



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 10:11 AM EDT

PDB ID : 6WEO
Title : IL-22 Signaling Complex with IL-22R1 and IL-10Rbeta
Authors : Saxton, R.A.; Jude, K.M.; Henneberg, L.T.; Garcia, K.C.
Deposited on : 2020-04-02
Resolution : 2.60 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 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 : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

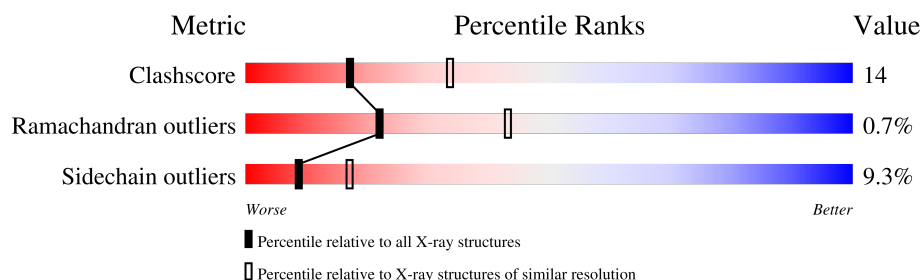
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 3518 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |


























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

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 0 | 204 | |
| 1 | 3 | 204 | |
| 1 | 6 | 204 | |
| 1 | 9 | 204 | |
| 1 | C | 204 | |
| 1 | E | 204 | |
| 1 | H | 204 | |
| 1 | K | 204 | |




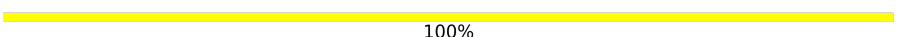
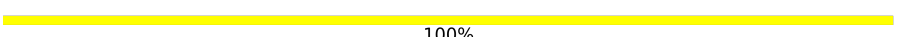

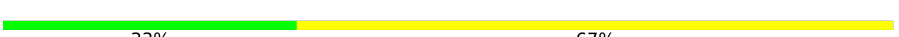

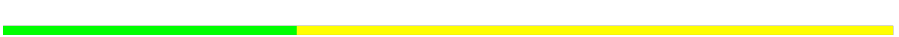

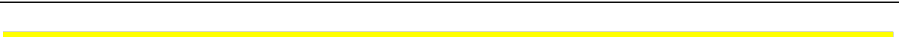
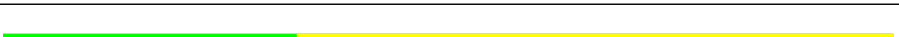

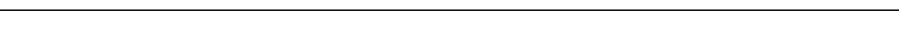
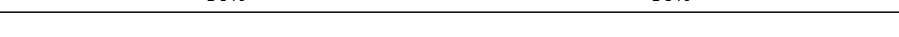
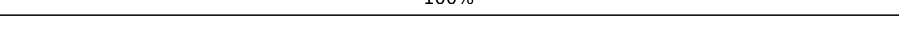
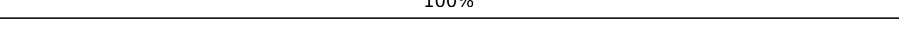
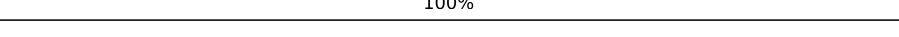
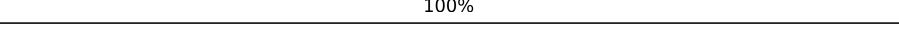
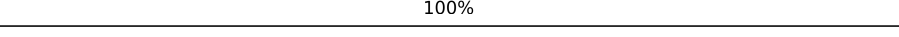





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | O | 204 |  |
| 1 | R | 204 |  |
| 1 | U | 204 |  |
| 1 | X | 204 |  |
| 2 | 1 | 204 |  |
| 2 | 4 | 204 |  |
| 2 | 7 | 204 |  |
| 2 | A | 204 |  |
| 2 | B | 204 |  |
| 2 | F | 204 |  |
| 2 | I | 204 |  |
| 2 | M | 204 |  |
| 2 | P | 204 |  |
| 2 | S | 204 |  |
| 2 | V | 204 |  |
| 2 | Y | 204 |  |
| 3 | 2 | 149 |  |
| 3 | 5 | 149 |  |
| 3 | 8 | 149 |  |
| 3 | D | 149 |  |
| 3 | G | 149 |  |
| 3 | J | 149 |  |
| 3 | L | 149 |  |
| 3 | N | 149 |  |
| 3 | Q | 149 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | T | 149 |  |
| 3 | W | 149 |  |
| 3 | Z | 149 |  |
| 4 | a | 4 |  |
| 4 | c | 4 |  |
| 4 | n | 4 |  |
| 5 | b | 3 |  |
| 5 | e | 3 |  |
| 5 | i | 3 |  |
| 5 | j | 3 |  |
| 5 | l | 3 |  |
| 5 | m | 3 |  |
| 5 | s | 3 |  |
| 6 | d | 2 |  |
| 6 | o | 2 |  |
| 6 | p | 2 |  |
| 6 | r | 2 |  |
| 6 | t | 2 |  |
| 6 | u | 2 |  |
| 6 | v | 2 |  |
| 7 | f | 2 |  |
| 8 | g | 3 |  |
| 9 | h | 5 |  |
| 9 | k | 5 |  |
| 10 | q | 2 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 11 | w | 3 |  33% 67% |

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 53140 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 Interleukin-10 receptor subunit beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | 0 | 193 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1579 | 1007 | 261 | 303 | 8 | | | |
| 1 | 3 | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1595 | 1016 | 263 | 308 | 8 | | | |
| 1 | 6 | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1607 | 1024 | 266 | 309 | 8 | | | |
| 1 | 9 | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1532 | 980 | 254 | 290 | 8 | | | |
| 1 | C | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1614 | 1026 | 270 | 310 | 8 | | | |
| 1 | E | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1593 | 1014 | 263 | 308 | 8 | | | |
| 1 | H | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1602 | 1021 | 264 | 309 | 8 | | | |
| 1 | K | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1022 | 267 | 308 | 8 | | | |
| 1 | O | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1025 | 268 | 308 | 8 | | | |
| 1 | R | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1611 | 1025 | 269 | 309 | 8 | | | |
| 1 | U | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1603 | 1020 | 266 | 309 | 8 | | | |
| 1 | X | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1619 | 1031 | 269 | 311 | 8 | | | |

There are 84 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| 0 | 49 | GLN | ASN | conflict | UNP Q61190 |
| 0 | 102 | GLN | ASN | conflict | UNP Q61190 |
| 0 | 161 | GLN | ASN | conflict | UNP Q61190 |
| 0 | 199 | GLN | ASN | conflict | UNP Q61190 |
| 0 | 221 | GLY | - | expression tag | UNP Q61190 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| 0 | 222 | GLY | - | expression tag | UNP Q61190 |
| 0 | 223 | SER | - | expression tag | UNP Q61190 |
| 3 | 49 | GLN | ASN | conflict | UNP Q61190 |
| 3 | 102 | GLN | ASN | conflict | UNP Q61190 |
| 3 | 161 | GLN | ASN | conflict | UNP Q61190 |
| 3 | 199 | GLN | ASN | conflict | UNP Q61190 |
| 3 | 221 | GLY | - | expression tag | UNP Q61190 |
| 3 | 222 | GLY | - | expression tag | UNP Q61190 |
| 3 | 223 | SER | - | expression tag | UNP Q61190 |
| 6 | 49 | GLN | ASN | conflict | UNP Q61190 |
| 6 | 102 | GLN | ASN | conflict | UNP Q61190 |
| 6 | 161 | GLN | ASN | conflict | UNP Q61190 |
| 6 | 199 | GLN | ASN | conflict | UNP Q61190 |
| 6 | 221 | GLY | - | expression tag | UNP Q61190 |
| 6 | 222 | GLY | - | expression tag | UNP Q61190 |
| 6 | 223 | SER | - | expression tag | UNP Q61190 |
| 9 | 49 | GLN | ASN | conflict | UNP Q61190 |
| 9 | 102 | GLN | ASN | conflict | UNP Q61190 |
| 9 | 161 | GLN | ASN | conflict | UNP Q61190 |
| 9 | 199 | GLN | ASN | conflict | UNP Q61190 |
| 9 | 221 | GLY | - | expression tag | UNP Q61190 |
| 9 | 222 | GLY | - | expression tag | UNP Q61190 |
| 9 | 223 | SER | - | expression tag | UNP Q61190 |
| C | 49 | GLN | ASN | conflict | UNP Q61190 |
| C | 102 | GLN | ASN | conflict | UNP Q61190 |
| C | 161 | GLN | ASN | conflict | UNP Q61190 |
| C | 199 | GLN | ASN | conflict | UNP Q61190 |
| C | 221 | GLY | - | expression tag | UNP Q61190 |
| C | 222 | GLY | - | expression tag | UNP Q61190 |
| C | 223 | SER | - | expression tag | UNP Q61190 |
| E | 49 | GLN | ASN | conflict | UNP Q61190 |
| E | 102 | GLN | ASN | conflict | UNP Q61190 |
| E | 161 | GLN | ASN | conflict | UNP Q61190 |
| E | 199 | GLN | ASN | conflict | UNP Q61190 |
| E | 221 | GLY | - | expression tag | UNP Q61190 |
| E | 222 | GLY | - | expression tag | UNP Q61190 |
| E | 223 | SER | - | expression tag | UNP Q61190 |
| H | 49 | GLN | ASN | conflict | UNP Q61190 |
| H | 102 | GLN | ASN | conflict | UNP Q61190 |
| H | 161 | GLN | ASN | conflict | UNP Q61190 |
| H | 199 | GLN | ASN | conflict | UNP Q61190 |
| H | 221 | GLY | - | expression tag | UNP Q61190 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| H | 222 | GLY | - | expression tag | UNP Q61190 |
| H | 223 | SER | - | expression tag | UNP Q61190 |
| K | 49 | GLN | ASN | conflict | UNP Q61190 |
| K | 102 | GLN | ASN | conflict | UNP Q61190 |
| K | 161 | GLN | ASN | conflict | UNP Q61190 |
| K | 199 | GLN | ASN | conflict | UNP Q61190 |
| K | 221 | GLY | - | expression tag | UNP Q61190 |
| K | 222 | GLY | - | expression tag | UNP Q61190 |
| K | 223 | SER | - | expression tag | UNP Q61190 |
| O | 49 | GLN | ASN | conflict | UNP Q61190 |
| O | 102 | GLN | ASN | conflict | UNP Q61190 |
| O | 161 | GLN | ASN | conflict | UNP Q61190 |
| O | 199 | GLN | ASN | conflict | UNP Q61190 |
| O | 221 | GLY | - | expression tag | UNP Q61190 |
| O | 222 | GLY | - | expression tag | UNP Q61190 |
| O | 223 | SER | - | expression tag | UNP Q61190 |
| R | 49 | GLN | ASN | conflict | UNP Q61190 |
| R | 102 | GLN | ASN | conflict | UNP Q61190 |
| R | 161 | GLN | ASN | conflict | UNP Q61190 |
| R | 199 | GLN | ASN | conflict | UNP Q61190 |
| R | 221 | GLY | - | expression tag | UNP Q61190 |
| R | 222 | GLY | - | expression tag | UNP Q61190 |
| R | 223 | SER | - | expression tag | UNP Q61190 |
| U | 49 | GLN | ASN | conflict | UNP Q61190 |
| U | 102 | GLN | ASN | conflict | UNP Q61190 |
| U | 161 | GLN | ASN | conflict | UNP Q61190 |
| U | 199 | GLN | ASN | conflict | UNP Q61190 |
| U | 221 | GLY | - | expression tag | UNP Q61190 |
| U | 222 | GLY | - | expression tag | UNP Q61190 |
| U | 223 | SER | - | expression tag | UNP Q61190 |
| X | 49 | GLN | ASN | conflict | UNP Q61190 |
| X | 102 | GLN | ASN | conflict | UNP Q61190 |
| X | 161 | GLN | ASN | conflict | UNP Q61190 |
| X | 199 | GLN | ASN | conflict | UNP Q61190 |
| X | 221 | GLY | - | expression tag | UNP Q61190 |
| X | 222 | GLY | - | expression tag | UNP Q61190 |
| X | 223 | SER | - | expression tag | UNP Q61190 |

- Molecule 2 is a protein called Interleukin-22 receptor subunit alpha-1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | 1 | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1613 | 1032 | 270 | 303 | 8 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | 4 | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1610 | 1030 | 269 | 303 | 8 | | | |
| 2 | 7 | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1604 | 1027 | 266 | 303 | 8 | | | |
| 2 | A | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1026 | 268 | 303 | 8 | | | |
| 2 | B | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1029 | 269 | 303 | 8 | | | |
| 2 | F | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1608 | 1030 | 267 | 303 | 8 | | | |
| 2 | I | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1614 | 1032 | 269 | 305 | 8 | | | |
| 2 | M | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1029 | 265 | 303 | 8 | | | |
| 2 | P | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1621 | 1037 | 271 | 305 | 8 | | | |
| 2 | S | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1617 | 1035 | 271 | 303 | 8 | | | |
| 2 | V | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1611 | 1032 | 268 | 303 | 8 | | | |
| 2 | Y | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1610 | 1032 | 265 | 305 | 8 | | | |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| 1 | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| 1 | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| 1 | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| 1 | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| 1 | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| 1 | 227 | SER | - | expression tag | UNP Q80XZ4 |
| 4 | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| 4 | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| 4 | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| 4 | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| 4 | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| 4 | 227 | SER | - | expression tag | UNP Q80XZ4 |
| 7 | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| 7 | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| 7 | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| 7 | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| 7 | 226 | GLY | - | expression tag | UNP Q80XZ4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| 7 | 227 | SER | - | expression tag | UNP Q80XZ4 |
| A | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| A | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| A | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| A | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| A | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| A | 227 | SER | - | expression tag | UNP Q80XZ4 |
| B | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| B | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| B | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| B | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| B | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| B | 227 | SER | - | expression tag | UNP Q80XZ4 |
| F | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| F | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| F | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| F | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| F | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| F | 227 | SER | - | expression tag | UNP Q80XZ4 |
| I | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| I | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| I | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| I | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| I | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| I | 227 | SER | - | expression tag | UNP Q80XZ4 |
| M | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| M | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| M | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| M | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| M | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| M | 227 | SER | - | expression tag | UNP Q80XZ4 |
| P | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| P | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| P | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| P | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| P | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| P | 227 | SER | - | expression tag | UNP Q80XZ4 |
| S | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| S | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| S | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| S | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| S | 226 | GLY | - | expression tag | UNP Q80XZ4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| S | 227 | SER | - | expression tag | UNP Q80XZ4 |
| V | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| V | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| V | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| V | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| V | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| V | 227 | SER | - | expression tag | UNP Q80XZ4 |
| Y | 80 | ASP | ASN | conflict | UNP Q80XZ4 |
| Y | 87 | ASP | ASN | conflict | UNP Q80XZ4 |
| Y | 89 | GLN | THR | conflict | UNP Q80XZ4 |
| Y | 225 | GLY | - | expression tag | UNP Q80XZ4 |
| Y | 226 | GLY | - | expression tag | UNP Q80XZ4 |
| Y | 227 | SER | - | expression tag | UNP Q80XZ4 |

- Molecule 3 is a protein called Interleukin-22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | 2 | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1096 | 700 | 186 | 202 | 8 | | | |
| 3 | 5 | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1126 | 715 | 197 | 206 | 8 | | | |
| 3 | 8 | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1107 | 704 | 191 | 204 | 8 | | | |
| 3 | D | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 718 | 198 | 207 | 8 | | | |
| 3 | G | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1123 | 715 | 196 | 204 | 8 | | | |
| 3 | J | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 711 | 193 | 205 | 8 | | | |
| 3 | L | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1125 | 716 | 195 | 206 | 8 | | | |
| 3 | N | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1093 | 695 | 187 | 203 | 8 | | | |
| 3 | Q | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1120 | 713 | 191 | 208 | 8 | | | |
| 3 | T | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 720 | 196 | 209 | 8 | | | |
| 3 | W | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1124 | 714 | 195 | 207 | 8 | | | |
| 3 | Z | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 718 | 197 | 206 | 8 | | | |

There are 120 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| 2 | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| 2 | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| 2 | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| 2 | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| 2 | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| 2 | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| 2 | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| 2 | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| 2 | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| 2 | 182 | SER | - | expression tag | UNP Q9JJY9 |
| 5 | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| 5 | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| 5 | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| 5 | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| 5 | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| 5 | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| 5 | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| 5 | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| 5 | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| 5 | 182 | SER | - | expression tag | UNP Q9JJY9 |
| 8 | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| 8 | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| 8 | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| 8 | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| 8 | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| 8 | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| 8 | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| 8 | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| 8 | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| 8 | 182 | SER | - | expression tag | UNP Q9JJY9 |
| D | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| D | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| D | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| D | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| D | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| D | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| D | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| D | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| D | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| D | 182 | SER | - | expression tag | UNP Q9JJY9 |
| G | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| G | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| G | 49 | SER | GLN | conflict | UNP Q9JJY9 |

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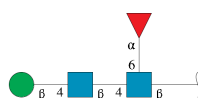
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| G | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| G | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| G | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| G | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| G | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| G | 182 | SER | - | expression tag | UNP Q9JJY9 |
| J | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| J | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| J | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| J | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| J | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| J | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| J | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| J | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| J | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| J | 182 | SER | - | expression tag | UNP Q9JJY9 |
| L | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| L | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| L | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| L | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| L | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| L | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| L | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| L | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| L | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| L | 182 | SER | - | expression tag | UNP Q9JJY9 |
| N | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| N | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| N | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| N | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| N | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| N | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| N | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| N | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| N | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| N | 182 | SER | - | expression tag | UNP Q9JJY9 |
| Q | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| Q | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| Q | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| Q | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| Q | 97 | GLN | ASN | conflict | UNP Q9JJY9 |

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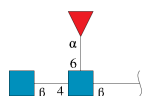
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Q | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| Q | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| Q | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| Q | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| Q | 182 | SER | - | expression tag | UNP Q9JJY9 |
| T | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| T | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| T | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| T | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| T | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| T | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| T | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| T | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| T | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| T | 182 | SER | - | expression tag | UNP Q9JJY9 |
| W | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| W | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| W | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| W | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| W | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| W | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| W | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| W | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| W | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| W | 182 | SER | - | expression tag | UNP Q9JJY9 |
| Z | 43 | HIS | GLU | conflict | UNP Q9JJY9 |
| Z | 45 | ARG | SER | conflict | UNP Q9JJY9 |
| Z | 49 | SER | GLN | conflict | UNP Q9JJY9 |
| Z | 68 | GLN | ASN | conflict | UNP Q9JJY9 |
| Z | 97 | GLN | ASN | conflict | UNP Q9JJY9 |
| Z | 116 | TRP | GLN | conflict | UNP Q9JJY9 |
| Z | 128 | LYS | GLN | conflict | UNP Q9JJY9 |
| Z | 180 | GLY | - | expression tag | UNP Q9JJY9 |
| Z | 181 | GLY | - | expression tag | UNP Q9JJY9 |
| Z | 182 | SER | - | expression tag | UNP Q9JJY9 |

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



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4 | a | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 49 | 28 | 2 | 19 | | | |
| 4 | c | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 49 | 28 | 2 | 19 | | | |
| 4 | n | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 49 | 28 | 2 | 19 | | | |

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5 | b | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 38 | 22 | 2 | 14 | | | |
| 5 | e | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 38 | 22 | 2 | 14 | | | |
| 5 | i | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 38 | 22 | 2 | 14 | | | |
| 5 | j | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 38 | 22 | 2 | 14 | | | |
| 5 | l | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 38 | 22 | 2 | 14 | | | |
| 5 | m | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 38 | 22 | 2 | 14 | | | |
| 5 | s | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 38 | 22 | 2 | 14 | | | |

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|---------|-------|
| 6 | d | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |
| 6 | o | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |

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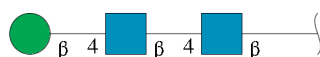
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|---------|-------|
| 6 | p | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |
| 6 | r | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |
| 6 | t | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |
| 6 | u | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |
| 6 | v | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



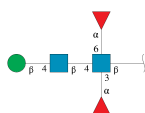
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|---------|-------|
| 7 | f | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 24 | 14 | 1 | 9 | | | |

- 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 | g | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



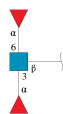
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 9 | h | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 59 | 34 | 2 | 23 | | | |
| 9 | k | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 59 | 34 | 2 | 23 | | | |

- Molecule 10 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 |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 10 | q | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 11 | w | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 34 | 20 | 1 | 13 | | | |

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 12 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 12 | H | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 12 | J | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 12 | K | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 12 | M | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 12 | O | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 12 | Y | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 13 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

- Molecule 14 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14 | 1 | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 14 | 2 | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 14 | 3 | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 14 | 4 | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 14 | 5 | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 14 | 6 | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 14 | 7 | 12 | Total | O | 0 | 0 |
| | | | 12 | 12 | | |
| 14 | 8 | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 14 | 9 | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 14 | A | 22 | Total | O | 0 | 0 |
| | | | 22 | 22 | | |
| 14 | B | 16 | Total | O | 0 | 0 |
| | | | 16 | 16 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 14 | C | 22 | Total O 22 22 | 0 | 0 |
| 14 | D | 14 | Total O 14 14 | 0 | 0 |
| 14 | E | 15 | Total O 15 15 | 0 | 0 |
| 14 | F | 10 | Total O 10 10 | 0 | 0 |
| 14 | G | 5 | Total O 5 5 | 0 | 0 |
| 14 | H | 17 | Total O 17 17 | 0 | 0 |
| 14 | I | 9 | Total O 9 9 | 0 | 0 |
| 14 | J | 6 | Total O 6 6 | 0 | 0 |
| 14 | K | 9 | Total O 9 9 | 0 | 0 |
| 14 | L | 8 | Total O 8 8 | 0 | 0 |
| 14 | M | 8 | Total O 8 8 | 0 | 0 |
| 14 | N | 5 | Total O 5 5 | 0 | 0 |
| 14 | O | 14 | Total O 14 14 | 0 | 0 |
| 14 | P | 6 | Total O 6 6 | 0 | 0 |
| 14 | Q | 7 | Total O 7 7 | 0 | 0 |
| 14 | R | 9 | Total O 9 9 | 0 | 0 |
| 14 | S | 13 | Total O 13 13 | 0 | 0 |
| 14 | T | 6 | Total O 6 6 | 0 | 0 |
| 14 | U | 14 | Total O 14 14 | 0 | 0 |
| 14 | V | 12 | Total O 12 12 | 0 | 0 |
| 14 | W | 1 | Total O 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 14 | X | 11 | Total 11 | O 11 | 0 | 0 |
| 14 | Y | 20 | Total 20 | O 20 | 0 | 0 |
| 14 | Z | 5 | Total 5 | O 5 | 0 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

