 11/12 | 0.71 | 0.37 | 43,47,56,63 | 0 |
| 7 | NAG | c | 2 | 14/15 | 0.76 | 0.40 | 90,90,90,90 | 0 |
| 7 | NAG | a | 1 | 14/15 | 0.76 | 0.23 | 90,90,90,90 | 0 |
| 5 | NAG | f | 2 | 14/15 | 0.77 | 0.25 | 90,90,90,90 | 0 |
| 6 | NAG | Z | 2 | 14/15 | 0.77 | 0.32 | 90,90,90,90 | 0 |
| 6 | MAN | Z | 5 | 11/12 | 0.77 | 0.48 | 90,90,90,90 | 0 |
| 5 | NAG | d | 1 | 14/15 | 0.77 | 0.44 | 90,90,90,90 | 0 |
| 6 | MAN | Z | 8 | 11/12 | 0.78 | 0.32 | 90,90,90,90 | 0 |
| 5 | NAG | Y | 1 | 14/15 | 0.80 | 0.42 | 90,90,90,90 | 0 |
| 7 | NAG | c | 1 | 14/15 | 0.80 | 0.48 | 90,90,90,90 | 0 |
| 6 | MAN | Z | 4 | 11/12 | 0.83 | 0.31 | 90,90,90,90 | 0 |
| 9 | NAG | e | 2 | 14/15 | 0.83 | 0.41 | 37,38,39,42 | 0 |
| 6 | BMA | Z | 3 | 11/12 | 0.84 | 0.35 | 90,90,90,90 | 0 |
| 8 | NAG | b | 1 | 14/15 | 0.88 | 0.25 | 38,47,53,63 | 0 |
| 6 | MAN | Z | 7 | 11/12 | 0.91 | 0.35 | 90,90,90,90 | 0 |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

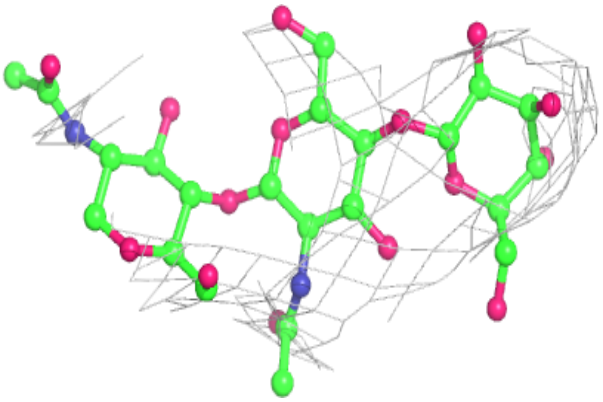
**Electron density around Chain Y:**

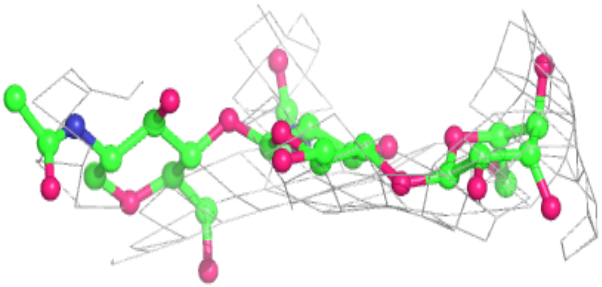
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