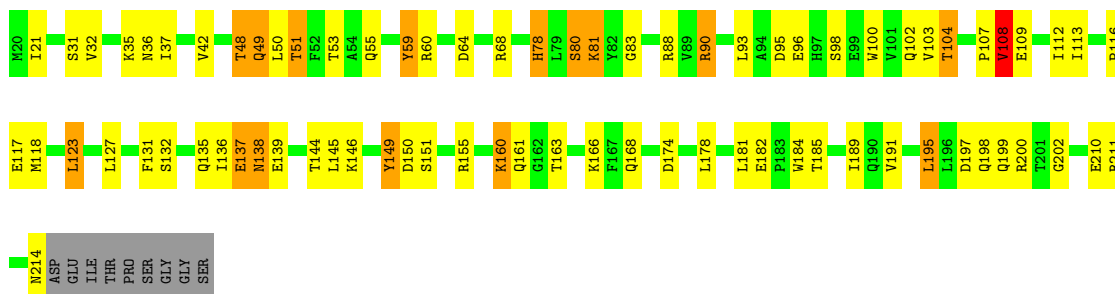
- Molecule 1: Interleukin-10 receptor subunit beta

Chain 0: 



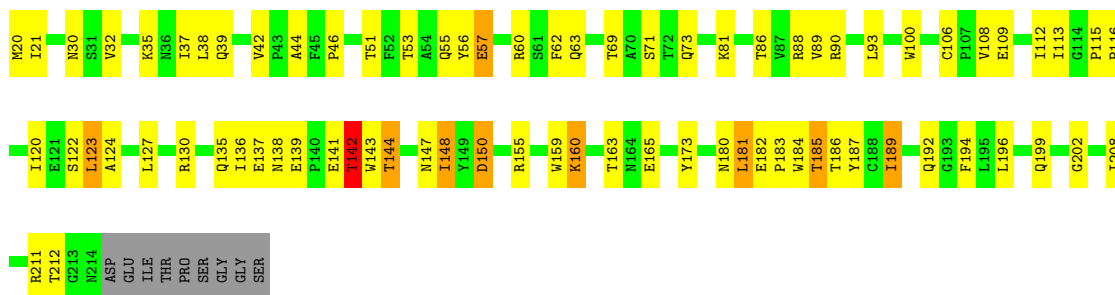
- Molecule 1: Interleukin-10 receptor subunit beta

Chain 3: 

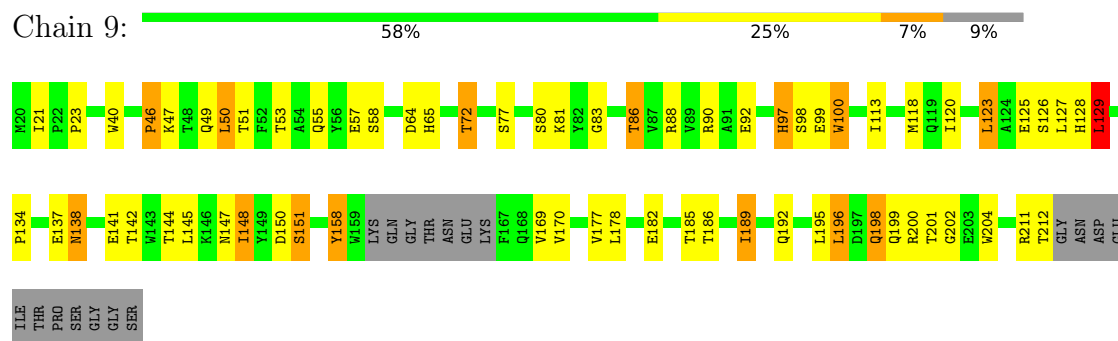


- Molecule 1: Interleukin-10 receptor subunit beta

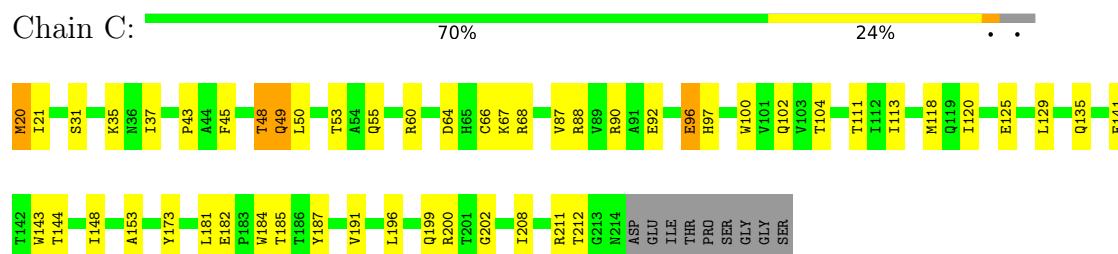
Chain 6: 



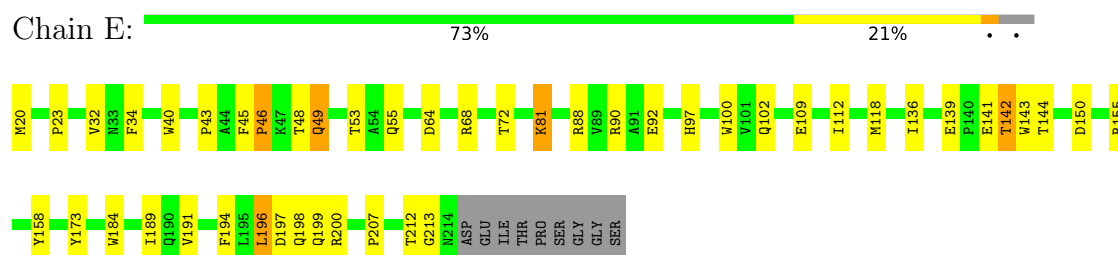
- Molecule 1: Interleukin-10 receptor subunit beta



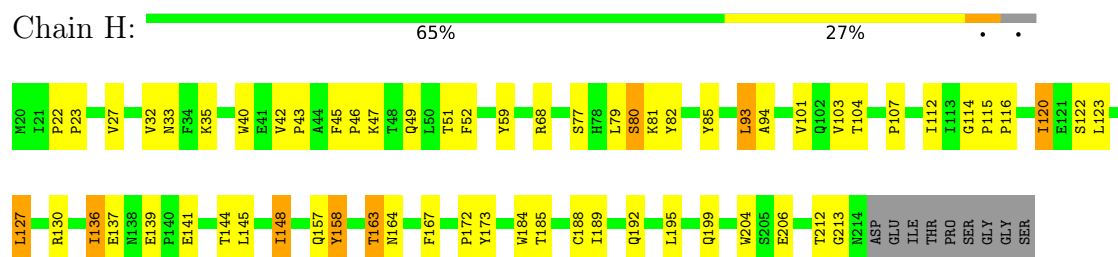
- Molecule 1: Interleukin-10 receptor subunit beta



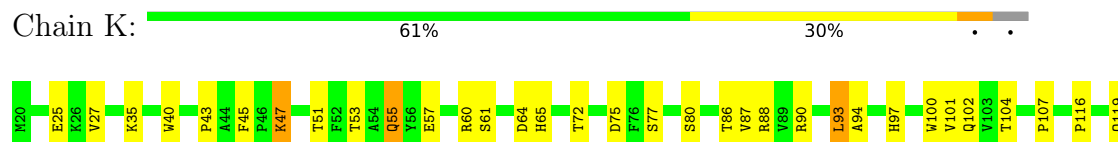
- Molecule 1: Interleukin-10 receptor subunit beta

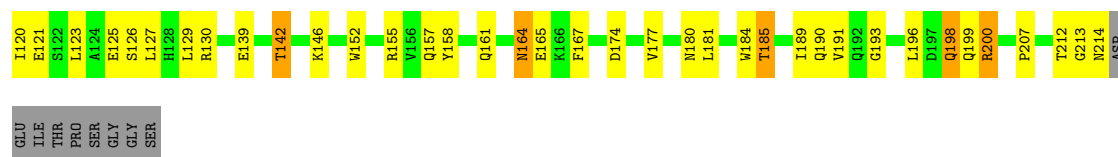


- Molecule 1: Interleukin-10 receptor subunit beta



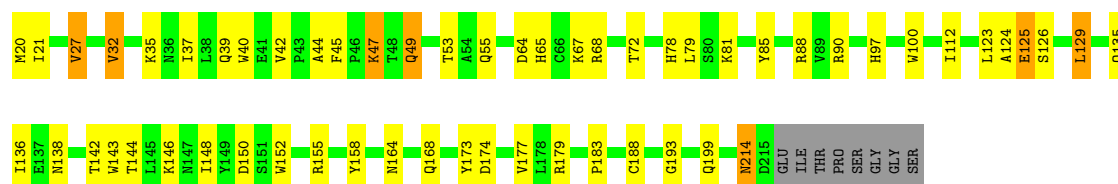
- Molecule 1: Interleukin-10 receptor subunit beta





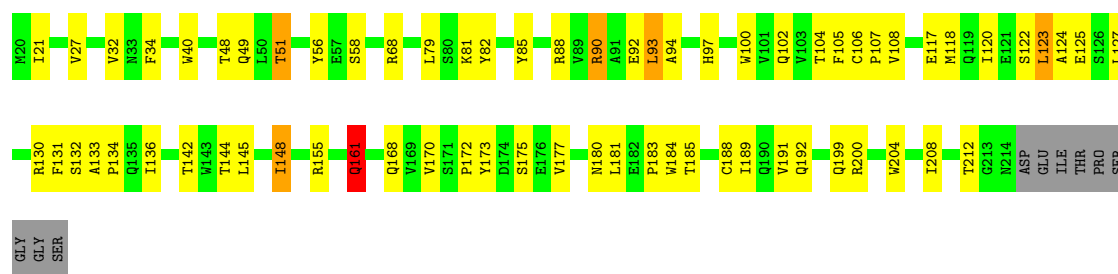
- Molecule 1: Interleukin-10 receptor subunit beta

Chain O: 68% 25%



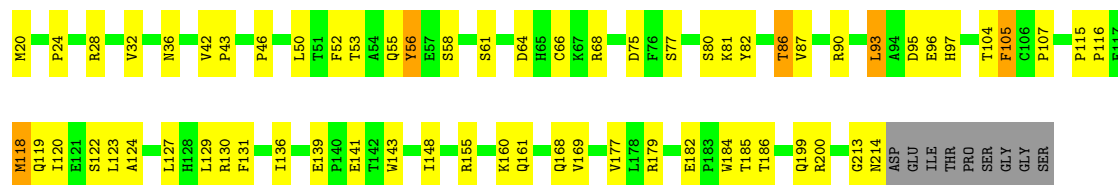
- Molecule 1: Interleukin-10 receptor subunit beta

Chain R: 62% 30%



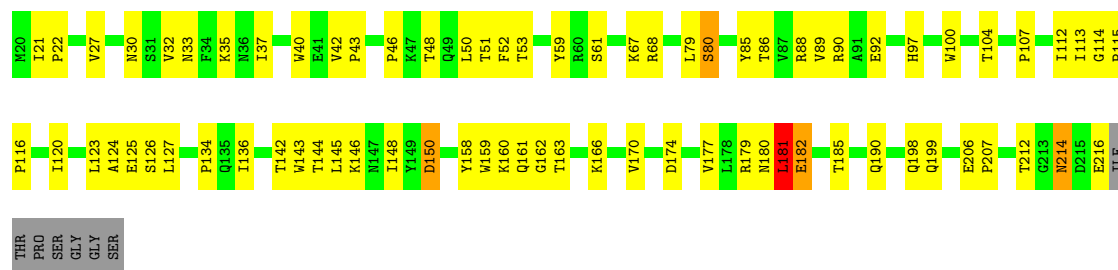
- Molecule 1: Interleukin-10 receptor subunit beta

Chain U: 64% 29%

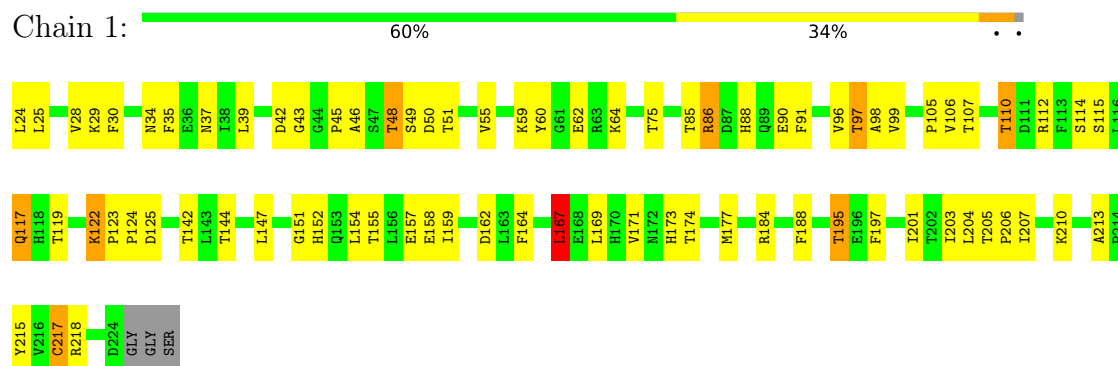


- Molecule 1: Interleukin-10 receptor subunit beta

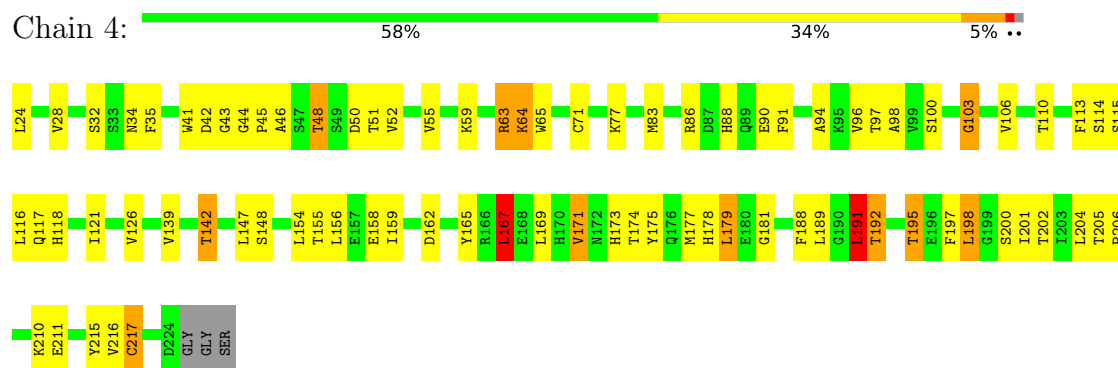
Chain X: 59% 35%



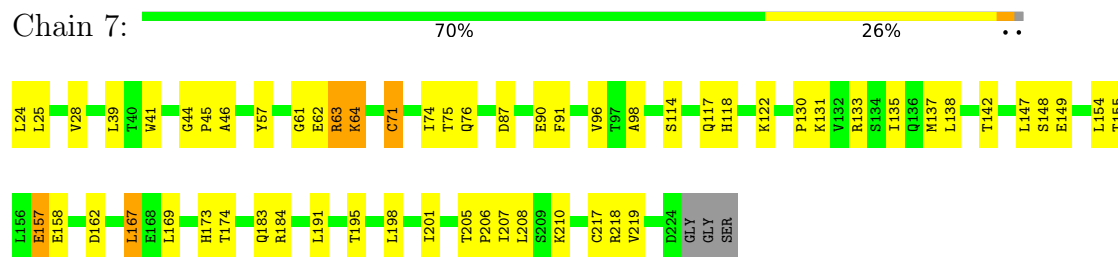
- Molecule 2: Interleukin-22 receptor subunit alpha-1



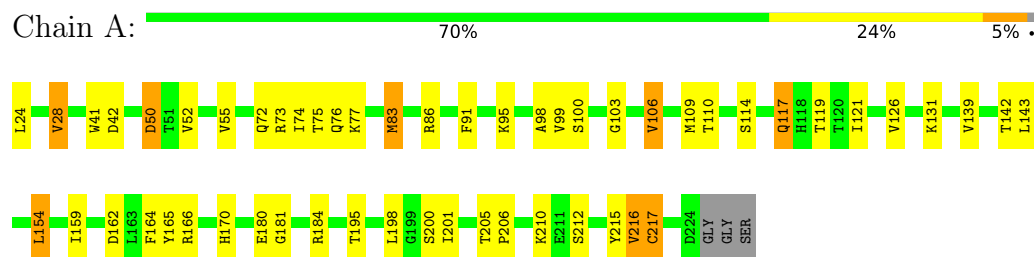
- Molecule 2: Interleukin-22 receptor subunit alpha-1



- Molecule 2: Interleukin-22 receptor subunit alpha-1

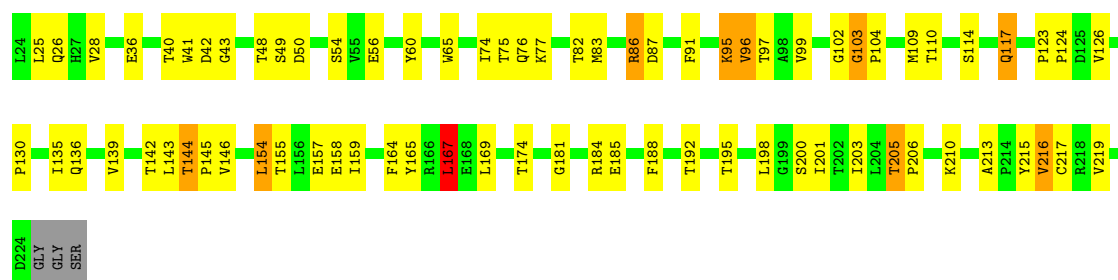


- Molecule 2: Interleukin-22 receptor subunit alpha-1



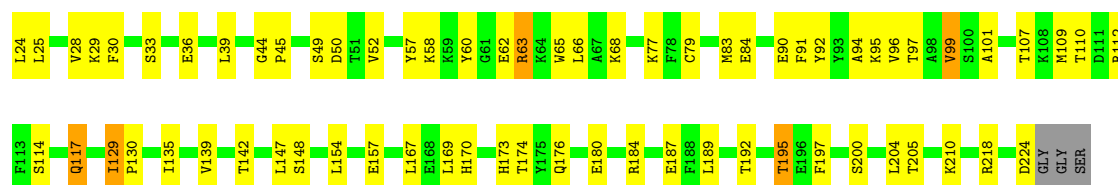
- Molecule 2: Interleukin-22 receptor subunit alpha-1





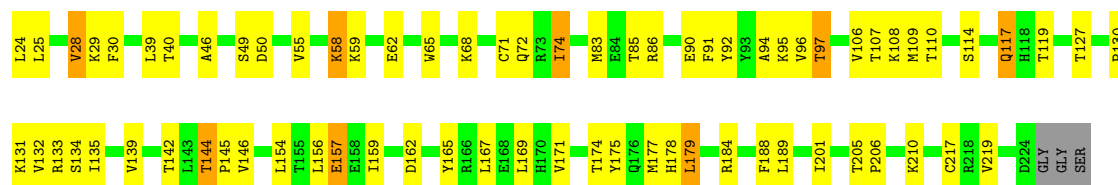
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain F: 65% 31% ..



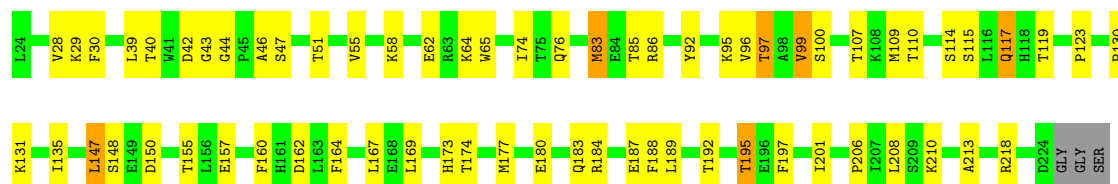
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain I: 63% 31% ..



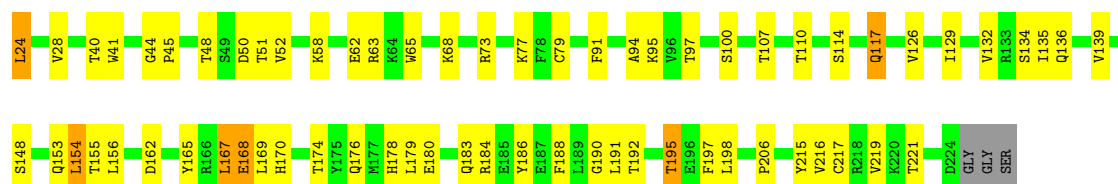
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain M: 66% 29% ..



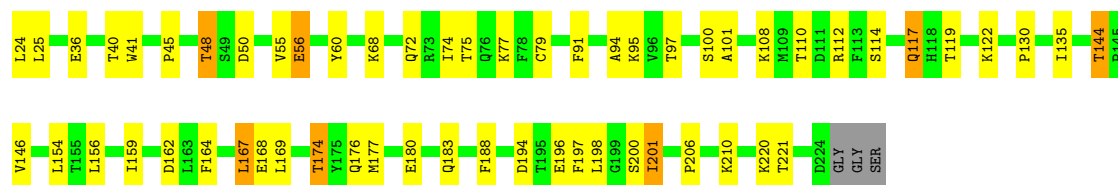
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain P: 66% 29% ..



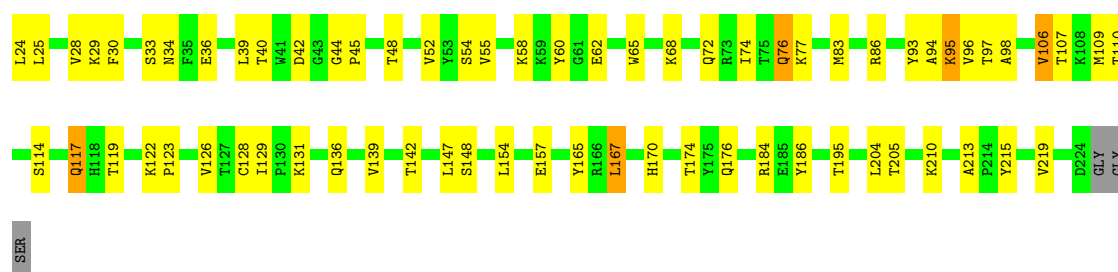
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain S:  70% 25% ..



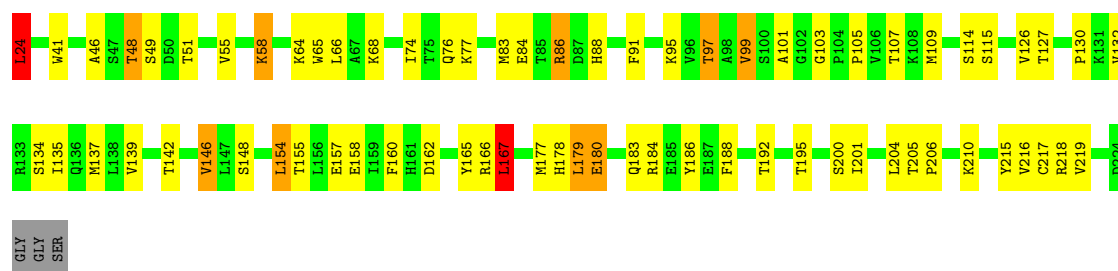
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain V:  65% 31% ..



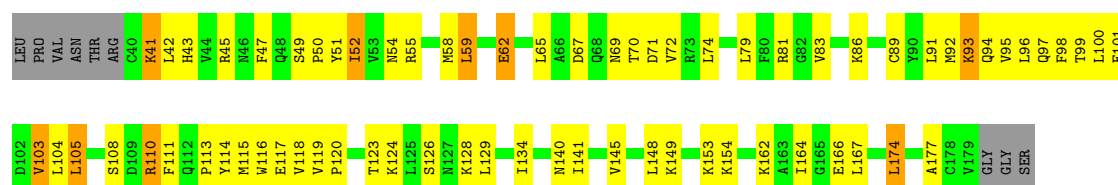
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain Y:  64% 29% ..



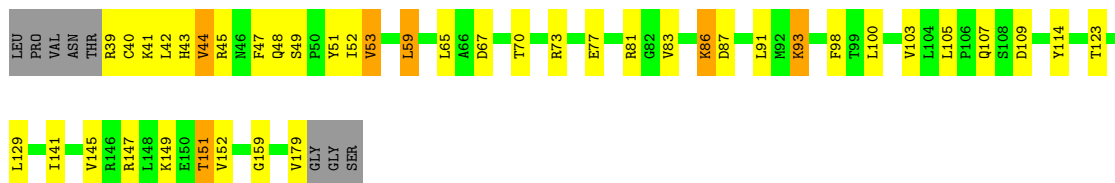
- Molecule 3: Interleukin-22

Chain 2:  47% 41% 6% 6%



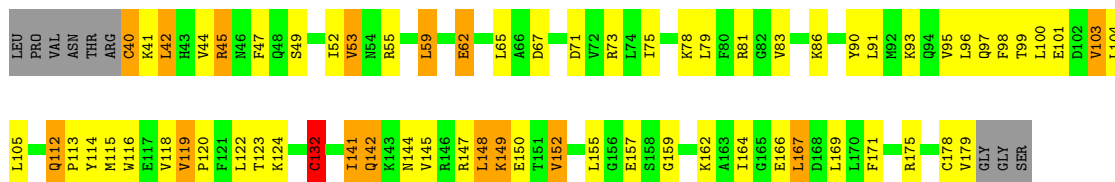
- Molecule 3: Interleukin-22

Chain 5:  66% 24% 5%



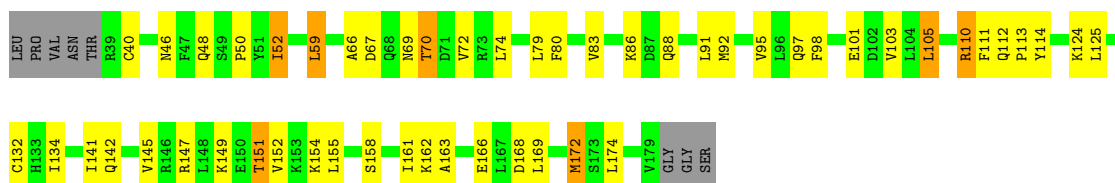
- Molecule 3: Interleukin-22

Chain 8: 48% 35% 10% 6%



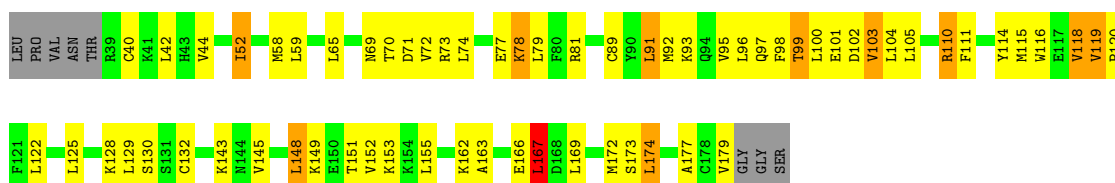
- Molecule 3: Interleukin-22

Chain D: 60% 30% 5% 5%



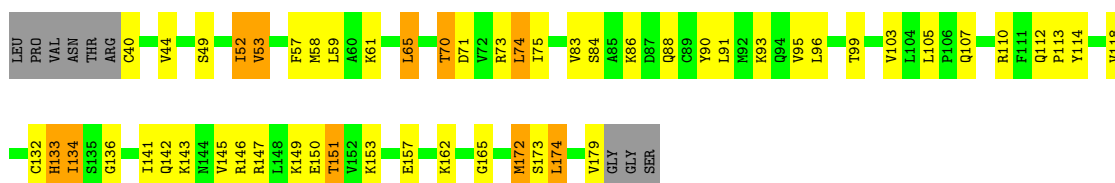
- Molecule 3: Interleukin-22

Chain G: 52% 36% 7% 5%



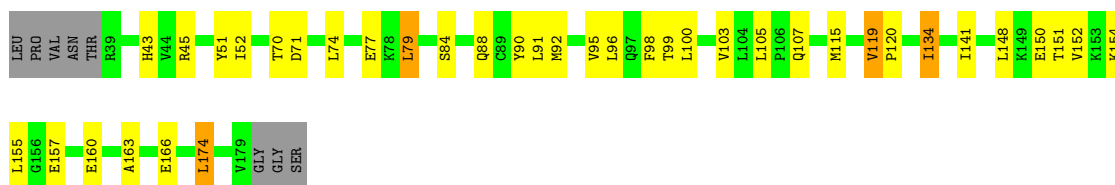
- Molecule 3: Interleukin-22

Chain J: 58% 30% 7% 6%



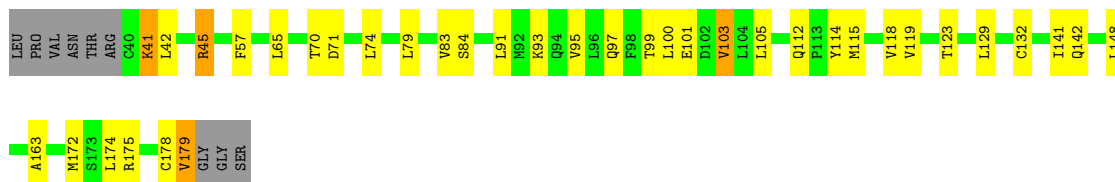
- Molecule 3: Interleukin-22

Chain L: 69% 23% 5%



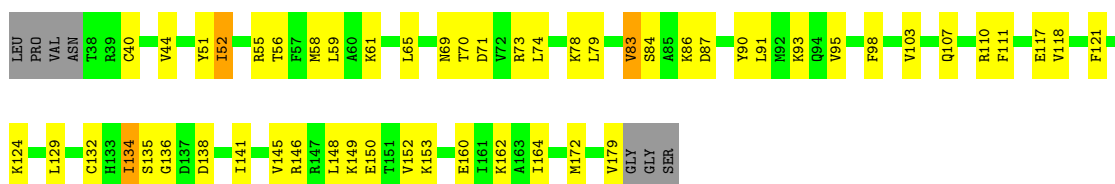
• Molecule 3: Interleukin-22

Chain N: 69% 22% 6%



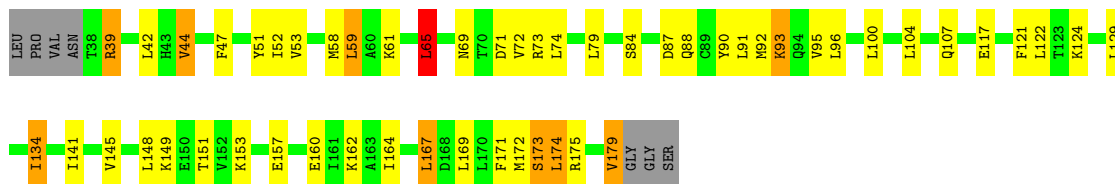
• Molecule 3: Interleukin-22

Chain Q: 60% 34% 5%



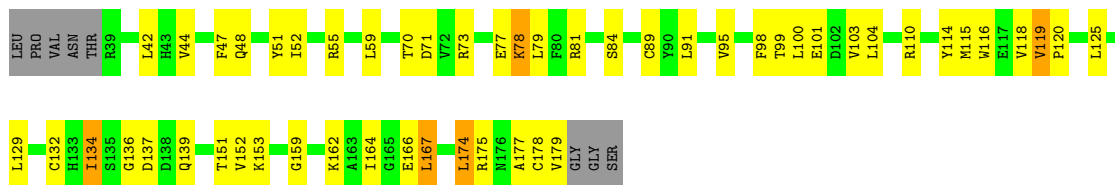
• Molecule 3: Interleukin-22

Chain T: 60% 29% 6% 5%



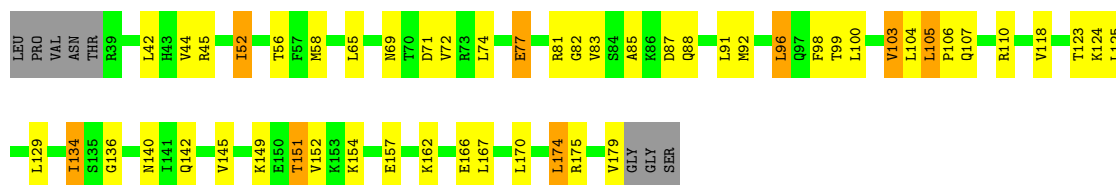
• Molecule 3: Interleukin-22

Chain W: 60% 32% 5%



• Molecule 3: Interleukin-22

Chain Z: 60% 30% 5% 5%



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

Chain a:  100%



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

Chain c:  100%



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

Chain n:  50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  33%

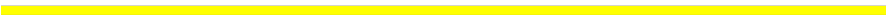


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  33% 67%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  67% 33%



- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50% 50%



- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%




- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%

MAG1
FUC2

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%MAG1
FUC2

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  100%MAG1
FUC2

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:  100%MAG1
FUC2

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  50% 50%MAG1
FUC2

- Molecule 7: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  50% 50%MAG1
FUC2

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

Chain g:  67% 33%MAG1
MAG2
BMA3

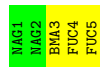
- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  20% 80%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