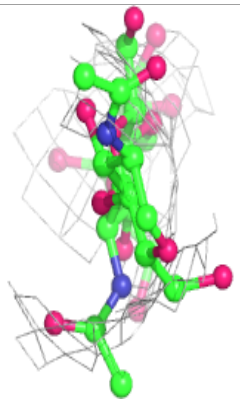


**Electron density around Chain d:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

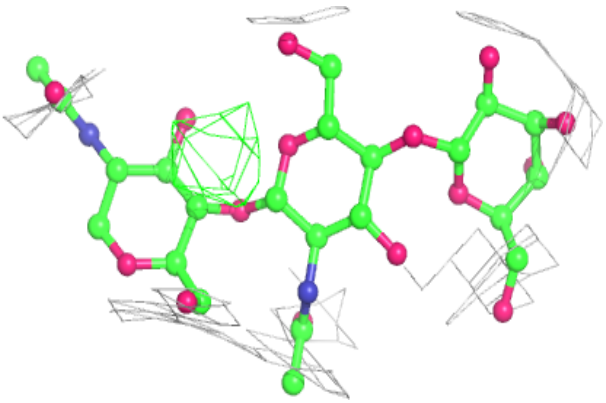


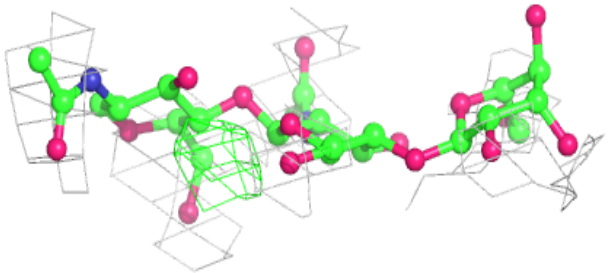


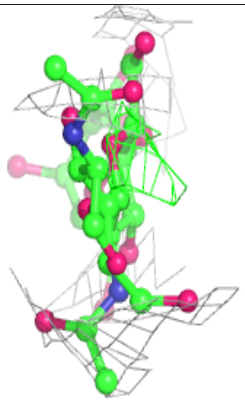


**Electron density around Chain f:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

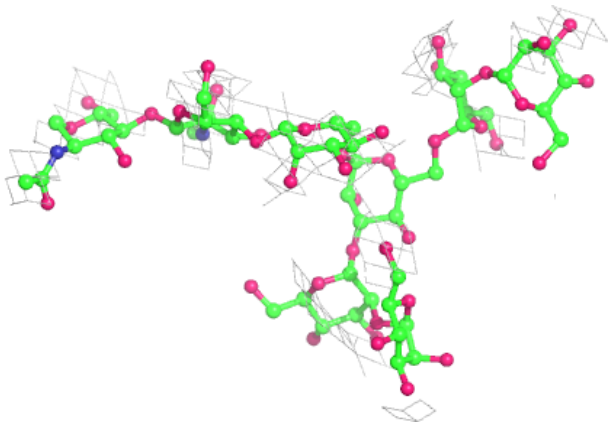


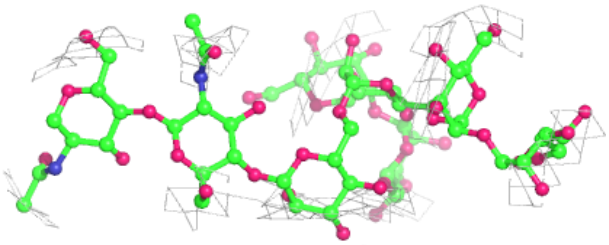


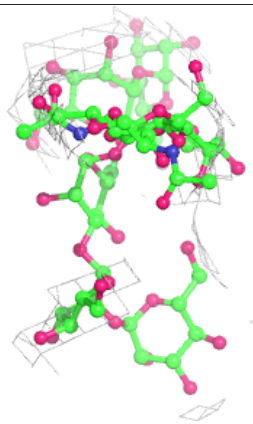


**Electron density around Chain Z:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

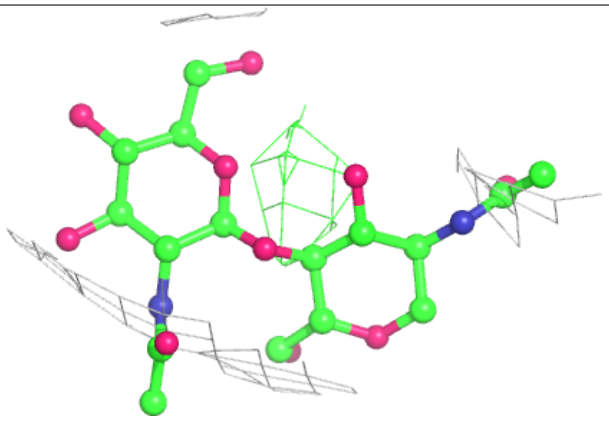