- Molecule 11: alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 134.49Å 145.22Å 152.04Å 71.06° 81.84° 62.48° | Depositor |
| Resolution (Å) | 48.09 – 2.60 | Depositor |
| % Data completeness (in resolution range) | 97.5 (48.09-2.60) | Depositor |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.23 (at 2.61Å) | Xtriage |
| Refinement program | PHENIX 1.17.1_3660 | Depositor |
| R, R_{free} | 0.236 , 0.296 | Depositor |
| Wilson B-factor (Å ²) | 69.1 | Xtriage |
| Anisotropy | 0.199 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 53140 | wwPDB-VP |
| Average B, all atoms (Å ²) | 101.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5066e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0 | 0.53 | 0/1627 | 0.74 | 1/2223 (0.0%) |
| 1 | 3 | 0.45 | 1/1643 (0.1%) | 0.67 | 0/2244 |
| 1 | 6 | 0.48 | 0/1655 | 0.67 | 0/2258 |
| 1 | 9 | 0.46 | 0/1579 | 0.72 | 2/2155 (0.1%) |
| 1 | C | 0.60 | 0/1662 | 0.75 | 0/2267 |
| 1 | E | 0.57 | 0/1641 | 0.72 | 1/2242 (0.0%) |
| 1 | H | 0.58 | 1/1650 (0.1%) | 0.74 | 0/2252 |
| 1 | K | 0.54 | 0/1653 | 0.71 | 0/2256 |
| 1 | O | 0.56 | 0/1657 | 0.76 | 2/2261 (0.1%) |
| 1 | R | 0.54 | 0/1659 | 0.69 | 0/2263 |
| 1 | U | 0.55 | 0/1651 | 0.72 | 1/2254 (0.0%) |
| 1 | X | 0.49 | 0/1667 | 0.73 | 1/2274 (0.0%) |
| 2 | 1 | 0.53 | 1/1655 (0.1%) | 0.75 | 1/2250 (0.0%) |
| 2 | 4 | 0.57 | 1/1652 (0.1%) | 0.81 | 4/2247 (0.2%) |
| 2 | 7 | 0.52 | 1/1646 (0.1%) | 0.73 | 1/2240 (0.0%) |
| 2 | A | 0.60 | 1/1647 (0.1%) | 0.78 | 1/2242 (0.0%) |
| 2 | B | 0.56 | 0/1651 | 0.78 | 1/2246 (0.0%) |
| 2 | F | 0.55 | 0/1650 | 0.72 | 0/2244 |
| 2 | I | 0.53 | 0/1656 | 0.74 | 0/2252 |
| 2 | M | 0.56 | 0/1647 | 0.74 | 0/2240 |
| 2 | P | 0.61 | 0/1663 | 0.83 | 0/2259 |
| 2 | S | 0.59 | 0/1659 | 0.77 | 1/2254 (0.0%) |
| 2 | V | 0.53 | 0/1653 | 0.70 | 0/2247 |
| 2 | Y | 0.60 | 0/1652 | 0.82 | 3/2246 (0.1%) |
| 3 | 2 | 0.59 | 1/1113 (0.1%) | 0.79 | 1/1500 (0.1%) |
| 3 | 5 | 0.45 | 0/1143 | 0.65 | 0/1536 |
| 3 | 8 | 0.62 | 2/1124 (0.2%) | 0.79 | 1/1513 (0.1%) |
| 3 | D | 0.52 | 0/1148 | 0.77 | 2/1543 (0.1%) |
| 3 | G | 0.48 | 0/1140 | 0.77 | 2/1533 (0.1%) |
| 3 | J | 0.45 | 0/1134 | 0.68 | 0/1525 |
| 3 | L | 0.54 | 0/1142 | 0.72 | 0/1536 |
| 3 | N | 0.49 | 0/1110 | 0.72 | 0/1498 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 3 | Q | 0.60 | 0/1137 | 0.84 | 2/1532 (0.1%) |
| 3 | T | 0.54 | 0/1150 | 0.77 | 1/1547 (0.1%) |
| 3 | W | 0.49 | 0/1141 | 0.70 | 0/1534 |
| 3 | Z | 0.57 | 0/1146 | 0.79 | 0/1540 |
| All | All | 0.54 | 9/53203 (0.0%) | 0.74 | 29/72253 (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 |
|-----|-------|---------------------|---------------------|
| 2 | 4 | 0 | 1 |
| 2 | Y | 0 | 1 |
| 3 | 2 | 0 | 1 |
| All | All | 0 | 3 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 8 | 40 | CYS | CB-SG | -9.55 | 1.66 | 1.82 |
| 3 | 2 | 62 | GLU | CG-CD | 9.31 | 1.66 | 1.51 |
| 3 | 8 | 132 | CYS | CB-SG | 8.11 | 1.96 | 1.82 |
| 2 | 7 | 71 | CYS | CB-SG | -7.13 | 1.70 | 1.82 |
| 2 | 4 | 217 | CYS | CB-SG | -6.00 | 1.72 | 1.82 |
| 2 | 1 | 217 | CYS | CB-SG | -5.84 | 1.72 | 1.81 |
| 1 | H | 82 | TYR | CD1-CE1 | 5.63 | 1.47 | 1.39 |
| 2 | A | 217 | CYS | CB-SG | -5.22 | 1.73 | 1.81 |
| 1 | 3 | 108 | VAL | CB-CG1 | -5.13 | 1.42 | 1.52 |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3 | 8 | 148 | LEU | CB-CG-CD2 | -10.11 | 93.81 | 111.00 |
| 3 | Q | 110 | ARG | NE-CZ-NH2 | 9.99 | 125.29 | 120.30 |
| 2 | Y | 167 | LEU | CA-CB-CG | 7.51 | 132.57 | 115.30 |
| 2 | 4 | 167 | LEU | CA-CB-CG | 6.99 | 131.37 | 115.30 |
| 2 | B | 167 | LEU | CB-CG-CD1 | -6.89 | 99.28 | 111.00 |
| 3 | T | 65 | LEU | CA-CB-CG | 6.59 | 130.45 | 115.30 |
| 1 | 0 | 178 | LEU | CB-CG-CD1 | -6.57 | 99.82 | 111.00 |
| 3 | D | 110 | ARG | NE-CZ-NH2 | 6.24 | 123.42 | 120.30 |
| 1 | 9 | 129 | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | Q | 73 | ARG | NE-CZ-NH2 | -6.01 | 117.29 | 120.30 |
| 2 | Y | 179 | LEU | CA-CB-CG | 5.93 | 128.93 | 115.30 |
| 2 | A | 154 | LEU | CB-CG-CD1 | -5.57 | 101.53 | 111.00 |
| 1 | 9 | 150 | ASP | CB-CG-OD2 | -5.56 | 113.29 | 118.30 |
| 1 | O | 129 | LEU | CA-CB-CG | 5.40 | 127.73 | 115.30 |
| 3 | 2 | 59 | LEU | CB-CG-CD2 | 5.40 | 120.17 | 111.00 |
| 2 | 7 | 167 | LEU | CA-CB-CG | 5.28 | 127.44 | 115.30 |
| 1 | X | 181 | LEU | CA-CB-CG | 5.26 | 127.39 | 115.30 |
| 1 | U | 75 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | E | 197 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 2 | S | 112 | ARG | NE-CZ-NH1 | -5.21 | 117.70 | 120.30 |
| 3 | G | 155 | LEU | CA-CB-CG | 5.17 | 127.20 | 115.30 |
| 1 | O | 138 | ASN | C-N-CA | -5.12 | 108.91 | 121.70 |
| 2 | 4 | 191 | LEU | CA-CB-CG | 5.11 | 127.04 | 115.30 |
| 2 | 1 | 167 | LEU | CA-CB-CG | 5.07 | 126.96 | 115.30 |
| 2 | 4 | 198 | LEU | CB-CG-CD2 | -5.06 | 102.40 | 111.00 |
| 3 | G | 167 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 2 | 4 | 191 | LEU | CB-CG-CD1 | 5.03 | 119.55 | 111.00 |
| 3 | D | 59 | LEU | CB-CG-CD1 | -5.01 | 102.48 | 111.00 |
| 2 | Y | 24 | LEU | CA-CB-CG | 5.01 | 126.82 | 115.30 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | 2 | 58 | MET | Mainchain |
| 2 | 4 | 103 | GLY | Peptide |
| 2 | Y | 103 | GLY | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 0 | 1579 | 0 | 1468 | 51 | 0 |
| 1 | 3 | 1595 | 0 | 1479 | 53 | 0 |
| 1 | 6 | 1607 | 0 | 1505 | 44 | 0 |
| 1 | 9 | 1532 | 0 | 1422 | 53 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | C | 1614 | 0 | 1516 | 31 | 0 |
| 1 | E | 1593 | 0 | 1474 | 26 | 0 |
| 1 | H | 1602 | 0 | 1499 | 46 | 0 |
| 1 | K | 1605 | 0 | 1500 | 41 | 0 |
| 1 | O | 1609 | 0 | 1508 | 25 | 0 |
| 1 | R | 1611 | 0 | 1512 | 46 | 0 |
| 1 | U | 1603 | 0 | 1491 | 41 | 0 |
| 1 | X | 1619 | 0 | 1516 | 50 | 0 |
| 2 | 1 | 1613 | 0 | 1583 | 54 | 0 |
| 2 | 4 | 1610 | 0 | 1574 | 58 | 0 |
| 2 | 7 | 1604 | 0 | 1563 | 39 | 0 |
| 2 | A | 1605 | 0 | 1561 | 39 | 0 |
| 2 | B | 1609 | 0 | 1572 | 59 | 0 |
| 2 | F | 1608 | 0 | 1574 | 40 | 0 |
| 2 | I | 1614 | 0 | 1578 | 53 | 0 |
| 2 | M | 1605 | 0 | 1572 | 43 | 0 |
| 2 | P | 1621 | 0 | 1598 | 44 | 0 |
| 2 | S | 1617 | 0 | 1594 | 39 | 0 |
| 2 | V | 1611 | 0 | 1583 | 42 | 0 |
| 2 | Y | 1610 | 0 | 1578 | 47 | 0 |
| 3 | 2 | 1096 | 0 | 1100 | 58 | 0 |
| 3 | 5 | 1126 | 0 | 1144 | 33 | 0 |
| 3 | 8 | 1107 | 0 | 1114 | 52 | 0 |
| 3 | D | 1131 | 0 | 1155 | 44 | 0 |
| 3 | G | 1123 | 0 | 1142 | 50 | 0 |
| 3 | J | 1117 | 0 | 1138 | 30 | 0 |
| 3 | L | 1125 | 0 | 1143 | 21 | 0 |
| 3 | N | 1093 | 0 | 1083 | 16 | 0 |
| 3 | Q | 1120 | 0 | 1127 | 33 | 0 |
| 3 | T | 1133 | 0 | 1153 | 36 | 0 |
| 3 | W | 1124 | 0 | 1139 | 30 | 0 |
| 3 | Z | 1129 | 0 | 1153 | 40 | 0 |
| 4 | a | 49 | 0 | 43 | 0 | 0 |
| 4 | c | 49 | 0 | 43 | 0 | 0 |
| 4 | n | 49 | 0 | 43 | 0 | 0 |
| 5 | b | 38 | 0 | 34 | 0 | 0 |
| 5 | e | 38 | 0 | 34 | 0 | 0 |
| 5 | i | 38 | 0 | 34 | 0 | 0 |
| 5 | j | 38 | 0 | 34 | 0 | 0 |
| 5 | l | 38 | 0 | 34 | 0 | 0 |
| 5 | m | 38 | 0 | 34 | 0 | 0 |
| 5 | s | 38 | 0 | 34 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | d | 24 | 0 | 22 | 0 | 0 |
| 6 | o | 24 | 0 | 22 | 0 | 0 |
| 6 | p | 24 | 0 | 22 | 0 | 0 |
| 6 | r | 24 | 0 | 22 | 0 | 0 |
| 6 | t | 24 | 0 | 22 | 0 | 0 |
| 6 | u | 24 | 0 | 22 | 0 | 0 |
| 6 | v | 24 | 0 | 22 | 0 | 0 |
| 7 | f | 24 | 0 | 22 | 0 | 0 |
| 8 | g | 39 | 0 | 34 | 0 | 0 |
| 9 | h | 59 | 0 | 52 | 0 | 0 |
| 9 | k | 59 | 0 | 52 | 0 | 0 |
| 10 | q | 28 | 0 | 25 | 0 | 0 |
| 11 | w | 34 | 0 | 31 | 0 | 0 |
| 12 | A | 6 | 0 | 8 | 0 | 0 |
| 12 | H | 6 | 0 | 8 | 0 | 0 |
| 12 | J | 6 | 0 | 8 | 0 | 0 |
| 12 | K | 6 | 0 | 8 | 0 | 0 |
| 12 | M | 6 | 0 | 8 | 2 | 0 |
| 12 | O | 6 | 0 | 8 | 0 | 0 |
| 12 | Y | 6 | 0 | 8 | 1 | 0 |
| 13 | B | 14 | 0 | 13 | 0 | 0 |
| 14 | 1 | 9 | 0 | 0 | 4 | 0 |
| 14 | 2 | 6 | 0 | 0 | 1 | 0 |
| 14 | 3 | 6 | 0 | 0 | 4 | 0 |
| 14 | 4 | 7 | 0 | 0 | 2 | 0 |
| 14 | 5 | 2 | 0 | 0 | 1 | 0 |
| 14 | 6 | 5 | 0 | 0 | 4 | 0 |
| 14 | 7 | 12 | 0 | 0 | 2 | 0 |
| 14 | 8 | 6 | 0 | 0 | 3 | 0 |
| 14 | 9 | 3 | 0 | 0 | 1 | 0 |
| 14 | A | 22 | 0 | 0 | 2 | 0 |
| 14 | B | 16 | 0 | 0 | 5 | 0 |
| 14 | C | 22 | 0 | 0 | 0 | 0 |
| 14 | D | 14 | 0 | 0 | 2 | 0 |
| 14 | E | 15 | 0 | 0 | 2 | 0 |
| 14 | F | 10 | 0 | 0 | 0 | 0 |
| 14 | G | 5 | 0 | 0 | 4 | 0 |
| 14 | H | 17 | 0 | 0 | 3 | 0 |
| 14 | I | 9 | 0 | 0 | 2 | 0 |
| 14 | J | 6 | 0 | 0 | 1 | 0 |
| 14 | K | 9 | 0 | 0 | 3 | 0 |
| 14 | L | 8 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14 | M | 8 | 0 | 0 | 0 | 0 |
| 14 | N | 5 | 0 | 0 | 0 | 0 |
| 14 | O | 14 | 0 | 0 | 0 | 0 |
| 14 | P | 6 | 0 | 0 | 0 | 0 |
| 14 | Q | 7 | 0 | 0 | 2 | 0 |
| 14 | R | 9 | 0 | 0 | 5 | 0 |
| 14 | S | 13 | 0 | 0 | 6 | 0 |
| 14 | T | 6 | 0 | 0 | 1 | 0 |
| 14 | U | 14 | 0 | 0 | 1 | 0 |
| 14 | V | 12 | 0 | 0 | 2 | 0 |
| 14 | W | 1 | 0 | 0 | 0 | 0 |
| 14 | X | 11 | 0 | 0 | 0 | 0 |
| 14 | Y | 20 | 0 | 0 | 2 | 0 |
| 14 | Z | 5 | 0 | 0 | 0 | 0 |
| All | All | 53140 | 0 | 51217 | 1419 | 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 (1419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:136:ILE:HD13 | 1:0:148:ILE:HD11 | 1.43 | 1.01 |
| 3:2:59:LEU:HD22 | 3:2:118:VAL:HG11 | 1.39 | 0.99 |
| 2:V:157:GLU:OE1 | 2:V:184:ARG:NH2 | 1.97 | 0.98 |
| 2:B:146:VAL:O | 14:B:401:HOH:O | 1.83 | 0.96 |
| 1:0:32:VAL:HG12 | 1:0:112:ILE:HB | 1.51 | 0.93 |
| 2:B:205:THR:HG23 | 2:B:210:LYS:HB2 | 1.52 | 0.92 |
| 3:G:102:ASP:O | 14:G:301:HOH:O | 1.90 | 0.90 |
| 1:9:123:LEU:HD22 | 1:9:128:HIS:CE1 | 2.07 | 0.89 |
| 1:0:111:THR:O | 1:0:200:ARG:NH2 | 2.06 | 0.89 |
| 3:T:92:MET:HB3 | 3:T:174:LEU:HD12 | 1.54 | 0.88 |
| 1:6:71:SER:O | 14:6:301:HOH:O | 1.91 | 0.88 |
| 2:7:205:THR:HB | 2:7:210:LYS:HB2 | 1.55 | 0.87 |
| 2:A:83:MET:SD | 2:A:86:ARG:NH1 | 2.48 | 0.87 |
| 3:2:100:LEU:HD23 | 3:2:104:LEU:HD21 | 1.57 | 0.86 |
| 2:P:139:VAL:HG23 | 2:P:184:ARG:HD2 | 1.58 | 0.86 |
| 1:U:184:TRP:HD1 | 1:U:213:GLY:HA2 | 1.41 | 0.86 |
| 1:3:210:GLU:O | 14:3:301:HOH:O | 1.93 | 0.86 |
| 2:I:25:LEU:HD21 | 2:I:96:VAL:HG13 | 1.59 | 0.85 |
| 1:9:123:LEU:HD22 | 1:9:128:HIS:HE1 | 1.41 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:184:TRP:CD1 | 1:U:213:GLY:HA2 | 2.12 | 0.84 |
| 1:K:88:ARG:HB3 | 1:K:102:GLN:HG2 | 1.59 | 0.84 |
| 1:K:161:GLN:O | 14:K:401:HOH:O | 1.94 | 0.84 |
| 1:R:106:CYS:SG | 14:R:301:HOH:O | 2.36 | 0.83 |
| 1:3:100:TRP:O | 14:3:302:HOH:O | 1.95 | 0.83 |
| 2:M:83:MET:SD | 2:M:86:ARG:NH1 | 2.51 | 0.83 |
| 2:V:25:LEU:HD21 | 2:V:96:VAL:HG23 | 1.60 | 0.83 |
| 2:Y:216:VAL:H | 12:Y:303:GOL:H31 | 1.45 | 0.82 |
| 3:T:107:GLN:NE2 | 3:T:157:GLU:OE2 | 2.10 | 0.82 |
| 2:I:144:THR:HG23 | 2:I:146:VAL:H | 1.45 | 0.82 |
| 3:D:147:ARG:O | 3:D:151:THR:OG1 | 1.98 | 0.81 |
| 3:G:162:LYS:O | 14:G:302:HOH:O | 1.98 | 0.81 |
| 3:G:77:GLU:OE1 | 3:G:81:ARG:NH1 | 2.14 | 0.81 |
| 1:X:120:ILE:HD11 | 1:X:127:LEU:HD22 | 1.63 | 0.81 |
| 3:8:83:VAL:HG21 | 3:8:91:LEU:HD22 | 1.61 | 0.80 |
| 1:H:136:ILE:HG21 | 1:H:148:ILE:HD11 | 1.62 | 0.80 |
| 2:Y:157:GLU:OE1 | 2:Y:184:ARG:NH2 | 2.14 | 0.80 |
| 3:5:67:ASP:OD2 | 14:5:301:HOH:O | 2.01 | 0.79 |
| 1:9:55:GLN:NE2 | 1:9:64:ASP:OD1 | 2.14 | 0.79 |
| 1:C:182:GLU:O | 1:C:212:THR:HG21 | 1.82 | 0.79 |
| 3:Q:153:LYS:NZ | 14:Q:301:HOH:O | 2.15 | 0.78 |
| 1:R:123:LEU:HD13 | 1:R:124:ALA:H | 1.47 | 0.78 |
| 2:A:50:ASP:N | 2:A:50:ASP:OD1 | 2.16 | 0.77 |
| 2:Y:24:LEU:HD12 | 2:Y:46:ALA:HB3 | 1.66 | 0.77 |
| 3:N:103:VAL:HG11 | 3:N:163:ALA:HB3 | 1.66 | 0.76 |
| 3:Z:103:VAL:O | 3:Z:107:GLN:HB3 | 1.85 | 0.76 |
| 2:B:74:ILE:HD12 | 2:B:76:GLN:HG2 | 1.67 | 0.76 |
| 3:Z:92:MET:HB3 | 3:Z:174:LEU:HD12 | 1.68 | 0.76 |
| 1:3:108:VAL:O | 1:3:200:ARG:NH2 | 2.13 | 0.76 |
| 2:B:87:ASP:OD2 | 14:B:402:HOH:O | 2.04 | 0.76 |
| 2:F:205:THR:HB | 2:F:210:LYS:HB2 | 1.68 | 0.76 |
| 2:I:83:MET:SD | 2:I:86:ARG:NH1 | 2.59 | 0.76 |
| 2:S:220:LYS:O | 14:S:401:HOH:O | 2.03 | 0.76 |
| 1:9:65:HIS:ND1 | 14:9:401:HOH:O | 2.17 | 0.75 |
| 2:Y:148:SER:HB2 | 2:Y:154:LEU:HD11 | 1.67 | 0.75 |
| 2:P:129:ILE:HB | 2:P:136:GLN:HB3 | 1.68 | 0.75 |
| 1:X:185:THR:H | 1:X:212:THR:HG22 | 1.50 | 0.75 |
| 3:5:49:SER:HB3 | 3:5:52:ILE:HG12 | 1.68 | 0.75 |
| 1:9:81:LYS:NZ | 1:9:138:ASN:OD1 | 2.19 | 0.75 |
| 2:7:184:ARG:NH2 | 14:7:401:HOH:O | 2.11 | 0.74 |
| 1:C:20:MET:N | 1:C:96:GLU:OE2 | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:90:ARG:HD2 | 1:0:97:HIS:HB2 | 1.68 | 0.74 |
| 1:0:122:SER:HB2 | 1:0:127:LEU:HD23 | 1.69 | 0.74 |
| 1:0:84:ASP:OD2 | 3:Z:124:LYS:HE2 | 1.87 | 0.74 |
| 2:1:157:GLU:OE1 | 2:1:184:ARG:NH2 | 2.20 | 0.73 |
| 2:I:97:THR:HG23 | 2:I:107:THR:OG1 | 1.88 | 0.73 |
| 2:B:126:VAL:HG21 | 2:B:201:ILE:HG21 | 1.70 | 0.73 |
| 3:5:44:VAL:HG13 | 3:5:179:VAL:HG21 | 1.69 | 0.73 |
| 3:G:92:MET:HB3 | 3:G:174:LEU:HD12 | 1.71 | 0.73 |
| 3:Q:107:GLN:NE2 | 3:Q:160:GLU:OE1 | 2.19 | 0.73 |
| 1:R:81:LYS:O | 14:R:301:HOH:O | 2.06 | 0.73 |
| 2:I:157:GLU:OE1 | 2:I:184:ARG:NH2 | 2.22 | 0.73 |
| 3:2:83:VAL:HG21 | 3:2:91:LEU:HD22 | 1.70 | 0.73 |
| 1:6:185:THR:H | 1:6:212:THR:HG22 | 1.53 | 0.73 |
| 1:6:35:LYS:HE2 | 1:6:37:ILE:HD11 | 1.69 | 0.73 |
| 2:F:157:GLU:OE1 | 2:F:184:ARG:NH2 | 2.20 | 0.73 |
| 3:5:41:LYS:NZ | 3:5:86:LYS:HD3 | 2.04 | 0.73 |
| 3:8:95:VAL:HG13 | 3:8:148:LEU:HD21 | 1.70 | 0.72 |
| 1:9:90:ARG:HH11 | 1:9:97:HIS:HB3 | 1.54 | 0.72 |
| 3:D:83:VAL:HG11 | 3:D:91:LEU:HD22 | 1.71 | 0.72 |
| 3:T:121:PHE:HD2 | 3:T:122:LEU:HD12 | 1.54 | 0.72 |
| 1:X:42:VAL:HG12 | 1:X:52:PHE:HZ | 1.51 | 0.72 |
| 2:Y:48:THR:HG23 | 2:Y:51:THR:HB | 1.72 | 0.72 |
| 3:W:98:PHE:HZ | 3:W:152:VAL:HG11 | 1.55 | 0.72 |
| 2:1:86:ARG:HD2 | 2:1:147:LEU:HD23 | 1.70 | 0.72 |
| 1:6:32:VAL:HG12 | 1:6:112:ILE:HB | 1.72 | 0.71 |
| 2:Y:97:THR:HG23 | 2:Y:107:THR:OG1 | 1.89 | 0.71 |
| 2:A:24:LEU:N | 14:A:403:HOH:O | 2.23 | 0.71 |
| 1:0:195:LEU:HD13 | 1:0:200:ARG:HB3 | 1.71 | 0.71 |
| 2:7:25:LEU:HD11 | 2:7:96:VAL:HG23 | 1.73 | 0.71 |
| 3:5:107:GLN:HE21 | 3:5:109:ASP:HB2 | 1.54 | 0.71 |
| 2:M:177:MET:HE2 | 2:M:188:PHE:HD1 | 1.54 | 0.71 |
| 1:H:120:ILE:HD11 | 1:H:127:LEU:HG | 1.73 | 0.71 |
| 2:4:42:ASP:HA | 2:4:77:LYS:HD3 | 1.72 | 0.70 |
| 2:V:58:LYS:HE3 | 2:V:65:TRP:CD1 | 2.26 | 0.70 |
| 2:1:144:THR:OG1 | 14:1:401:HOH:O | 2.09 | 0.70 |
| 3:J:147:ARG:O | 3:J:151:THR:HG22 | 1.92 | 0.70 |
| 1:0:145:LEU:HA | 1:0:148:ILE:HD12 | 1.72 | 0.70 |
| 2:7:74:ILE:HD12 | 2:7:76:GLN:HG2 | 1.73 | 0.70 |
| 2:F:58:LYS:HD3 | 2:F:65:TRP:CD1 | 2.27 | 0.70 |
| 3:2:62:GLU:N | 3:2:62:GLU:OE1 | 2.25 | 0.70 |
| 1:6:39:GLN:NE2 | 14:6:302:HOH:O | 2.24 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:9:123:LEU:HD23 | 1:9:126:SER:H | 1.56 | 0.69 |
| 1:R:177:VAL:O | 14:R:302:HOH:O | 2.10 | 0.69 |
| 1:U:86:THR:HG23 | 1:U:104:THR:HG22 | 1.74 | 0.69 |
| 1:3:35:LYS:HE2 | 1:3:37:ILE:HD11 | 1.75 | 0.69 |
| 2:A:52:VAL:HG21 | 2:A:73:ARG:HG3 | 1.75 | 0.69 |
| 1:C:185:THR:H | 1:C:212:THR:HG22 | 1.56 | 0.69 |
| 3:T:96:LEU:HD22 | 3:T:174:LEU:HD21 | 1.74 | 0.69 |
| 2:A:162:ASP:OD2 | 14:A:401:HOH:O | 2.10 | 0.69 |
| 3:J:114:TYR:O | 3:J:118:VAL:HG23 | 1.93 | 0.69 |
| 3:W:59:LEU:HD13 | 3:W:114:TYR:HB2 | 1.75 | 0.69 |
| 3:5:93:LYS:HB2 | 3:5:129:LEU:HD13 | 1.74 | 0.69 |
| 2:I:58:LYS:NZ | 3:J:70:THR:OG1 | 2.23 | 0.69 |
| 2:A:74:ILE:HD12 | 2:A:76:GLN:HG2 | 1.75 | 0.68 |
| 3:T:87:ASP:HB3 | 3:T:141:ILE:HD11 | 1.73 | 0.68 |
| 2:1:97:THR:HG23 | 2:1:107:THR:OG1 | 1.94 | 0.68 |
| 1:E:88:ARG:HB3 | 1:E:102:GLN:HG2 | 1.76 | 0.68 |
| 2:1:167:LEU:HB3 | 2:1:201:ILE:HG13 | 1.75 | 0.68 |
| 2:A:144:THR:HG23 | 2:A:146:VAL:H | 1.58 | 0.68 |
| 2:B:165:TYR:HB3 | 2:B:201:ILE:HD11 | 1.74 | 0.68 |
| 1:O:214:ASN:OD1 | 1:O:214:ASN:N | 2.27 | 0.68 |
| 1:O:35:LYS:HE2 | 1:O:37:ILE:HD11 | 1.76 | 0.68 |
| 2:S:97:THR:O | 14:S:402:HOH:O | 2.12 | 0.68 |
| 2:4:83:MET:SD | 2:4:86:ARG:NH1 | 2.67 | 0.67 |
| 2:F:58:LYS:NZ | 2:F:62:GLU:O | 2.27 | 0.67 |
| 1:R:51:THR:OG1 | 1:R:92:GLU:OE2 | 2.12 | 0.67 |
| 2:1:218:ARG:NH2 | 1:C:50:LEU:O | 2.27 | 0.67 |
| 1:0:156:VAL:HB | 1:0:169:VAL:HG12 | 1.77 | 0.67 |
| 1:6:135:GLN:HA | 1:6:144:THR:HA | 1.76 | 0.67 |
| 3:D:110:ARG:NH2 | 3:D:161:ILE:HG22 | 2.08 | 0.67 |
| 2:V:58:LYS:NZ | 2:V:62:GLU:O | 2.28 | 0.67 |
| 2:B:126:VAL:HB | 2:B:215:TYR:CD2 | 2.30 | 0.67 |
| 3:Z:85:ALA:HA | 3:Z:88:GLN:HG3 | 1.76 | 0.67 |
| 1:0:163:THR:HG22 | 1:0:165:GLU:H | 1.60 | 0.66 |
| 2:V:58:LYS:HG2 | 2:V:95:LYS:HZ1 | 1.60 | 0.66 |
| 3:D:151:THR:HG22 | 3:D:154:LYS:HE2 | 1.76 | 0.66 |
| 2:F:192:THR:HG23 | 2:F:195:THR:OG1 | 1.95 | 0.66 |
| 2:4:173:HIS:HB2 | 1:E:68:ARG:HB2 | 1.78 | 0.66 |
| 2:7:71:CYS:HB3 | 2:7:74:ILE:HD13 | 1.77 | 0.66 |
| 3:D:97:GLN:NE2 | 14:D:301:HOH:O | 2.27 | 0.66 |
| 2:S:144:THR:HG23 | 2:S:146:VAL:H | 1.59 | 0.66 |
| 1:K:86:THR:HG22 | 1:K:104:THR:HG22 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:9:120:ILE:HD12 | 1:9:129:LEU:HD12 | 1.78 | 0.66 |
| 2:A:126:VAL:HG22 | 2:A:139:VAL:HG22 | 1.76 | 0.66 |
| 3:G:42:LEU:HG | 3:G:129:LEU:HD21 | 1.78 | 0.66 |
| 3:2:120:PRO:HB3 | 1:3:83:GLY:HA2 | 1.78 | 0.66 |
| 2:I:130:PRO:HA | 2:I:135:ILE:HD13 | 1.78 | 0.66 |
| 3:L:151:THR:HA | 3:L:154:LYS:HE2 | 1.78 | 0.66 |
| 2:4:48:THR:HG23 | 2:4:50:ASP:H | 1.61 | 0.65 |
| 1:K:155:ARG:NH1 | 14:K:402:HOH:O | 2.28 | 0.65 |
| 1:K:196:LEU:O | 1:K:198:GLN:NE2 | 2.29 | 0.65 |
| 3:T:74:LEU:HB3 | 3:T:148:LEU:HD11 | 1.78 | 0.65 |
| 2:4:178:HIS:CD2 | 1:6:130:ARG:HD2 | 2.32 | 0.65 |
| 2:B:65:TRP:CG | 2:B:95:LYS:HE3 | 2.31 | 0.65 |
| 2:F:33:SER:O | 2:F:36:GLU:HG2 | 1.95 | 0.65 |
| 1:K:57:GLU:OE1 | 2:M:64:LYS:NZ | 2.23 | 0.65 |
| 2:A:144:THR:HG23 | 2:A:146:VAL:HG13 | 1.77 | 0.65 |
| 2:M:97:THR:HG22 | 2:M:107:THR:HG23 | 1.77 | 0.65 |
| 3:Q:146:ARG:NH1 | 3:Q:150:GLU:OE2 | 2.29 | 0.65 |
| 1:9:90:ARG:NH1 | 1:9:97:HIS:HB3 | 2.11 | 0.65 |
| 3:N:93:LYS:NZ | 3:N:132:CYS:O | 2.25 | 0.65 |
| 3:G:115:MET:O | 3:G:119:VAL:HG13 | 1.96 | 0.65 |
| 2:M:58:LYS:HE3 | 2:M:65:TRP:CE2 | 2.32 | 0.65 |
| 2:Y:205:THR:HB | 2:Y:210:LYS:HB2 | 1.77 | 0.65 |
| 2:1:177:MET:HE2 | 2:1:188:PHE:CD1 | 2.31 | 0.65 |
| 3:2:116:TRP:HD1 | 1:3:80:SER:OG | 1.79 | 0.65 |
| 3:2:99:THR:HA | 3:2:103:VAL:HG23 | 1.78 | 0.65 |
| 3:N:97:GLN:NE2 | 3:N:101:GLU:OE2 | 2.30 | 0.65 |
| 2:P:63:ARG:NH1 | 3:Q:71:ASP:OD2 | 2.28 | 0.65 |
| 2:F:58:LYS:HD3 | 2:F:65:TRP:HD1 | 1.61 | 0.65 |
| 2:7:62:GLU:HB3 | 2:7:64:LYS:HD2 | 1.78 | 0.65 |
| 2:I:95:LYS:HA | 2:I:109:MET:HA | 1.78 | 0.65 |
| 3:5:98:PHE:HZ | 3:5:152:VAL:HG11 | 1.61 | 0.64 |
| 3:G:166:GLU:HG3 | 14:G:302:HOH:O | 1.96 | 0.64 |
| 2:4:63:ARG:HB3 | 2:4:63:ARG:HH11 | 1.62 | 0.64 |
| 3:Z:107:GLN:HE21 | 3:Z:110:ARG:HG2 | 1.60 | 0.64 |
| 3:2:96:LEU:HD13 | 3:2:126:SER:HB3 | 1.80 | 0.64 |
| 3:8:67:ASP:CG | 3:8:162:LYS:HE2 | 2.18 | 0.64 |
| 3:G:116:TRP:O | 1:H:80:SER:OG | 2.15 | 0.64 |
| 1:O:90:ARG:HD2 | 1:O:97:HIS:HB2 | 1.80 | 0.64 |
| 3:G:110:ARG:HD3 | 3:G:111:PHE:H | 1.63 | 0.64 |
| 3:L:103:VAL:HG11 | 3:L:163:ALA:HB3 | 1.80 | 0.64 |
| 1:9:123:LEU:HG | 1:9:125:GLU:H | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:188:CYS:C | 1:H:189:ILE:HD13 | 2.18 | 0.64 |
| 1:R:161:GLN:HG2 | 1:R:188:CYS:SG | 2.38 | 0.64 |
| 3:8:59:LEU:HD12 | 3:8:118:VAL:HG11 | 1.77 | 0.63 |
| 3:G:59:LEU:HD13 | 3:G:114:TYR:HB2 | 1.80 | 0.63 |
| 2:Y:48:THR:HG21 | 2:Y:101:ALA:H | 1.62 | 0.63 |
| 1:R:120:ILE:HD13 | 1:R:189:ILE:HD12 | 1.80 | 0.63 |
| 1:3:146:LYS:NZ | 1:3:174:ASP:OD1 | 2.31 | 0.63 |
| 2:4:167:LEU:HB3 | 2:4:201:ILE:HG13 | 1.81 | 0.63 |
| 2:M:157:GLU:OE1 | 2:M:184:ARG:NH2 | 2.31 | 0.63 |
| 3:8:164:ILE:HA | 3:8:167:LEU:HD13 | 1.80 | 0.63 |
| 1:3:116:PRO:HG2 | 1:3:191:VAL:HG13 | 1.81 | 0.63 |
| 2:S:24:LEU:HD22 | 2:S:45:PRO:HD2 | 1.80 | 0.63 |
| 1:3:104:THR:O | 14:3:303:HOH:O | 2.16 | 0.63 |
| 2:M:148:SER:OG | 2:M:150:ASP:OD1 | 2.11 | 0.63 |
| 2:S:176:GLN:HE21 | 1:U:130:ARG:HH12 | 1.46 | 0.63 |
| 1:H:32:VAL:HG22 | 1:H:112:ILE:HB | 1.80 | 0.63 |
| 3:Z:145:VAL:O | 3:Z:149:LYS:HG3 | 1.99 | 0.63 |
| 3:2:98:PHE:CD1 | 3:2:149:LYS:HE2 | 2.34 | 0.62 |
| 3:D:151:THR:HA | 3:D:154:LYS:HG2 | 1.80 | 0.62 |
| 3:Z:107:GLN:NE2 | 3:Z:110:ARG:HG2 | 2.14 | 0.62 |
| 2:1:25:LEU:HD12 | 2:1:98:ALA:HB2 | 1.82 | 0.62 |
| 2:B:103:GLY:H | 2:B:104:PRO:HD2 | 1.64 | 0.62 |
| 1:H:195:LEU:O | 14:H:401:HOH:O | 2.15 | 0.62 |
| 2:P:168:GLU:HG3 | 2:P:170:HIS:NE2 | 2.13 | 0.62 |
| 3:T:121:PHE:CD2 | 3:T:122:LEU:HD12 | 2.34 | 0.62 |
| 3:W:98:PHE:CZ | 3:W:152:VAL:HG11 | 2.34 | 0.62 |
| 3:Z:110:ARG:NH2 | 3:Z:157:GLU:OE2 | 2.32 | 0.62 |
| 1:9:77:SER:O | 1:9:138:ASN:ND2 | 2.26 | 0.62 |
| 2:B:157:GLU:OE1 | 2:B:184:ARG:NH2 | 2.33 | 0.62 |
| 1:3:160:LYS:NZ | 1:3:182:GLU:OE1 | 2.25 | 0.62 |
| 2:P:52:VAL:HG21 | 2:P:73:ARG:HG3 | 1.81 | 0.62 |
| 2:P:126:VAL:HB | 2:P:215:TYR:CD2 | 2.34 | 0.62 |
| 2:A:131:LYS:HE2 | 2:Y:41:TRP:O | 2.00 | 0.62 |
| 1:0:134:PRO:HB2 | 1:0:145:LEU:HD13 | 1.80 | 0.62 |
| 3:J:142:GLN:HA | 3:J:145:VAL:HG22 | 1.81 | 0.62 |
| 1:X:42:VAL:HG12 | 1:X:52:PHE:CZ | 2.34 | 0.62 |
| 3:2:98:PHE:HA | 3:2:101:GLU:HG2 | 1.82 | 0.62 |
| 3:L:98:PHE:HZ | 3:L:152:VAL:HG11 | 1.64 | 0.62 |
| 2:V:94:ALA:O | 2:V:110:THR:HG23 | 1.99 | 0.62 |
| 3:W:79:LEU:HD21 | 3:W:95:VAL:HG21 | 1.82 | 0.62 |
| 1:0:130:ARG:HD2 | 2:Y:178:HIS:CD2 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:7:24:LEU:HB2 | 2:7:46:ALA:HB3 | 1.82 | 0.62 |
| 1:9:123:LEU:HD21 | 1:9:125:GLU:HB2 | 1.81 | 0.62 |
| 3:D:172:MET:HA | 3:D:172:MET:CE | 2.30 | 0.62 |
| 2:M:160:PHE:HD1 | 12:M:305:GOL:H12 | 1.65 | 0.62 |
| 2:P:24:LEU:HB3 | 2:P:44:GLY:HA3 | 1.81 | 0.62 |
| 3:5:49:SER:O | 3:5:53:VAL:HG13 | 2.00 | 0.61 |
| 2:P:165:TYR:OH | 2:P:184:ARG:NH1 | 2.33 | 0.61 |
| 1:3:48:THR:O | 1:3:50:LEU:N | 2.33 | 0.61 |
| 3:G:73:ARG:HB3 | 3:G:78:LYS:HZ2 | 1.65 | 0.61 |
| 2:M:95:LYS:HA | 2:M:109:MET:HA | 1.82 | 0.61 |
| 2:I:139:VAL:O | 2:I:184:ARG:HD3 | 2.00 | 0.61 |
| 2:V:28:VAL:HG22 | 2:V:110:THR:HG22 | 1.83 | 0.61 |
| 3:Z:77:GLU:HB2 | 3:Z:81:ARG:HH12 | 1.65 | 0.61 |
| 1:0:79:LEU:HB3 | 1:0:85:TYR:CE2 | 2.34 | 0.61 |
| 1:3:88:ARG:HB3 | 1:3:102:GLN:HG2 | 1.82 | 0.61 |
| 2:1:91:PHE:CE2 | 2:1:114:SER:HB2 | 2.35 | 0.61 |
| 3:2:96:LEU:HD12 | 3:2:97:GLN:N | 2.16 | 0.61 |
| 1:6:160:LYS:HE3 | 1:6:165:GLU:HB2 | 1.81 | 0.61 |
| 1:9:88:ARG:HD3 | 1:9:100:TRP:CG | 2.36 | 0.61 |
| 2:4:204:LEU:HG | 2:4:211:GLU:HG3 | 1.82 | 0.61 |
| 2:P:48:THR:OG1 | 2:P:50:ASP:OD1 | 2.12 | 0.61 |
| 2:4:91:PHE:CE2 | 2:4:114:SER:HB2 | 2.35 | 0.61 |
| 2:A:98:ALA:HB3 | 2:A:106:VAL:HG23 | 1.82 | 0.61 |
| 2:4:155:THR:HG23 | 2:4:158:GLU:H | 1.66 | 0.60 |
| 2:P:195:THR:O | 2:P:221:THR:HG22 | 2.01 | 0.60 |
| 3:Z:72:VAL:HG13 | 3:Z:162:LYS:HE3 | 1.83 | 0.60 |
| 3:Z:170:LEU:HD23 | 3:Z:174:LEU:HD22 | 1.83 | 0.60 |
| 2:B:91:PHE:CE2 | 2:B:114:SER:HB2 | 2.36 | 0.60 |
| 1:U:55:GLN:NE2 | 1:U:64:ASP:OD1 | 2.30 | 0.60 |
| 1:0:51:THR:O | 1:0:92:GLU:N | 2.32 | 0.60 |
| 3:2:96:LEU:HD21 | 3:2:129:LEU:HD12 | 1.83 | 0.60 |
| 3:2:141:ILE:O | 3:2:145:VAL:HG23 | 2.02 | 0.60 |
| 2:M:167:LEU:HG | 2:M:201:ILE:HG23 | 1.84 | 0.60 |
| 1:H:80:SER:O | 1:H:107:PRO:HG2 | 2.02 | 0.60 |
| 2:I:144:THR:HG21 | 2:I:159:ILE:HD11 | 1.83 | 0.60 |
| 3:Z:100:LEU:HD23 | 3:Z:104:LEU:HD12 | 1.84 | 0.60 |
| 3:8:49:SER:OG | 1:9:148:ILE:O | 2.11 | 0.60 |
| 3:W:115:MET:O | 3:W:119:VAL:HG13 | 2.01 | 0.60 |
| 2:S:114:SER:HB3 | 2:S:117:GLN:HG3 | 1.83 | 0.60 |
| 3:W:42:LEU:N | 3:W:178:CYS:O | 2.32 | 0.60 |
| 3:Z:92:MET:HB3 | 3:Z:174:LEU:CD1 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:24:LEU:HB3 | 2:F:44:GLY:HA3 | 1.83 | 0.59 |
| 3:Z:103:VAL:O | 3:Z:107:GLN:CB | 2.50 | 0.59 |
| 3:Z:98:PHE:HZ | 3:Z:152:VAL:HG11 | 1.66 | 0.59 |
| 2:S:194:ASP:HA | 2:S:221:THR:O | 2.02 | 0.59 |
| 3:L:98:PHE:CZ | 3:L:152:VAL:HG11 | 2.36 | 0.59 |
| 1:U:119:GLN:OE1 | 14:U:301:HOH:O | 2.17 | 0.59 |
| 2:V:170:HIS:ND1 | 2:V:176:GLN:HG2 | 2.18 | 0.59 |
| 1:H:35:LYS:HD3 | 1:H:137:GLU:HG3 | 1.83 | 0.59 |
| 2:1:154:LEU:O | 14:1:401:HOH:O | 2.17 | 0.59 |
| 1:K:116:PRO:HG2 | 1:K:191:VAL:HG22 | 1.84 | 0.59 |
| 2:M:58:LYS:NZ | 2:M:62:GLU:O | 2.24 | 0.59 |
| 2:S:25:LEU:O | 2:S:108:LYS:NZ | 2.28 | 0.59 |
| 2:4:51:THR:HA | 2:4:100:SER:HB3 | 1.85 | 0.59 |
| 2:A:148:SER:HB3 | 2:A:154:LEU:HD21 | 1.84 | 0.59 |
| 2:P:94:ALA:H | 2:P:110:THR:HG22 | 1.66 | 0.59 |
| 1:C:120:ILE:HD12 | 1:C:208:ILE:HG22 | 1.84 | 0.59 |
| 3:T:117:GLU:HG3 | 14:T:301:HOH:O | 2.02 | 0.59 |
| 3:8:119:VAL:HG22 | 3:8:120:PRO:HD3 | 1.85 | 0.59 |
| 3:G:149:LYS:O | 3:G:153:LYS:HG2 | 2.03 | 0.59 |
| 2:V:131:LYS:NZ | 14:V:402:HOH:O | 2.34 | 0.59 |
| 1:X:32:VAL:HG22 | 1:X:112:ILE:HB | 1.84 | 0.59 |
| 2:7:130:PRO:HA | 2:7:135:ILE:HD13 | 1.85 | 0.59 |
| 1:R:79:LEU:HB3 | 1:R:85:TYR:CE2 | 2.38 | 0.59 |
| 2:V:33:SER:O | 2:V:36:GLU:HG2 | 2.02 | 0.59 |
| 2:V:148:SER:HB3 | 2:V:154:LEU:HD21 | 1.84 | 0.59 |
| 1:X:179:ARG:O | 1:X:181:LEU:HD13 | 2.03 | 0.59 |
| 2:7:133:ARG:HG3 | 2:7:191:LEU:O | 2.02 | 0.58 |
| 2:1:123:PRO:HG3 | 2:1:213:ALA:HB3 | 1.85 | 0.58 |
| 1:R:21:ILE:HG12 | 1:R:93:LEU:HD23 | 1.85 | 0.58 |
| 2:4:126:VAL:HG22 | 2:4:139:VAL:HG22 | 1.84 | 0.58 |
| 1:9:127:LEU:HD21 | 1:9:212:THR:HG22 | 1.85 | 0.58 |
| 1:E:136:ILE:HD12 | 1:E:143:TRP:HB3 | 1.85 | 0.58 |
| 1:H:145:LEU:HA | 1:H:148:ILE:HD12 | 1.85 | 0.58 |
| 3:W:137:ASP:OD1 | 3:W:139:GLN:HG2 | 2.04 | 0.58 |
| 1:E:142:THR:O | 1:E:142:THR:OG1 | 2.21 | 0.58 |
| 1:X:146:LYS:NZ | 1:X:174:ASP:OD1 | 2.32 | 0.58 |
| 2:7:155:THR:HG23 | 2:7:158:GLU:H | 1.67 | 0.58 |
| 1:R:145:LEU:HA | 1:R:148:ILE:HD12 | 1.86 | 0.58 |