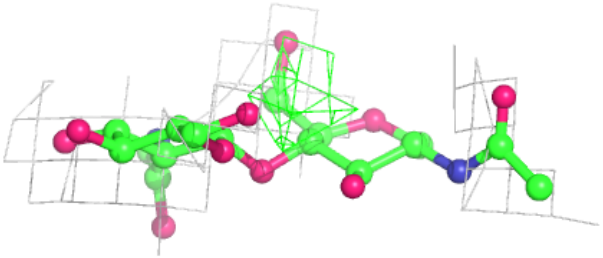


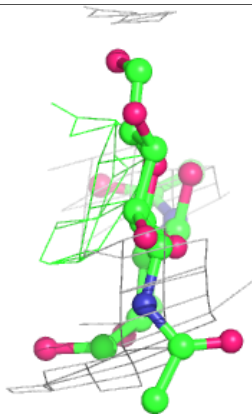


**Electron density around Chain a:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

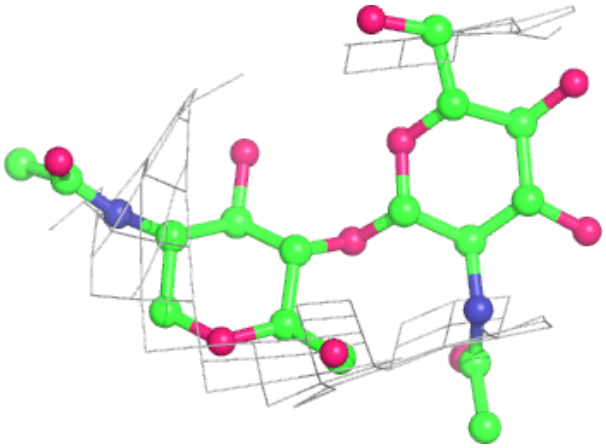


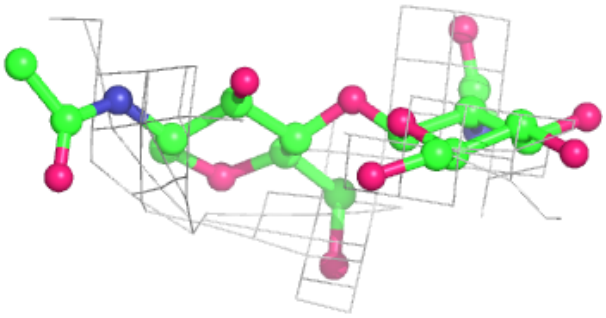


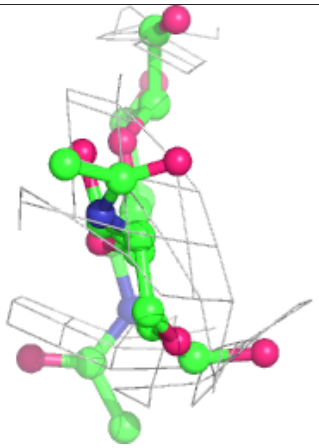


**Electron density around Chain c:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

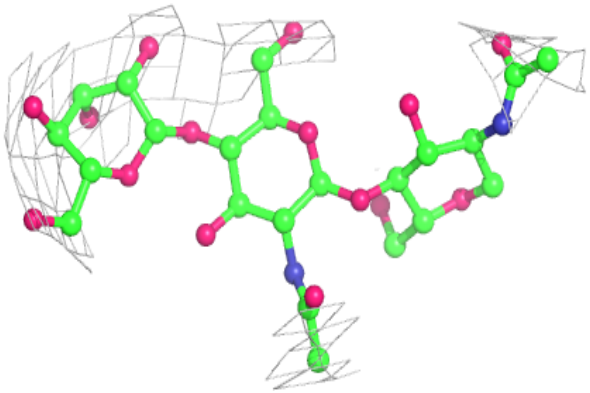


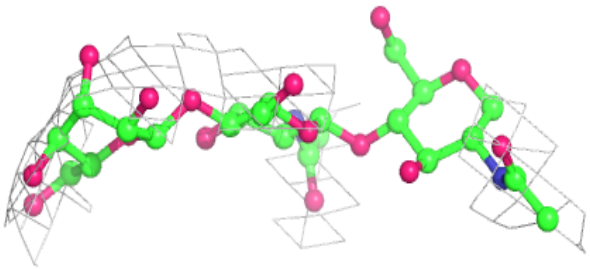


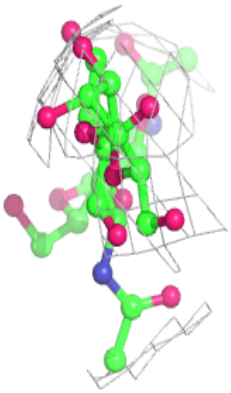


**Electron density around Chain b:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

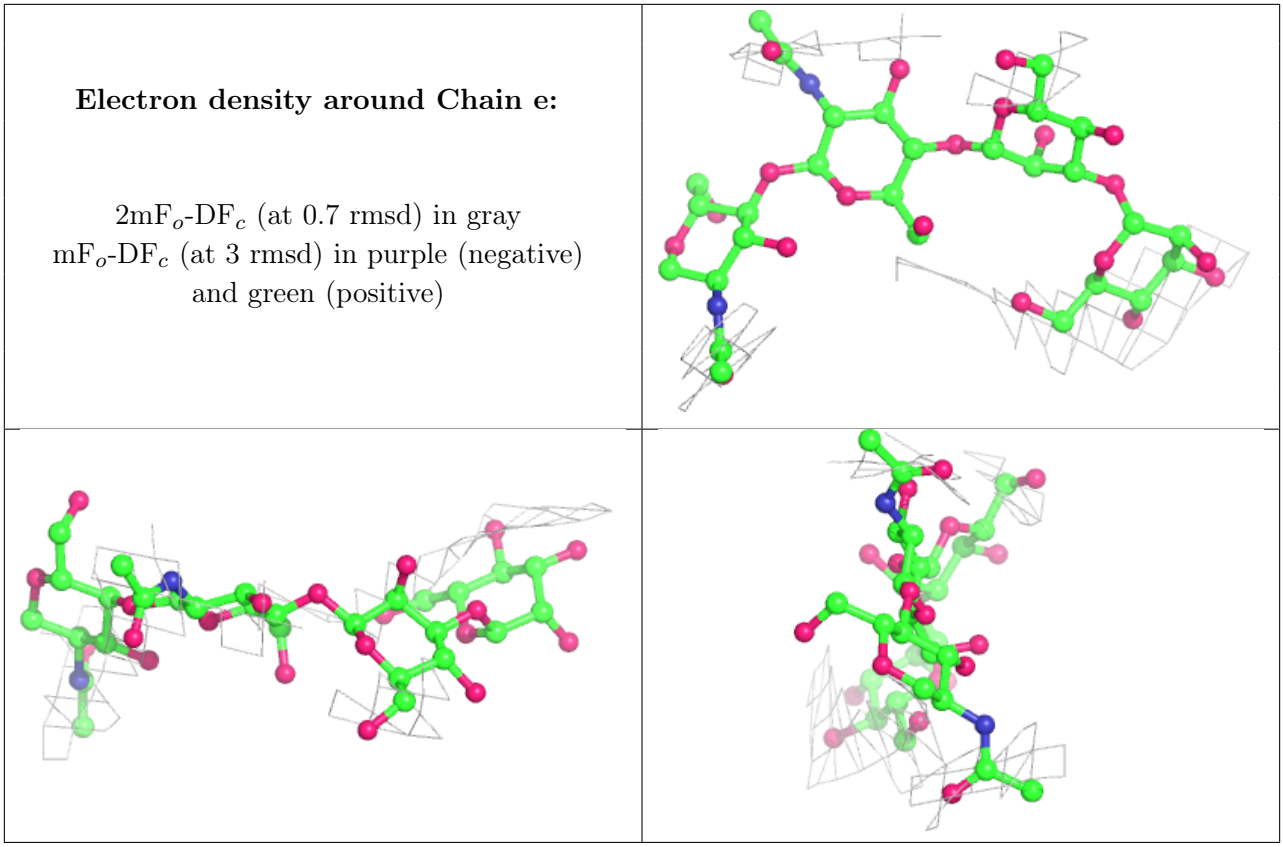






**Electron density around Chain e:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 10 | NAG | S | 2004 | 14/15 | 0.67 | 0.43 | 90,90,90,90 | 0 |
| 10 | NAG | M | 2003 | 14/15 | 0.68 | 0.40 | 90,90,90,90 | 0 |
| 10 | NAG | A | 2004 | 14/15 | 0.70 | 0.42 | 90,90,90,90 | 0 |
| 10 | NAG | P | 2001 | 14/15 | 0.73 | 0.43 | 90,90,90,90 | 0 |
| 10 | NAG | C | 2001 | 14/15 | 0.81 | 0.39 | 90,90,90,90 | 0 |
| 10 | NAG | O | 2004 | 14/15 | 0.87 | 0.24 | 90,90,90,90 | 0 |

## 6.5 Other polymers

There are no such residues in this entry.