| 1:R:183:PRO:HB2 | 1:R:184:TRP:CE3 | 2.38 | 0.58 |
| 1:X:136:ILE:CD1 | 1:X:148:ILE:HD11 | 2.34 | 0.58 |
| 1:6:142:THR:O | 1:6:142:THR:OG1 | 2.16 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:198:LEU:HD12 | 2:B:217:CYS:O | 2.04 | 0.58 |
| 1:0:125:GLU:HG2 | 1:0:183:PRO:HB3 | 1.86 | 0.58 |
| 3:G:58:MET:HG2 | 3:G:114:TYR:CZ | 2.39 | 0.58 |
| 3:5:41:LYS:HZ1 | 3:5:86:LYS:HD3 | 1.69 | 0.57 |
| 1:6:81:LYS:O | 1:6:108:VAL:HG13 | 2.05 | 0.57 |
| 1:X:136:ILE:HG23 | 1:X:145:LEU:HD12 | 1.86 | 0.57 |
| 3:N:99:THR:HA | 3:N:103:VAL:HG23 | 1.85 | 0.57 |
| 2:V:24:LEU:HD22 | 2:V:45:PRO:HD2 | 1.86 | 0.57 |
| 2:1:34:ASN:HB2 | 2:1:122:LYS:HD2 | 1.85 | 0.57 |
| 3:8:45:ARG:NH2 | 1:9:151:SER:OG | 2.37 | 0.57 |
| 1:R:108:VAL:HG12 | 14:R:301:HOH:O | 2.04 | 0.57 |
| 1:H:22:PRO:HG2 | 1:H:43:PRO:HB2 | 1.86 | 0.57 |
| 2:P:195:THR:H | 2:P:221:THR:HG23 | 1.70 | 0.57 |
| 3:W:175:ARG:O | 3:W:179:VAL:HG12 | 2.04 | 0.57 |
| 2:4:216:VAL:HG11 | 1:E:48:THR:HG23 | 1.85 | 0.57 |
| 1:6:183:PRO:HB2 | 1:6:184:TRP:CE3 | 2.39 | 0.57 |
| 1:9:195:LEU:HD13 | 1:9:200:ARG:HD2 | 1.87 | 0.57 |
| 1:K:35:LYS:HD2 | 1:K:77:SER:OG | 2.04 | 0.57 |
| 1:6:123:LEU:HD13 | 1:6:124:ALA:H | 1.69 | 0.57 |
| 3:T:169:LEU:O | 3:T:173:SER:OG | 2.23 | 0.57 |
| 3:N:91:LEU:O | 3:N:95:VAL:HG23 | 2.05 | 0.57 |
| 3:W:100:LEU:HD23 | 3:W:104:LEU:HD12 | 1.86 | 0.57 |
| 1:X:136:ILE:HD11 | 1:X:143:TRP:HB2 | 1.86 | 0.57 |
| 2:7:218:ARG:NH2 | 1:X:50:LEU:O | 2.35 | 0.57 |
| 2:B:144:THR:HG22 | 14:B:401:HOH:O | 2.05 | 0.57 |
| 2:F:114:SER:HB3 | 2:F:117:GLN:HG3 | 1.87 | 0.57 |
| 1:H:136:ILE:HG22 | 1:H:145:LEU:HD12 | 1.87 | 0.57 |
| 3:8:120:PRO:HB3 | 1:9:83:GLY:HA2 | 1.87 | 0.57 |
| 3:L:79:LEU:HD21 | 3:L:148:LEU:HB2 | 1.87 | 0.57 |
| 2:4:177:MET:HE2 | 2:4:188:PHE:CD1 | 2.40 | 0.56 |
| 1:X:30:ASN:N | 1:X:37:ILE:O | 2.36 | 0.56 |
| 2:4:64:LYS:HD3 | 2:4:65:TRP:N | 2.20 | 0.56 |
| 2:B:48:THR:C | 2:B:50:ASP:H | 2.09 | 0.56 |
| 2:I:58:LYS:HZ2 | 2:I:65:TRP:HE1 | 1.53 | 0.56 |
| 3:J:83:VAL:HG13 | 3:J:141:ILE:HG12 | 1.87 | 0.56 |
| 2:P:169:LEU:HD11 | 2:P:197:PHE:HB3 | 1.87 | 0.56 |
| 3:W:120:PRO:HG2 | 1:X:80:SER:OG | 2.05 | 0.56 |
| 1:X:48:THR:HG22 | 1:X:48:THR:O | 2.04 | 0.56 |
| 2:1:173:HIS:HB2 | 1:C:68:ARG:HB2 | 1.87 | 0.56 |
| 1:3:109:GLU:N | 1:3:109:GLU:OE1 | 2.36 | 0.56 |
| 2:4:192:THR:HG23 | 2:4:195:THR:OG1 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:9:186:THR:OG1 | 1:9:212:THR:HG23 | 2.05 | 0.56 |
| 2:B:65:TRP:CD2 | 2:B:95:LYS:HE3 | 2.41 | 0.56 |
| 2:A:181:GLY:HA2 | 1:C:173:TYR:CZ | 2.41 | 0.56 |
| 1:X:214:ASN:ND2 | 1:X:216:GLU:O | 2.38 | 0.56 |
| 1:3:21:ILE:HG13 | 1:3:98:SER:HB2 | 1.87 | 0.56 |
| 3:8:55:ARG:NH2 | 1:9:141:GLU:OE1 | 2.39 | 0.56 |
| 1:9:134:PRO:HB2 | 1:9:145:LEU:HD13 | 1.87 | 0.56 |
| 3:D:103:VAL:HG11 | 3:D:163:ALA:HB3 | 1.88 | 0.56 |
| 3:G:93:LYS:HZ1 | 3:G:130:SER:HA | 1.70 | 0.56 |
| 3:J:49:SER:O | 3:J:53:VAL:HG13 | 2.05 | 0.56 |
| 2:M:173:HIS:HB2 | 1:U:68:ARG:HB2 | 1.88 | 0.56 |
| 3:W:99:THR:O | 3:W:103:VAL:HG22 | 2.06 | 0.56 |
| 3:8:98:PHE:HZ | 3:8:152:VAL:HG21 | 1.71 | 0.56 |
| 1:9:123:LEU:CD2 | 1:9:125:GLU:HB2 | 2.35 | 0.56 |
| 1:9:158:TYR:HB3 | 1:9:189:ILE:HG22 | 1.86 | 0.56 |
| 2:V:65:TRP:CZ2 | 2:V:95:LYS:HD2 | 2.41 | 0.56 |
| 3:2:99:THR:HA | 3:2:103:VAL:CG2 | 2.36 | 0.56 |
| 1:3:31:SER:OG | 1:3:36:ASN:OD1 | 2.20 | 0.56 |
| 2:4:91:PHE:CD2 | 2:4:114:SER:HB2 | 2.41 | 0.56 |
| 3:8:67:ASP:OD2 | 3:8:162:LYS:HE2 | 2.05 | 0.56 |
| 3:D:59:LEU:HD13 | 3:D:114:TYR:HB2 | 1.87 | 0.56 |
| 2:I:59:LYS:O | 2:I:62:GLU:HG2 | 2.06 | 0.56 |
| 3:J:99:THR:HA | 3:J:103:VAL:HG13 | 1.87 | 0.56 |
| 3:L:107:GLN:NE2 | 3:L:160:GLU:OE1 | 2.39 | 0.56 |
| 2:M:218:ARG:NH2 | 1:U:50:LEU:O | 2.39 | 0.56 |
| 2:1:88:HIS:HA | 2:1:115:SER:OG | 2.06 | 0.55 |
| 2:P:126:VAL:HG22 | 2:P:139:VAL:HG12 | 1.87 | 0.55 |
| 1:R:180:ASN:O | 1:R:181:LEU:HD23 | 2.06 | 0.55 |
| 1:U:160:LYS:NZ | 1:U:182:GLU:OE1 | 2.32 | 0.55 |
| 2:1:91:PHE:HD2 | 2:1:112:ARG:HG2 | 1.71 | 0.55 |
| 1:3:127:LEU:HB2 | 1:3:178:LEU:HD12 | 1.88 | 0.55 |
| 3:L:107:GLN:NE2 | 3:L:157:GLU:OE2 | 2.39 | 0.55 |
| 2:M:162:ASP:HB2 | 2:M:206:PRO:HD2 | 1.88 | 0.55 |
| 1:E:194:PHE:CE2 | 1:E:196:LEU:HD12 | 2.42 | 0.55 |
| 2:V:34:ASN:CG | 2:V:122:LYS:HG2 | 2.27 | 0.55 |
| 3:W:42:LEU:HD13 | 3:W:125:LEU:HD22 | 1.89 | 0.55 |
| 2:4:178:HIS:O | 2:4:179:LEU:HD22 | 2.06 | 0.55 |
| 2:4:191:LEU:HD23 | 2:4:197:PHE:CE1 | 2.41 | 0.55 |
| 1:O:32:VAL:HG12 | 1:O:112:ILE:HB | 1.88 | 0.55 |
| 3:2:124:LYS:HE3 | 1:3:109:GLU:OE2 | 2.07 | 0.55 |
| 1:9:21:ILE:HG13 | 1:9:98:SER:HB2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:9:126:SER:HB3 | 1:9:178:LEU:O | 2.05 | 0.55 |
| 3:J:143:LYS:O | 3:J:146:ARG:HG2 | 2.07 | 0.55 |
| 1:K:120:ILE:HD13 | 1:K:189:ILE:HD13 | 1.89 | 0.55 |
| 2:S:146:VAL:HG23 | 2:S:154:LEU:HD12 | 1.88 | 0.55 |
| 2:V:65:TRP:CH2 | 2:V:95:LYS:HD2 | 2.42 | 0.55 |
| 2:7:61:GLY:HA3 | 3:8:73:ARG:HB2 | 1.89 | 0.55 |
| 2:B:167:LEU:HD23 | 2:B:167:LEU:N | 2.22 | 0.55 |
| 3:Q:51:TYR:HD2 | 3:Q:52:ILE:HD13 | 1.72 | 0.55 |
| 3:T:145:VAL:O | 3:T:149:LYS:HG3 | 2.06 | 0.55 |
| 1:X:35:LYS:HE2 | 1:X:37:ILE:HD11 | 1.87 | 0.55 |
| 1:0:136:ILE:HG21 | 1:0:148:ILE:HD11 | 1.89 | 0.54 |
| 1:0:172:PRO:HG2 | 1:0:173:TYR:CE2 | 2.41 | 0.54 |
| 2:1:35:PHE:CE2 | 2:1:159:ILE:HD13 | 2.43 | 0.54 |
| 1:K:40:TRP:O | 1:K:72:THR:OG1 | 2.25 | 0.54 |
| 2:M:164:PHE:HE1 | 2:M:206:PRO:HG3 | 1.72 | 0.54 |
| 1:0:113:ILE:HD12 | 1:0:145:LEU:HD23 | 1.89 | 0.54 |
| 2:1:119:THR:O | 2:1:210:LYS:HE3 | 2.07 | 0.54 |
| 1:E:23:PRO:O | 1:E:43:PRO:HB3 | 2.08 | 0.54 |
| 1:H:122:SER:OG | 1:H:212:THR:O | 2.25 | 0.54 |
| 3:J:146:ARG:O | 3:J:150:GLU:HG2 | 2.07 | 0.54 |
| 2:S:144:THR:HG21 | 2:S:159:ILE:HD11 | 1.88 | 0.54 |
| 1:X:160:LYS:NZ | 1:X:185:THR:HG21 | 2.21 | 0.54 |
| 1:9:55:GLN:HG2 | 1:9:64:ASP:HA | 1.87 | 0.54 |
| 2:A:139:VAL:HG11 | 2:A:165:TYR:CZ | 2.42 | 0.54 |
| 2:F:200:SER:OG | 1:U:46:PRO:HG2 | 2.07 | 0.54 |
| 1:X:159:TRP:HZ3 | 1:X:162:GLY:H | 1.54 | 0.54 |
| 2:1:24:LEU:HB2 | 2:1:46:ALA:HB3 | 1.89 | 0.54 |
| 2:7:207:ILE:HG22 | 2:7:208:LEU:HD12 | 1.90 | 0.54 |
| 1:K:142:THR:O | 1:K:142:THR:OG1 | 2.25 | 0.54 |
| 2:V:83:MET:HE3 | 2:V:86:ARG:HD2 | 1.89 | 0.54 |
| 1:0:40:TRP:NE1 | 1:0:72:THR:HA | 2.22 | 0.54 |
| 1:0:197:ASP:OD2 | 3:Z:45:ARG:HD3 | 2.07 | 0.54 |
| 1:H:45:PHE:CD1 | 1:H:46:PRO:HD2 | 2.43 | 0.54 |
| 2:1:147:LEU:HD12 | 2:1:151:GLY:O | 2.07 | 0.54 |
| 1:3:135:GLN:NE2 | 14:3:304:HOH:O | 2.40 | 0.54 |
| 1:E:53:THR:N | 14:E:303:HOH:O | 2.39 | 0.54 |
| 3:G:77:GLU:CD | 3:G:81:ARG:NH1 | 2.60 | 0.54 |
| 2:V:126:VAL:HB | 2:V:215:TYR:CD2 | 2.43 | 0.54 |
| 1:6:159:TRP:HZ3 | 1:6:163:THR:H | 1.56 | 0.54 |
| 1:U:155:ARG:NH1 | 1:U:168:GLN:OE1 | 2.37 | 0.54 |
| 3:W:47:PHE:HE2 | 3:W:174:LEU:HB3 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Z:151:THR:HG22 | 3:Z:154:LYS:HE2 | 1.90 | 0.54 |
| 3:8:100:LEU:O | 3:8:105:LEU:HD13 | 2.08 | 0.54 |
| 3:D:88:GLN:O | 3:D:92:MET:HG2 | 2.07 | 0.54 |
| 3:J:93:LYS:NZ | 3:J:132:CYS:O | 2.37 | 0.54 |
| 3:L:91:LEU:O | 3:L:95:VAL:HG13 | 2.08 | 0.54 |
| 2:S:60:TYR:CE2 | 3:T:73:ARG:HG3 | 2.43 | 0.54 |
| 3:8:75:ILE:HG22 | 3:8:166:GLU:OE1 | 2.08 | 0.54 |
| 2:M:29:LYS:HA | 2:M:110:THR:HG22 | 1.90 | 0.54 |
| 1:O:67:LYS:HE3 | 1:O:68:ARG:NH2 | 2.23 | 0.54 |
| 1:R:117:GLU:HB2 | 1:R:132:SER:HB2 | 1.89 | 0.54 |
| 3:2:108:SER:HA | 3:2:115:MET:HE1 | 1.90 | 0.54 |
| 2:4:156:LEU:N | 14:4:401:HOH:O | 2.41 | 0.54 |
| 3:D:67:ASP:OD1 | 3:D:162:LYS:NZ | 2.39 | 0.54 |
| 3:G:44:VAL:HG13 | 3:G:179:VAL:HG21 | 1.90 | 0.54 |
| 3:J:75:ILE:HD11 | 3:J:173:SER:HB2 | 1.90 | 0.54 |
| 2:V:24:LEU:CD2 | 2:V:45:PRO:HD2 | 2.38 | 0.54 |
| 2:V:74:ILE:HD13 | 2:V:76:GLN:HG2 | 1.90 | 0.54 |
| 2:A:42:ASP:OD2 | 2:Y:132:VAL:HG22 | 2.08 | 0.53 |
| 3:D:147:ARG:HH22 | 3:D:154:LYS:HD3 | 1.73 | 0.53 |
| 1:H:188:CYS:O | 1:H:189:ILE:HD13 | 2.07 | 0.53 |
| 1:U:141:GLU:HB2 | 1:U:143:TRP:CD1 | 2.43 | 0.53 |
| 1:U:184:TRP:HD1 | 1:U:213:GLY:CA | 2.18 | 0.53 |
| 3:8:115:MET:O | 3:8:119:VAL:HG13 | 2.07 | 0.53 |
| 1:9:192:GLN:HG2 | 1:9:204:TRP:CZ3 | 2.44 | 0.53 |
| 1:C:181:LEU:HB3 | 1:C:187:TYR:CZ | 2.43 | 0.53 |
| 3:D:48:GLN:O | 3:D:50:PRO:HD3 | 2.07 | 0.53 |
| 1:K:164:ASN:OD1 | 1:K:164:ASN:N | 2.41 | 0.53 |
| 2:Y:130:PRO:HA | 2:Y:135:ILE:HD13 | 1.89 | 0.53 |
| 2:4:86:ARG:HH21 | 2:4:147:LEU:HD11 | 1.73 | 0.53 |
| 3:T:79:LEU:HD21 | 3:T:95:VAL:HG21 | 1.90 | 0.53 |
| 1:9:51:THR:O | 1:9:92:GLU:N | 2.41 | 0.53 |
| 2:A:144:THR:CG2 | 2:A:146:VAL:HG13 | 2.38 | 0.53 |
| 2:F:94:ALA:O | 2:F:110:THR:HG23 | 2.07 | 0.53 |
| 1:H:158:TYR:CB | 1:H:189:ILE:HD12 | 2.38 | 0.53 |
| 1:H:184:TRP:CD2 | 1:H:213:GLY:HA2 | 2.44 | 0.53 |
| 2:M:123:PRO:HG3 | 2:M:213:ALA:HB3 | 1.91 | 0.53 |
| 1:0:135:GLN:HG3 | 1:0:143:TRP:O | 2.08 | 0.53 |
| 1:3:55:GLN:HG2 | 1:3:64:ASP:HA | 1.90 | 0.53 |
| 2:7:173:HIS:HB2 | 1:X:68:ARG:HB2 | 1.90 | 0.53 |
| 3:8:116:TRP:N | 14:8:302:HOH:O | 2.41 | 0.53 |
| 3:N:57:PHE:HZ | 3:N:172:MET:HE2 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:131:PHE:CE1 | 1:R:191:VAL:HG11 | 2.44 | 0.53 |
| 2:7:24:LEU:HD13 | 2:7:45:PRO:HD2 | 1.91 | 0.53 |
| 2:7:173:HIS:HA | 1:X:68:ARG:HH21 | 1.74 | 0.53 |
| 2:M:58:LYS:HE3 | 2:M:65:TRP:CZ2 | 2.44 | 0.53 |
| 1:R:68:ARG:HA | 1:R:92:GLU:OE2 | 2.09 | 0.53 |
| 2:S:162:ASP:HB2 | 2:S:206:PRO:HD2 | 1.90 | 0.53 |
| 3:2:51:TYR:OH | 1:3:139:GLU:OE2 | 2.20 | 0.53 |
| 2:4:177:MET:HE2 | 2:4:188:PHE:HD1 | 1.73 | 0.53 |
| 3:8:67:ASP:OD1 | 3:8:162:LYS:HE2 | 2.09 | 0.53 |
| 2:B:86:ARG:HD3 | 2:B:145:PRO:O | 2.09 | 0.53 |
| 2:F:29:LYS:O | 2:F:39:LEU:HD12 | 2.09 | 0.53 |
| 1:C:48:THR:O | 1:C:50:LEU:N | 2.37 | 0.53 |
| 1:C:184:TRP:HD1 | 1:C:211:ARG:HH21 | 1.56 | 0.53 |
| 2:I:83:MET:O | 2:I:86:ARG:HG3 | 2.08 | 0.53 |
| 2:V:58:LYS:HE3 | 2:V:65:TRP:NE1 | 2.23 | 0.53 |
| 2:1:110:THR:HB | 14:1:407:HOH:O | 2.10 | 0.53 |
| 3:8:78:LYS:HD2 | 3:8:78:LYS:N | 2.24 | 0.53 |
| 3:8:120:PRO:HG2 | 1:9:80:SER:OG | 2.09 | 0.53 |
| 1:9:57:GLU:HB3 | 1:9:86:THR:HG23 | 1.90 | 0.53 |
| 3:J:134:ILE:HD13 | 3:J:136:GLY:N | 2.24 | 0.53 |
| 3:W:164:ILE:HA | 3:W:167:LEU:HD13 | 1.90 | 0.53 |
| 1:X:124:ALA:O | 1:X:126:SER:N | 2.42 | 0.53 |
| 2:Y:115:SER:HA | 14:Y:406:HOH:O | 2.09 | 0.53 |
| 3:5:147:ARG:O | 3:5:151:THR:OG1 | 2.27 | 0.52 |
| 2:M:195:THR:HB | 2:M:197:PHE:CE1 | 2.44 | 0.52 |
| 2:V:114:SER:HB3 | 2:V:117:GLN:HG3 | 1.91 | 0.52 |
| 2:4:142:THR:O | 14:4:401:HOH:O | 2.19 | 0.52 |
| 1:9:51:THR:HG23 | 1:9:92:GLU:HB2 | 1.90 | 0.52 |
| 1:6:57:GLU:HA | 1:6:62:PHE:HA | 1.92 | 0.52 |
| 1:6:143:TRP:O | 1:6:147:ASN:ND2 | 2.43 | 0.52 |
| 3:J:143:LYS:HA | 3:J:146:ARG:HG2 | 1.89 | 0.52 |
| 1:O:124:ALA:O | 1:O:126:SER:N | 2.42 | 0.52 |
| 1:U:139:GLU:HG2 | 1:U:143:TRP:CD1 | 2.44 | 0.52 |
| 2:Y:74:ILE:HD12 | 2:Y:76:GLN:HG2 | 1.90 | 0.52 |
| 2:1:155:THR:HG23 | 2:1:158:GLU:H | 1.75 | 0.52 |
| 1:3:151:SER:HB3 | 1:3:195:LEU:HD12 | 1.91 | 0.52 |
| 1:X:190:GLN:HE21 | 1:X:207:PRO:N | 2.08 | 0.52 |
| 2:Y:146:VAL:HG22 | 2:Y:154:LEU:HD23 | 1.92 | 0.52 |
| 3:2:116:TRP:O | 1:3:80:SER:OG | 2.28 | 0.52 |
| 2:P:155:THR:OG1 | 2:P:156:LEU:N | 2.43 | 0.52 |
| 2:7:25:LEU:HD21 | 2:7:28:VAL:CG2 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:201:ILE:HG23 | 2:B:215:TYR:HB3 | 1.91 | 0.52 |
| 1:C:55:GLN:HG2 | 1:C:64:ASP:HA | 1.92 | 0.52 |
| 1:O:143:TRP:HB3 | 1:O:148:ILE:HD11 | 1.91 | 0.52 |
| 1:X:33:ASN:HD21 | 1:X:114:GLY:HA3 | 1.75 | 0.52 |
| 3:G:44:VAL:HG12 | 3:G:179:VAL:HG11 | 1.91 | 0.52 |
| 1:O:125:GLU:HG2 | 1:O:183:PRO:HB3 | 1.91 | 0.52 |
| 1:O:177:VAL:HG11 | 1:O:179:ARG:NH2 | 2.24 | 0.52 |
| 3:Q:69:ASN:O | 3:Q:162:LYS:NZ | 2.38 | 0.52 |
| 1:R:68:ARG:HG2 | 1:R:92:GLU:OE2 | 2.10 | 0.52 |
| 2:S:156:LEU:HA | 14:S:410:HOH:O | 2.09 | 0.52 |
| 2:V:58:LYS:HG2 | 2:V:95:LYS:NZ | 2.25 | 0.52 |
| 3:8:49:SER:O | 3:8:53:VAL:HG12 | 2.09 | 0.52 |
| 3:G:163:ALA:O | 3:G:167:LEU:HD13 | 2.09 | 0.52 |
| 3:Q:145:VAL:O | 3:Q:149:LYS:HG3 | 2.10 | 0.52 |
| 2:7:162:ASP:HB2 | 2:7:206:PRO:HD2 | 1.92 | 0.52 |
| 1:C:35:LYS:HE2 | 1:C:37:ILE:HD11 | 1.91 | 0.52 |
| 1:C:111:THR:O | 1:C:200:ARG:NH2 | 2.43 | 0.52 |
| 3:N:41:LYS:HG3 | 3:N:178:CYS:O | 2.10 | 0.52 |
| 3:Q:103:VAL:O | 3:Q:107:GLN:HB2 | 2.10 | 0.52 |
| 2:B:123:PRO:O | 14:B:403:HOH:O | 2.19 | 0.52 |
| 2:I:90:GLU:OE2 | 3:J:73:ARG:NH2 | 2.29 | 0.52 |
| 3:2:92:MET:HA | 3:2:95:VAL:HG22 | 1.92 | 0.51 |
| 2:7:25:LEU:HD12 | 2:7:98:ALA:HB2 | 1.92 | 0.51 |
| 1:9:51:THR:CG2 | 1:9:92:GLU:HB2 | 2.40 | 0.51 |
| 1:9:151:SER:HB3 | 1:9:196:LEU:HB3 | 1.92 | 0.51 |
| 2:P:180:GLU:OE1 | 1:R:173:TYR:HB3 | 2.10 | 0.51 |
| 2:P:195:THR:H | 2:P:221:THR:CG2 | 2.22 | 0.51 |
| 3:T:47:PHE:CD2 | 3:T:175:ARG:HB2 | 2.44 | 0.51 |
| 1:X:159:TRP:CZ3 | 1:X:161:GLN:HA | 2.45 | 0.51 |
| 2:Y:155:THR:HG23 | 2:Y:158:GLU:H | 1.75 | 0.51 |
| 3:Z:69:ASN:OD1 | 3:Z:72:VAL:HG12 | 2.10 | 0.51 |
| 3:Z:99:THR:HA | 3:Z:103:VAL:HG13 | 1.92 | 0.51 |
| 1:H:33:ASN:HD21 | 1:H:114:GLY:HA3 | 1.75 | 0.51 |
| 1:3:149:TYR:N | 1:3:149:TYR:HD1 | 2.08 | 0.51 |
| 1:6:184:TRP:HB3 | 1:6:211:ARG:NH2 | 2.25 | 0.51 |
| 3:G:99:THR:HA | 3:G:103:VAL:HG23 | 1.93 | 0.51 |
| 3:J:75:ILE:HD11 | 3:J:173:SER:CB | 2.40 | 0.51 |
| 1:O:40:TRP:O | 1:O:72:THR:OG1 | 2.28 | 0.51 |
| 1:O:177:VAL:HG11 | 1:O:179:ARG:HH21 | 1.76 | 0.51 |
| 2:P:195:THR:HB | 2:P:197:PHE:CE1 | 2.45 | 0.51 |
| 1:0:21:ILE:HD11 | 1:0:91:ALA:O | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:34:PHE:CD2 | 1:E:136:ILE:HG23 | 2.46 | 0.51 |
| 1:H:172:PRO:HG2 | 1:H:173:TYR:CE2 | 2.44 | 0.51 |
| 2:B:144:THR:HG23 | 2:B:146:VAL:HG13 | 1.93 | 0.51 |
| 1:E:184:TRP:H | 1:E:213:GLY:H | 1.57 | 0.51 |
| 1:H:27:VAL:HG22 | 1:H:40:TRP:HB3 | 1.92 | 0.51 |
| 2:P:168:GLU:HA | 2:P:178:HIS:HB3 | 1.91 | 0.51 |
| 1:U:55:GLN:HG2 | 1:U:64:ASP:HA | 1.92 | 0.51 |
| 1:3:149:TYR:N | 1:3:149:TYR:CD1 | 2.79 | 0.51 |
| 2:4:41:TRP:CE2 | 2:4:77:LYS:HA | 2.46 | 0.51 |
| 1:H:185:THR:O | 1:H:212:THR:HG23 | 2.10 | 0.51 |
| 1:U:118:MET:HE3 | 1:U:131:PHE:HE1 | 1.76 | 0.51 |
| 3:2:110:ARG:NE | 3:2:111:PHE:H | 2.08 | 0.51 |
| 3:D:98:PHE:HZ | 3:D:152:VAL:HG11 | 1.76 | 0.51 |
| 3:G:105:LEU:O | 1:H:59:TYR:OH | 2.19 | 0.51 |
| 3:T:53:VAL:HG22 | 3:T:171:PHE:CZ | 2.45 | 0.51 |
| 1:0:33:ASN:HD21 | 1:0:114:GLY:HA3 | 1.75 | 0.51 |
| 1:3:160:LYS:O | 1:3:163:THR:HG22 | 2.10 | 0.51 |
| 3:5:49:SER:HB3 | 3:5:52:ILE:CG1 | 2.38 | 0.51 |
| 3:Q:74:LEU:HB3 | 3:Q:148:LEU:HD11 | 1.93 | 0.51 |
| 2:V:60:TYR:CD1 | 2:V:93:TYR:HE1 | 2.29 | 0.51 |
| 2:4:117:GLN:HG3 | 2:4:118:HIS:CE1 | 2.46 | 0.51 |
| 1:C:48:THR:OG1 | 1:C:49:GLN:N | 2.41 | 0.51 |
| 1:E:155:ARG:O | 1:E:191:VAL:HA | 2.11 | 0.51 |
| 1:H:52:PHE:HE2 | 2:Y:218:ARG:NH2 | 2.08 | 0.51 |
| 1:H:206:GLU:N | 1:H:206:GLU:OE1 | 2.44 | 0.50 |
| 3:T:44:VAL:HG13 | 3:T:179:VAL:HG21 | 1.92 | 0.50 |
| 1:U:123:LEU:HG | 1:U:124:ALA:H | 1.75 | 0.50 |
| 2:F:28:VAL:HG12 | 2:F:110:THR:HG22 | 1.93 | 0.50 |
| 3:G:125:LEU:HD23 | 3:G:174:LEU:HD23 | 1.93 | 0.50 |
| 1:H:136:ILE:HD11 | 1:H:139:GLU:HG3 | 1.92 | 0.50 |
| 2:P:179:LEU:HD11 | 2:P:186:TYR:HD1 | 1.76 | 0.50 |
| 2:V:98:ALA:HB3 | 2:V:106:VAL:HG23 | 1.93 | 0.50 |
| 1:X:136:ILE:HD11 | 1:X:143:TRP:CB | 2.40 | 0.50 |
| 2:1:164:PHE:HE1 | 2:1:206:PRO:HG3 | 1.76 | 0.50 |
| 1:6:194:PHE:CE2 | 1:6:196:LEU:HG | 2.47 | 0.50 |
| 2:7:114:SER:H | 2:7:118:HIS:CD2 | 2.29 | 0.50 |
| 2:B:26:GLN:NE2 | 2:B:43:GLY:O | 2.43 | 0.50 |
| 1:E:92:GLU:HG3 | 14:E:303:HOH:O | 2.11 | 0.50 |
| 2:I:94:ALA:O | 2:I:110:THR:HG23 | 2.10 | 0.50 |
| 3:Z:175:ARG:O | 3:Z:179:VAL:HG12 | 2.12 | 0.50 |
| 2:A:126:VAL:HB | 2:A:215:TYR:CD2 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:90:ARG:HD2 | 1:E:97:HIS:HB2 | 1.94 | 0.50 |
| 2:A:91:PHE:CE2 | 2:A:114:SER:HB2 | 2.47 | 0.50 |
| 3:D:79:LEU:HD21 | 3:D:95:VAL:HG21 | 1.93 | 0.50 |
| 2:F:24:LEU:HG | 2:F:45:PRO:HG2 | 1.94 | 0.50 |
| 3:G:73:ARG:HB3 | 3:G:78:LYS:NZ | 2.26 | 0.50 |
| 3:G:95:VAL:HG13 | 3:G:148:LEU:HD11 | 1.93 | 0.50 |
| 1:H:136:ILE:CG2 | 1:H:148:ILE:HD11 | 2.38 | 0.50 |
| 3:T:72:VAL:CG2 | 3:T:162:LYS:HE3 | 2.42 | 0.50 |
| 1:U:105:PHE:CE2 | 1:U:107:PRO:HG3 | 2.47 | 0.50 |
| 2:1:29:LYS:HA | 2:1:110:THR:HG23 | 1.92 | 0.50 |
| 3:D:59:LEU:HD11 | 3:D:111:PHE:HB3 | 1.93 | 0.50 |
| 2:F:167:LEU:HD12 | 2:F:167:LEU:N | 2.27 | 0.50 |
| 3:J:61:LYS:O | 3:J:65:LEU:HD12 | 2.10 | 0.50 |
| 3:L:92:MET:HB3 | 3:L:174:LEU:HD13 | 1.93 | 0.50 |
| 2:B:201:ILE:CG2 | 2:B:215:TYR:HB3 | 2.41 | 0.50 |
| 1:C:88:ARG:HB3 | 1:C:102:GLN:HG2 | 1.93 | 0.50 |
| 3:T:100:LEU:HD23 | 3:T:104:LEU:HD12 | 1.93 | 0.50 |
| 2:7:28:VAL:HG22 | 2:7:41:TRP:HB3 | 1.93 | 0.50 |
| 3:8:78:LYS:HB2 | 14:8:301:HOH:O | 2.11 | 0.50 |
| 2:I:144:THR:HG22 | 2:I:154:LEU:O | 2.12 | 0.50 |
| 3:W:79:LEU:HG | 3:W:91:LEU:HD11 | 1.92 | 0.50 |
| 2:1:25:LEU:HD21 | 2:1:28:VAL:HG23 | 1.93 | 0.50 |
| 2:S:144:THR:CG2 | 2:S:146:VAL:H | 2.25 | 0.50 |
| 2:V:29:LYS:O | 2:V:39:LEU:HD12 | 2.12 | 0.50 |
| 1:0:21:ILE:HG13 | 1:0:98:SER:HB2 | 1.94 | 0.49 |
| 2:1:205:THR:OG1 | 2:1:210:LYS:HB2 | 2.11 | 0.49 |
| 2:4:41:TRP:O | 2:4:77:LYS:HB3 | 2.12 | 0.49 |
| 2:A:119:THR:O | 2:A:210:LYS:HE3 | 2.12 | 0.49 |
| 2:F:97:THR:HG23 | 2:F:107:THR:OG1 | 2.12 | 0.49 |
| 3:N:74:LEU:HB3 | 3:N:148:LEU:HD11 | 1.93 | 0.49 |
| 3:W:116:TRP:O | 1:X:80:SER:OG | 2.29 | 0.49 |
| 3:2:96:LEU:HD23 | 3:2:174:LEU:HD21 | 1.94 | 0.49 |
| 3:2:98:PHE:HD1 | 3:2:149:LYS:HE2 | 1.77 | 0.49 |
| 1:9:118:MET:HE2 | 1:9:120:ILE:HD11 | 1.94 | 0.49 |
| 2:F:139:VAL:O | 2:F:184:ARG:HD3 | 2.12 | 0.49 |
| 3:G:110:ARG:HD3 | 3:G:111:PHE:N | 2.27 | 0.49 |
| 1:U:177:VAL:HB | 1:U:179:ARG:NH2 | 2.26 | 0.49 |
| 1:X:160:LYS:HZ3 | 1:X:185:THR:HG21 | 1.77 | 0.49 |
| 1:3:81:LYS:O | 1:3:108:VAL:HG12 | 2.12 | 0.49 |
| 1:3:88:ARG:CB | 1:3:102:GLN:HG2 | 2.42 | 0.49 |
| 2:B:123:PRO:HG3 | 2:B:213:ALA:HB3 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:118:MET:HE2 | 1:C:191:VAL:HG12 | 1.93 | 0.49 |
| 2:P:162:ASP:HB2 | 2:P:206:PRO:HD2 | 1.94 | 0.49 |
| 2:P:178:HIS:NE2 | 1:R:130:ARG:CZ | 2.75 | 0.49 |
| 1:X:214:ASN:OD1 | 1:X:214:ASN:N | 2.38 | 0.49 |
| 3:5:48:GLN:NE2 | 1:6:150:ASP:OD2 | 2.44 | 0.49 |
| 2:P:97:THR:HG23 | 2:P:107:THR:OG1 | 2.12 | 0.49 |
| 1:R:27:VAL:HG22 | 1:R:40:TRP:HB3 | 1.94 | 0.49 |
| 1:3:48:THR:C | 1:3:50:LEU:H | 2.16 | 0.49 |
| 3:5:145:VAL:O | 3:5:149:LYS:HG2 | 2.13 | 0.49 |
| 2:F:169:LEU:HD11 | 2:F:197:PHE:HB3 | 1.94 | 0.49 |
| 3:Z:77:GLU:HB2 | 3:Z:81:ARG:NH1 | 2.28 | 0.49 |
| 2:F:170:HIS:ND1 | 2:F:176:GLN:HG2 | 2.27 | 0.49 |
| 1:K:185:THR:O | 1:K:212:THR:HG23 | 2.13 | 0.49 |
| 3:L:115:MET:O | 3:L:119:VAL:HG13 | 2.12 | 0.49 |
| 1:U:36:ASN:N | 1:U:77:SER:OG | 2.42 | 0.49 |
| 3:W:119:VAL:HG22 | 3:W:120:PRO:HD3 | 1.94 | 0.49 |
| 3:2:45:ARG:NE | 1:3:197:ASP:OD2 | 2.45 | 0.49 |
| 1:H:79:LEU:HB3 | 1:H:85:TYR:CE2 | 2.48 | 0.49 |
| 2:I:58:LYS:HG2 | 2:I:65:TRP:CD1 | 2.48 | 0.49 |
| 2:Y:126:VAL:HG11 | 2:Y:201:ILE:HD13 | 1.94 | 0.49 |
| 3:2:42:LEU:HD11 | 3:2:47:PHE:HE1 | 1.77 | 0.49 |
| 3:5:141:ILE:O | 3:5:145:VAL:HG13 | 2.13 | 0.49 |
| 1:6:184:TRP:HB3 | 1:6:211:ARG:HH21 | 1.78 | 0.49 |
| 3:8:99:THR:HA | 3:8:103:VAL:HG13 | 1.94 | 0.49 |
| 2:B:144:THR:HG21 | 2:B:159:ILE:HD11 | 1.94 | 0.49 |
| 2:B:200:SER:HA | 2:B:215:TYR:O | 2.12 | 0.49 |
| 3:D:91:LEU:HD13 | 3:D:141:ILE:HG23 | 1.95 | 0.49 |
| 2:F:173:HIS:HD1 | 1:U:20:MET:N | 2.10 | 0.49 |
| 2:I:167:LEU:HG | 2:I:201:ILE:HG23 | 1.95 | 0.49 |
| 3:Q:83:VAL:HG11 | 3:Q:91:LEU:HD22 | 1.95 | 0.49 |
| 2:V:139:VAL:HG11 | 2:V:165:TYR:CE1 | 2.48 | 0.49 |
| 2:Y:95:LYS:HA | 2:Y:109:MET:HA | 1.94 | 0.49 |
| 3:Z:82:GLY:O | 3:Z:140:ASN:ND2 | 2.34 | 0.49 |
| 3:Z:83:VAL:HG21 | 3:Z:91:LEU:HD22 | 1.94 | 0.49 |
| 1:3:88:ARG:HD2 | 1:3:100:TRP:CG | 2.48 | 0.49 |
| 2:7:137:MET:SD | 2:7:201:ILE:HD11 | 2.53 | 0.49 |
| 3:8:79:LEU:HD21 | 3:8:91:LEU:HD11 | 1.95 | 0.49 |
| 1:9:88:ARG:HD3 | 1:9:100:TRP:CD2 | 2.47 | 0.49 |
| 2:B:155:THR:HG23 | 2:B:158:GLU:H | 1.78 | 0.49 |
| 2:F:173:HIS:CD2 | 2:F:174:THR:HG23 | 2.47 | 0.49 |
| 2:V:54:SER:HA | 14:V:401:HOH:O | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:5:49:SER:CB | 3:5:52:ILE:HG12 | 2.40 | 0.49 |
| 1:9:90:ARG:NH1 | 1:9:92:GLU:HG2 | 2.28 | 0.49 |
| 2:B:136:GLN:NE2 | 2:B:185:GLU:OE2 | 2.45 | 0.49 |
| 3:D:162:LYS:HB2 | 3:D:162:LYS:HZ2 | 1.77 | 0.49 |
| 2:M:85:THR:HA | 2:M:92:TYR:CZ | 2.48 | 0.49 |
| 3:D:158:SER:O | 3:D:161:ILE:HG12 | 2.13 | 0.48 |
| 3:D:172:MET:HA | 3:D:172:MET:HE3 | 1.95 | 0.48 |
| 1:E:118:MET:HE2 | 1:E:191:VAL:HG12 | 1.95 | 0.48 |
| 1:H:42:VAL:HG12 | 1:H:52:PHE:CZ | 2.48 | 0.48 |
| 1:R:88:ARG:HB3 | 1:R:102:GLN:HG2 | 1.95 | 0.48 |
| 1:R:192:GLN:NE2 | 1:R:204:TRP:CE2 | 2.81 | 0.48 |
| 2:V:205:THR:HB | 2:V:210:LYS:HB2 | 1.94 | 0.48 |
| 3:2:79:LEU:HD23 | 3:2:148:LEU:HG | 1.95 | 0.48 |
| 3:2:116:TRP:CD1 | 1:3:80:SER:OG | 2.65 | 0.48 |
| 3:5:49:SER:HB3 | 3:5:52:ILE:CD1 | 2.43 | 0.48 |
| 1:6:35:LYS:HB2 | 1:6:137:GLU:HG3 | 1.95 | 0.48 |
| 2:7:91:PHE:CE2 | 2:7:114:SER:HB2 | 2.48 | 0.48 |
| 3:8:62:GLU:N | 3:8:62:GLU:OE1 | 2.45 | 0.48 |
| 1:C:53:THR:HA | 1:C:66:CYS:O | 2.12 | 0.48 |
| 2:M:74:ILE:HD12 | 2:M:76:GLN:HB2 | 1.93 | 0.48 |
| 2:S:159:ILE:HD12 | 14:S:410:HOH:O | 2.12 | 0.48 |
| 1:0:137:GLU:HG3 | 1:0:137:GLU:O | 2.13 | 0.48 |
| 2:1:55:VAL:HG22 | 2:1:96:VAL:HG22 | 1.94 | 0.48 |
| 2:1:117:GLN:O | 2:1:117:GLN:HG2 | 2.13 | 0.48 |
| 1:6:181:LEU:HB3 | 1:6:187:TYR:HE2 | 1.78 | 0.48 |
| 2:7:157:GLU:OE1 | 2:7:184:ARG:NH2 | 2.43 | 0.48 |
| 3:8:73:ARG:HH21 | 3:8:169:LEU:HD21 | 1.78 | 0.48 |
| 2:A:205:THR:OG1 | 2:A:210:LYS:HB2 | 2.13 | 0.48 |
| 2:Y:200:SER:HA | 2:Y:215:TYR:O | 2.13 | 0.48 |
| 1:0:122:SER:HB2 | 1:0:127:LEU:CD2 | 2.42 | 0.48 |
| 1:0:192:GLN:HG2 | 1:0:204:TRP:CZ3 | 2.49 | 0.48 |
| 1:C:90:ARG:HH11 | 1:C:97:HIS:CB | 2.27 | 0.48 |
| 3:G:72:VAL:HG23 | 3:G:162:LYS:NZ | 2.28 | 0.48 |
| 1:3:155:ARG:HD3 | 1:3:168:GLN:OE1 | 2.13 | 0.48 |
| 2:7:74:ILE:HB | 2:7:76:GLN:CD | 2.33 | 0.48 |
| 2:A:198:LEU:HD12 | 2:A:217:CYS:O | 2.14 | 0.48 |
| 2:B:124:PRO:HB3 | 2:B:203:ILE:HD11 | 1.95 | 0.48 |
| 2:P:24:LEU:HD22 | 2:P:45:PRO:HD2 | 1.94 | 0.48 |
| 3:T:39:ARG:HA | 3:T:39:ARG:HD3 | 1.53 | 0.48 |
| 1:3:184:TRP:HE3 | 1:3:211:ARG:HH21 | 1.60 | 0.48 |
| 3:8:141:ILE:HG13 | 3:8:142:GLN:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:21:ILE:HG13 | 1:C:96:GLU:HG2 | 1.95 | 0.48 |
| 3:D:124:LYS:NZ | 1:E:109:GLU:OE2 | 2.39 | 0.48 |
| 3:Q:160:GLU:O | 3:Q:164:ILE:HG13 | 2.13 | 0.48 |
| 3:5:100:LEU:O | 3:5:105:LEU:HB2 | 2.13 | 0.48 |
| 3:8:164:ILE:HG23 | 3:8:167:LEU:HD22 | 1.95 | 0.48 |
| 2:B:103:GLY:H | 2:B:104:PRO:CD | 2.25 | 0.48 |
| 3:D:69:ASN:OD1 | 3:D:72:VAL:HG22 | 2.14 | 0.48 |
| 1:U:86:THR:CG2 | 1:U:104:THR:HG22 | 2.42 | 0.48 |
| 3:W:91:LEU:O | 3:W:95:VAL:HG23 | 2.12 | 0.48 |
| 2:Y:58:LYS:HE3 | 2:Y:65:TRP:CE2 | 2.49 | 0.48 |
| 2:1:59:LYS:HB3 | 2:1:62:GLU:OE2 | 2.14 | 0.48 |
| 2:1:195:THR:HB | 2:1:197:PHE:CE1 | 2.49 | 0.48 |
| 3:5:42:LEU:HD11 | 3:5:47:PHE:HE1 | 1.79 | 0.48 |
| 1:6:120:ILE:HD13 | 1:6:208:ILE:HG21 | 1.94 | 0.48 |
| 3:8:47:PHE:HD1 | 3:8:171:PHE:CE1 | 2.32 | 0.48 |
| 1:H:127:LEU:HD11 | 1:H:212:THR:HG22 | 1.96 | 0.48 |
| 2:S:174:THR:O | 2:S:174:THR:OG1 | 2.31 | 0.48 |
| 3:T:124:LYS:HD2 | 1:U:82:TYR:HD2 | 1.77 | 0.48 |
| 1:X:134:PRO:HB2 | 1:X:145:LEU:HD13 | 1.96 | 0.48 |
| 3:Z:96:LEU:HD23 | 3:Z:170:LEU:HD21 | 1.96 | 0.48 |
| 1:0:160:LYS:HG3 | 1:0:187:TYR:CE2 | 2.49 | 0.48 |
| 2:A:143:LEU:HD13 | 2:A:143:LEU:HA | 1.74 | 0.48 |
| 2:I:29:LYS:O | 2:I:39:LEU:HD12 | 2.14 | 0.48 |
| 1:K:80:SER:O | 1:K:107:PRO:HG2 | 2.13 | 0.48 |
| 1:K:139:GLU:N | 1:K:139:GLU:OE1 | 2.47 | 0.48 |
| 3:L:154:LYS:HG3 | 3:L:155:LEU:HD22 | 1.96 | 0.48 |
| 2:S:169:LEU:HD11 | 2:S:197:PHE:HB3 | 1.95 | 0.48 |
| 3:T:93:LYS:HB2 | 3:T:129:LEU:HD13 | 1.94 | 0.48 |
| 2:Y:167:LEU:HD11 | 2:Y:186:TYR:HB2 | 1.96 | 0.48 |
| 1:0:88:ARG:HD2 | 1:0:100:TRP:CG | 2.49 | 0.48 |
| 2:B:42:ASP:OD1 | 2:B:43:GLY:N | 2.47 | 0.48 |
| 2:S:91:PHE:CE2 | 2:S:114:SER:HB2 | 2.48 | 0.48 |
| 1:U:53:THR:HA | 1:U:66:CYS:O | 2.13 | 0.48 |
| 1:U:122:SER:HA | 1:U:127:LEU:HD23 | 1.96 | 0.48 |
| 2:Y:167:LEU:HD11 | 2:Y:186:TYR:CB | 2.44 | 0.48 |
| 3:5:83:VAL:HG11 | 3:5:91:LEU:HD22 | 1.96 | 0.47 |
| 1:6:30:ASN:HB3 | 14:6:302:HOH:O | 2.14 | 0.47 |
| 2:7:131:LYS:HE2 | 2:B:41:TRP:O | 2.14 | 0.47 |
| 2:I:28:VAL:HG11 | 2:I:108:LYS:HB3 | 1.95 | 0.47 |
| 2:I:177:MET:HE2 | 2:I:188:PHE:CD1 | 2.49 | 0.47 |
| 3:Q:56:THR:HA | 3:Q:118:VAL:HG21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:21:ILE:HD11 | 1:X:97:HIS:HA | 1.96 | 0.47 |
| 2:4:162:ASP:OD2 | 2:4:206:PRO:HD2 | 2.15 | 0.47 |
| 1:6:122:SER:HA | 1:6:127:LEU:HD23 | 1.96 | 0.47 |
| 2:A:114:SER:HB3 | 2:A:117:GLN:HG3 | 1.97 | 0.47 |
| 1:K:184:TRP:HD1 | 1:K:213:GLY:HA2 | 1.78 | 0.47 |
| 1:R:134:PRO:HB2 | 1:R:145:LEU:HD13 | 1.95 | 0.47 |
| 2:V:24:LEU:HB3 | 2:V:44:GLY:HA3 | 1.97 | 0.47 |
| 2:1:125:ASP:OD1 | 14:1:402:HOH:O | 2.20 | 0.47 |
| 3:8:147:ARG:HA | 3:8:150:GLU:HG2 | 1.96 | 0.47 |
| 2:I:177:MET:HE2 | 2:I:188:PHE:HD1 | 1.79 | 0.47 |
| 1:K:27:VAL:HG22 | 1:K:40:TRP:HB3 | 1.96 | 0.47 |
| 3:T:164:ILE:O | 3:T:167:LEU:HD22 | 2.14 | 0.47 |
| 3:W:89:CYS:HB2 | 3:W:177:ALA:O | 2.14 | 0.47 |
| 2:1:24:LEU:HD23 | 2:1:45:PRO:HD2 | 1.96 | 0.47 |
| 1:3:81:LYS:O | 1:3:107:PRO:HD2 | 2.14 | 0.47 |
| 2:7:87:ASP:OD2 | 2:7:90:GLU:HG2 | 2.15 | 0.47 |
| 3:8:162:LYS:HE3 | 3:8:162:LYS:HB2 | 1.67 | 0.47 |
| 2:A:28:VAL:HG22 | 2:A:110:THR:HG22 | 1.95 | 0.47 |
| 3:Q:44:VAL:HG12 | 3:Q:179:VAL:HG11 | 1.95 | 0.47 |
| 1:6:44:ALA:O | 1:6:46:PRO:HD3 | 2.14 | 0.47 |
| 3:8:78:LYS:HD2 | 3:8:78:LYS:H | 1.79 | 0.47 |
| 3:8:97:GLN:NE2 | 3:8:101:GLU:OE2 | 2.44 | 0.47 |
| 3:G:73:ARG:NH1 | 3:G:169:LEU:HD21 | 2.29 | 0.47 |
| 1:K:152:TRP:CH2 | 1:K:193:GLY:HA3 | 2.50 | 0.47 |
| 1:0:92:GLU:CD | 1:0:97:HIS:HB3 | 2.35 | 0.47 |
| 3:8:40:CYS:HA | 3:8:132:CYS:HB2 | 1.94 | 0.47 |
| 3:Z:134:ILE:HG22 | 3:Z:136:GLY:H | 1.80 | 0.47 |
| 2:1:174:THR:O | 2:1:174:THR:OG1 | 2.32 | 0.47 |
| 2:4:205:THR:OG1 | 2:4:210:LYS:HB2 | 2.14 | 0.47 |
| 3:8:45:ARG:HH22 | 1:9:196:LEU:HD23 | 1.79 | 0.47 |
| 2:A:216:VAL:HG13 | 1:H:46:PRO:HB2 | 1.96 | 0.47 |
| 2:B:41:TRP:O | 2:B:77:LYS:HB3 | 2.14 | 0.47 |
| 3:D:40:CYS:HB2 | 3:D:132:CYS:HB2 | 1.72 | 0.47 |
| 1:H:192:GLN:HG2 | 1:H:204:TRP:CZ3 | 2.50 | 0.47 |
| 2:I:91:PHE:CE2 | 2:I:114:SER:HB2 | 2.49 | 0.47 |
| 2:I:167:LEU:HB2 | 2:I:179:LEU:HD12 | 1.96 | 0.47 |
| 3:Q:52:ILE:HG12 | 1:R:82:TYR:CE1 | 2.50 | 0.47 |
| 2:V:97:THR:HG23 | 2:V:107:THR:OG1 | 2.15 | 0.47 |
| 2:Y:88:HIS:HA | 2:Y:115:SER:OG | 2.14 | 0.47 |
| 1:0:93:LEU:HD23 | 1:0:93:LEU:HA | 1.77 | 0.47 |
| 3:2:93:LYS:HD3 | 3:2:94:GLN:OE1 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:4:24:LEU:HD13 | 2:4:45:PRO:HD2 | 1.97 | 0.47 |
| 2:B:181:GLY:HA2 | 1:E:173:TYR:CZ | 2.50 | 0.47 |
| 3:J:96:LEU:HB2 | 3:J:174:LEU:HD11 | 1.96 | 0.47 |
| 2:Y:215:TYR:HE1 | 2:Y:217:CYS:SG | 2.38 | 0.47 |
| 2:1:173:HIS:ND1 | 1:C:68:ARG:HD3 | 2.30 | 0.47 |
| 3:2:50:PRO:O | 3:2:54:ASN:N | 2.35 | 0.47 |
| 2:4:94:ALA:O | 2:4:110:THR:HG23 | 2.15 | 0.47 |
| 2:F:63:ARG:NH1 | 3:G:71:ASP:HB3 | 2.29 | 0.47 |
| 1:H:35:LYS:HD2 | 1:H:77:SER:OG | 2.13 | 0.47 |
| 1:O:79:LEU:HB3 | 1:O:85:TYR:CE2 | 2.50 | 0.47 |
| 2:P:135:ILE:HG21 | 2:P:169:LEU:HD22 | 1.97 | 0.47 |
| 3:T:72:VAL:HG23 | 3:T:162:LYS:HE3 | 1.96 | 0.47 |
| 2:Y:48:THR:O | 2:Y:51:THR:HG22 | 2.14 | 0.47 |
| 3:2:117:GLU:O | 14:2:301:HOH:O | 2.21 | 0.47 |
| 1:3:48:THR:C | 1:3:50:LEU:N | 2.68 | 0.47 |
| 3:5:45:ARG:HG2 | 1:6:150:ASP:OD1 | 2.15 | 0.47 |
| 1:K:190:GLN:HE21 | 1:K:207:PRO:HG3 | 1.80 | 0.47 |
| 2:P:51:THR:HA | 2:P:100:SER:HA | 1.96 | 0.47 |
| 3:Q:61:LYS:O | 3:Q:65:LEU:HD13 | 2.15 | 0.47 |
| 1:0:86:THR:OG1 | 1:0:102:GLN:NE2 | 2.47 | 0.46 |
| 3:2:164:ILE:HA | 3:2:167:LEU:HD13 | 1.95 | 0.46 |
| 2:4:97:THR:HA | 2:4:106:VAL:O | 2.15 | 0.46 |
| 3:D:147:ARG:HA | 3:D:147:ARG:HD2 | 1.64 | 0.46 |
| 1:K:123:LEU:HB3 | 1:K:126:SER:OG | 2.15 | 0.46 |
| 2:M:177:MET:HE2 | 2:M:188:PHE:CD1 | 2.43 | 0.46 |
| 3:T:69:ASN:O | 3:T:162:LYS:NZ | 2.43 | 0.46 |
| 2:P:148:SER:HB2 | 2:P:154:LEU:HD11 | 1.96 | 0.46 |
| 1:R:34:PHE:HE2 | 1:R:148:ILE:HD13 | 1.80 | 0.46 |
| 3:Z:44:VAL:HB | 3:Z:179:VAL:HG21 | 1.96 | 0.46 |
| 1:0:40:TRP:CE2 | 1:0:72:THR:HA | 2.51 | 0.46 |
| 3:2:89:CYS:HB2 | 3:2:177:ALA:O | 2.15 | 0.46 |
| 1:3:48:THR:HG22 | 1:3:49:GLN:H | 1.79 | 0.46 |
| 1:3:117:GLU:HB2 | 1:3:132:SER:HB2 | 1.97 | 0.46 |
| 2:P:114:SER:HB3 | 2:P:117:GLN:HG3 | 1.96 | 0.46 |
| 2:S:24:LEU:CD2 | 2:S:45:PRO:HD2 | 2.45 | 0.46 |
| 1:U:115:PRO:HA | 1:U:116:PRO:HD3 | 1.85 | 0.46 |
| 1:X:136:ILE:HD13 | 1:X:148:ILE:HD11 | 1.95 | 0.46 |
| 1:6:69:THR:HG23 | 14:6:301:HOH:O | 2.14 | 0.46 |
| 1:E:32:VAL:HG12 | 1:E:112:ILE:HB | 1.98 | 0.46 |
| 1:E:88:ARG:HD2 | 1:E:100:TRP:CG | 2.50 | 0.46 |
| 2:I:24:LEU:HB2 | 2:I:46:ALA:HB3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:217:CYS:HB3 | 2:P:219:VAL:HG13 | 1.97 | 0.46 |
| 2:Y:177:MET:HE2 | 2:Y:188:PHE:HB3 | 1.98 | 0.46 |
| 1:O:51:THR:OG1 | 1:O:68:ARG:HA | 2.15 | 0.46 |
| 2:4:24:LEU:HB3 | 2:4:44:GLY:HA3 | 1.96 | 0.46 |
| 3:N:175:ARG:O | 3:N:179:VAL:HB | 2.15 | 0.46 |
| 2:S:159:ILE:HB | 14:S:410:HOH:O | 2.15 | 0.46 |
| 3:W:42:LEU:HG | 3:W:129:LEU:HD21 | 1.97 | 0.46 |
| 1:X:182:GLU:O | 1:X:212:THR:HG21 | 2.15 | 0.46 |
| 3:2:42:LEU:CD1 | 3:2:47:PHE:HE1 | 2.28 | 0.46 |
| 2:4:24:LEU:HD23 | 2:4:24:LEU:HA | 1.56 | 0.46 |
| 2:A:41:TRP:O | 2:A:77:LYS:HB3 | 2.16 | 0.46 |
| 1:H:158:TYR:HB3 | 1:H:189:ILE:HD12 | 1.97 | 0.46 |
| 1:R:155:ARG:HD3 | 1:R:168:GLN:NE2 | 2.30 | 0.46 |
| 2:1:29:LYS:HA | 2:1:110:THR:CG2 | 2.46 | 0.46 |
| 2:B:114:SER:HB3 | 2:B:117:GLN:HG3 | 1.96 | 0.46 |
| 3:G:119:VAL:HG22 | 3:G:120:PRO:HD3 | 1.97 | 0.46 |
| 3:G:120:PRO:HG2 | 1:H:80:SER:OG | 2.16 | 0.46 |
| 3:N:83:VAL:HG13 | 3:N:141:ILE:HG12 | 1.98 | 0.46 |
| 3:T:61:LYS:O | 3:T:65:LEU:HD12 | 2.15 | 0.46 |
| 3:W:119:VAL:HG21 | 1:X:59:TYR:OH | 2.14 | 0.46 |
| 1:X:90:ARG:HD2 | 1:X:97:HIS:HB2 | 1.97 | 0.46 |
| 2:Y:99:VAL:CG1 | 2:Y:105:PRO:HB3 | 2.45 | 0.46 |
| 2:1:124:PRO:HB3 | 2:1:203:ILE:HD11 | 1.98 | 0.46 |
| 3:2:140:ASN:OD1 | 3:2:141:ILE:N | 2.49 | 0.46 |
| 2:B:144:THR:HG23 | 2:B:146:VAL:H | 1.80 | 0.46 |
| 2:B:167:LEU:HD22 | 2:B:201:ILE:CD1 | 2.46 | 0.46 |
| 2:M:114:SER:HB3 | 2:M:117:GLN:HG3 | 1.98 | 0.46 |
| 2:B:60:TYR:OH | 3:D:166:GLU:OE2 | 2.14 | 0.46 |
| 2:S:194:ASP:N | 2:S:221:THR:OG1 | 2.49 | 0.46 |
| 2:1:59:LYS:HD2 | 2:1:90:GLU:HG3 | 1.97 | 0.46 |
| 2:1:147:LEU:HD13 | 2:1:152:HIS:C | 2.36 | 0.46 |
| 1:3:90:ARG:HB2 | 1:3:100:TRP:CZ3 | 2.51 | 0.46 |
| 1:6:38:LEU:O | 1:6:73:GLN:HA | 2.16 | 0.46 |
| 1:9:118:MET:CE | 1:9:120:ILE:HD11 | 2.46 | 0.46 |
| 2:F:77:LYS:HB2 | 2:M:131:LYS:HE3 | 1.97 | 0.46 |
| 3:G:77:GLU:O | 3:G:81:ARG:NH1 | 2.49 | 0.46 |
| 3:L:92:MET:HA | 3:L:95:VAL:HG22 | 1.98 | 0.46 |
| 1:O:88:ARG:HD3 | 1:O:100:TRP:CD2 | 2.51 | 0.46 |
| 3:Z:170:LEU:CD2 | 3:Z:174:LEU:HD22 | 2.46 | 0.46 |
| 3:D:98:PHE:CZ | 3:D:152:VAL:HG11 | 2.52 | 0.45 |
| 2:I:72:GLN:H | 2:I:74:ILE:HD11 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:114:SER:HB3 | 2:I:117:GLN:HG3 | 1.98 | 0.45 |
| 1:R:122:SER:HA | 1:R:127:LEU:HD23 | 1.97 | 0.45 |
| 2:4:32:SER:HB2 | 2:4:113:PHE:HZ | 1.81 | 0.45 |
| 3:D:110:ARG:HG2 | 3:D:111:PHE:N | 2.31 | 0.45 |
| 2:F:52:VAL:HG23 | 2:F:99:VAL:HG13 | 1.99 | 0.45 |
| 2:I:55:VAL:HG13 | 2:I:68:LYS:HB3 | 1.99 | 0.45 |
| 2:P:129:ILE:HD12 | 2:P:136:GLN:HG2 | 1.98 | 0.45 |
| 3:Q:98:PHE:CD1 | 3:Q:149:LYS:HE3 | 2.51 | 0.45 |
| 3:Q:152:VAL:HG12 | 3:Q:153:LYS:HD2 | 1.99 | 0.45 |
| 3:Z:77:GLU:HB2 | 3:Z:81:ARG:HH22 | 1.82 | 0.45 |
| 2:1:48:THR:C | 2:1:50:ASP:H | 2.20 | 0.45 |
| 2:1:177:MET:HE2 | 2:1:188:PHE:HD1 | 1.80 | 0.45 |
| 2:B:25:LEU:HD21 | 2:B:96:VAL:HG22 | 1.98 | 0.45 |
| 3:D:147:ARG:NH2 | 3:D:154:LYS:HD3 | 2.31 | 0.45 |
| 2:F:57:TYR:CE2 | 2:F:84:GLU:HB3 | 2.52 | 0.45 |
| 2:F:96:VAL:O | 2:F:107:THR:HA | 2.17 | 0.45 |
| 3:G:97:GLN:O | 3:G:101:GLU:HG2 | 2.16 | 0.45 |
| 2:S:48:THR:HG23 | 2:S:100:SER:OG | 2.17 | 0.45 |
| 3:Z:87:ASP:HA | 3:Z:134:ILE:HD11 | 1.99 | 0.45 |
| 1:0:142:THR:O | 1:0:142:THR:OG1 | 2.23 | 0.45 |
| 3:8:98:PHE:CD1 | 3:8:149:LYS:HE2 | 2.51 | 0.45 |
| 1:9:113:ILE:HB | 1:9:202:GLY:CA | 2.46 | 0.45 |
| 2:B:36:GLU:HG3 | 2:B:82:THR:OG1 | 2.16 | 0.45 |
| 3:D:52:ILE:HD12 | 3:D:52:ILE:HA | 1.82 | 0.45 |
| 1:H:35:LYS:HB2 | 1:H:137:GLU:HG3 | 1.97 | 0.45 |
| 3:J:57:PHE:HZ | 3:J:172:MET:HE3 | 1.81 | 0.45 |
| 3:T:52:ILE:HD12 | 3:T:121:PHE:CE1 | 2.51 | 0.45 |
| 1:0:113:ILE:CD1 | 1:0:145:LEU:HD23 | 2.46 | 0.45 |
| 3:2:45:ARG:HG2 | 1:3:150:ASP:OD2 | 2.16 | 0.45 |
| 2:4:116:LEU:O | 2:4:116:LEU:HD22 | 2.17 | 0.45 |
| 2:4:179:LEU:HD13 | 2:4:179:LEU:HA | 1.65 | 0.45 |
| 3:8:42:LEU:HD12 | 3:8:42:LEU:HA | 1.76 | 0.45 |
| 3:D:125:LEU:HD23 | 3:D:125:LEU:HA | 1.84 | 0.45 |
| 1:E:189:ILE:O | 1:E:207:PRO:HA | 2.16 | 0.45 |
| 2:F:95:LYS:HA | 2:F:109:MET:HA | 1.98 | 0.45 |
| 3:G:52:ILE:HD12 | 3:G:52:ILE:HA | 1.83 | 0.45 |
| 3:G:145:VAL:O | 3:G:149:LYS:HG2 | 2.15 | 0.45 |
| 2:P:65:TRP:CD2 | 2:P:95:LYS:HE2 | 2.52 | 0.45 |
| 2:S:55:VAL:O | 2:S:72:GLN:NE2 | 2.49 | 0.45 |
| 1:X:88:ARG:HG3 | 1:X:100:TRP:CE3 | 2.52 | 0.45 |
| 2:4:59:LYS:NZ | 2:4:90:GLU:HG2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:9:169:VAL:HG21 | 1:9:178:LEU:HD21 | 1.97 | 0.45 |
| 2:I:175:TYR:HE1 | 1:K:121:GLU:OE2 | 2.00 | 0.45 |
| 1:X:27:VAL:HG22 | 1:X:40:TRP:HB3 | 1.98 | 0.45 |
| 2:4:167:LEU:HA | 2:4:200:SER:O | 2.15 | 0.45 |
| 2:7:41:TRP:CE3 | 2:7:96:VAL:HG11 | 2.51 | 0.45 |
| 3:L:119:VAL:HG22 | 3:L:120:PRO:HD3 | 1.99 | 0.45 |
| 3:Q:93:LYS:HB2 | 3:Q:129:LEU:HD13 | 1.99 | 0.45 |
| 1:R:192:GLN:HB3 | 1:R:204:TRP:HA | 1.98 | 0.45 |
| 1:U:118:MET:HE1 | 1:U:129:LEU:HD22 | 1.99 | 0.45 |
| 1:X:53:THR:O | 1:X:89:VAL:HA | 2.17 | 0.45 |
| 2:1:42:ASP:OD1 | 2:1:43:GLY:N | 2.50 | 0.45 |
| 1:E:81:LYS:HE2 | 1:E:139:GLU:OE2 | 2.16 | 0.45 |
| 2:F:224:ASP:OD1 | 2:F:224:ASP:N | 2.48 | 0.45 |
| 1:H:27:VAL:HG22 | 1:H:40:TRP:CB | 2.47 | 0.45 |
| 2:I:85:THR:HB | 2:I:92:TYR:CD2 | 2.52 | 0.45 |
| 3:J:74:LEU:HD22 | 3:J:162:LYS:HG2 | 1.98 | 0.45 |
| 1:O:27:VAL:HA | 1:O:39:GLN:O | 2.17 | 0.45 |
| 2:S:167:LEU:HB3 | 2:S:201:ILE:HG23 | 1.99 | 0.45 |
| 1:U:93:LEU:O | 1:U:95:ASP:N | 2.49 | 0.45 |
| 2:V:119:THR:O | 2:V:210:LYS:HE3 | 2.16 | 0.45 |
| 2:Y:137:MET:SD | 2:Y:201:ILE:HD11 | 2.57 | 0.45 |
| 1:C:148:ILE:HD12 | 3:L:51:TYR:HB3 | 1.99 | 0.45 |
| 1:K:116:PRO:HD3 | 14:K:405:HOH:O | 2.16 | 0.45 |
| 2:S:41:TRP:CE2 | 2:S:77:LYS:HA | 2.51 | 0.45 |
| 3:W:77:GLU:HG3 | 3:W:81:ARG:NH1 | 2.32 | 0.45 |
| 2:1:59:LYS:HD2 | 2:1:90:GLU:CG | 2.47 | 0.45 |
| 2:7:25:LEU:HD21 | 2:7:28:VAL:HG23 | 1.99 | 0.45 |
| 3:8:59:LEU:HG | 3:8:114:TYR:HB2 | 1.98 | 0.45 |
| 2:A:170:HIS:HB2 | 2:A:198:LEU:HB3 | 1.98 | 0.45 |
| 1:K:65:HIS:HE1 | 1:K:75:ASP:O | 2.00 | 0.45 |
| 1:O:155:ARG:HD3 | 1:O:168:GLN:OE1 | 2.17 | 0.45 |
| 3:Q:51:TYR:O | 3:Q:55:ARG:HG2 | 2.17 | 0.45 |
| 1:X:80:SER:HB2 | 1:X:85:TYR:OH | 2.17 | 0.45 |
| 1:9:137:GLU:HG3 | 1:9:137:GLU:O | 2.17 | 0.44 |
| 1:C:141:GLU:HB2 | 1:C:143:TRP:CD1 | 2.53 | 0.44 |
| 1:E:198:GLN:O | 1:E:200:ARG:HG3 | 2.16 | 0.44 |
| 3:G:79:LEU:CD1 | 3:G:91:LEU:HD11 | 2.47 | 0.44 |
| 1:K:90:ARG:HD2 | 1:K:97:HIS:HB2 | 1.98 | 0.44 |
| 2:M:55:VAL:HG22 | 2:M:96:VAL:HG22 | 1.99 | 0.44 |
| 1:R:34:PHE:CZ | 1:R:108:VAL:HA | 2.52 | 0.44 |
| 3:T:84:SER:O | 3:T:88:GLN:HG3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:146:VAL:O | 2:Y:154:LEU:HD22 | 2.17 | 0.44 |
| 2:1:169:LEU:HD12 | 2:1:169:LEU:HA | 1.74 | 0.44 |
| 2:4:90:GLU:OE1 | 3:5:73:ARG:NH2 | 2.29 | 0.44 |
| 2:7:198:LEU:HA | 2:7:198:LEU:HD23 | 1.83 | 0.44 |
| 2:M:130:PRO:HA | 2:M:135:ILE:HD13 | 1.98 | 0.44 |
| 1:R:105:PHE:CE2 | 1:R:107:PRO:HG3 | 2.52 | 0.44 |
| 2:V:123:PRO:HG3 | 2:V:213:ALA:HB3 | 1.98 | 0.44 |
| 2:Y:99:VAL:HG12 | 2:Y:105:PRO:HB3 | 2.00 | 0.44 |
| 2:M:147:LEU:HD12 | 2:M:147:LEU:H | 1.83 | 0.44 |
| 1:6:88:ARG:HD2 | 1:6:100:TRP:CG | 2.53 | 0.44 |
| 2:B:28:VAL:HG12 | 2:B:110:THR:HG22 | 1.99 | 0.44 |
| 2:F:187:GLU:O | 2:F:189:LEU:HD12 | 2.17 | 0.44 |
| 3:G:95:VAL:HG13 | 3:G:148:LEU:CD1 | 2.48 | 0.44 |
| 3:J:40:CYS:HB2 | 3:J:132:CYS:HB2 | 1.86 | 0.44 |
| 1:K:157:GLN:HA | 1:K:167:PHE:O | 2.17 | 0.44 |
| 1:U:24:PRO:HA | 1:U:43:PRO:HG3 | 1.98 | 0.44 |
| 1:6:90:ARG:HB3 | 1:6:100:TRP:CE3 | 2.53 | 0.44 |
| 2:B:86:ARG:NH1 | 2:B:145:PRO:O | 2.48 | 0.44 |
| 1:H:68:ARG:HD2 | 14:H:402:HOH:O | 2.16 | 0.44 |
| 1:K:45:PHE:CE1 | 1:K:47:LYS:HD2 | 2.52 | 0.44 |
| 2:M:44:GLY:C | 2:M:46:ALA:H | 2.20 | 0.44 |
| 3:W:51:TYR:O | 3:W:55:ARG:HG2 | 2.18 | 0.44 |
| 3:Z:56:THR:HA | 3:Z:118:VAL:HG21 | 1.98 | 0.44 |
| 3:2:49:SER:HB3 | 3:2:52:ILE:HD11 | 2.00 | 0.44 |
| 2:A:139:VAL:HG12 | 2:A:184:ARG:HH11 | 1.83 | 0.44 |
| 2:B:95:LYS:HA | 2:B:109:MET:HA | 1.98 | 0.44 |
| 2:B:198:LEU:HD12 | 2:B:198:LEU:HA | 1.71 | 0.44 |
| 2:F:50:ASP:HB3 | 2:F:101:ALA:HB2 | 1.98 | 0.44 |
| 2:F:90:GLU:HB3 | 2:F:92:TYR:CE1 | 2.53 | 0.44 |
| 2:M:97:THR:HG22 | 2:M:107:THR:CG2 | 2.47 | 0.44 |
| 1:R:118:MET:HB3 | 1:R:118:MET:HE2 | 1.77 | 0.44 |
| 1:R:136:ILE:CD1 | 1:R:148:ILE:HD11 | 2.48 | 0.44 |
| 2:S:168:GLU:HA | 2:S:177:MET:O | 2.18 | 0.44 |
| 1:X:177:VAL:HG22 | 1:X:179:ARG:HG3 | 2.00 | 0.44 |
| 2:Y:139:VAL:HG21 | 2:Y:165:TYR:CZ | 2.52 | 0.44 |
| 2:1:51:THR:HG23 | 2:1:99:VAL:O | 2.18 | 0.44 |
| 2:4:215:TYR:HE2 | 2:4:217:CYS:SG | 2.40 | 0.44 |
| 3:5:152:VAL:HG23 | 3:5:159:GLY:C | 2.38 | 0.44 |
| 2:7:122:LYS:HG3 | 14:7:402:HOH:O | 2.18 | 0.44 |
| 1:9:186:THR:OG1 | 1:9:211:ARG:HA | 2.18 | 0.44 |
| 2:1:147:LEU:HD12 | 2:1:151:GLY:C | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:2:134:ILE:HD12 | 3:2:134:ILE:HA | 1.80 | 0.44 |
| 1:3:118:MET:HE3 | 1:3:131:PHE:HE1 | 1.83 | 0.44 |
| 2:4:24:LEU:HB2 | 2:4:46:ALA:HB3 | 1.99 | 0.44 |
| 2:4:169:LEU:HD12 | 2:4:169:LEU:HA | 1.85 | 0.44 |
| 1:6:120:ILE:HD13 | 1:6:208:ILE:CG2 | 2.48 | 0.44 |
| 2:B:169:LEU:HD22 | 2:B:188:PHE:CB | 2.47 | 0.44 |
| 1:C:135:GLN:HG3 | 1:C:143:TRP:O | 2.18 | 0.44 |
| 2:F:24:LEU:HD13 | 2:F:24:LEU:HA | 1.78 | 0.44 |
| 3:G:44:VAL:CG1 | 3:G:179:VAL:HG21 | 2.47 | 0.44 |
| 3:W:134:ILE:HG22 | 3:W:136:GLY:H | 1.82 | 0.44 |
| 1:X:113:ILE:HD12 | 1:X:145:LEU:HD23 | 2.00 | 0.44 |
| 2:1:86:ARG:HG3 | 2:1:86:ARG:O | 2.16 | 0.44 |
| 3:2:74:LEU:HB2 | 3:2:166:GLU:OE1 | 2.17 | 0.44 |
| 1:6:38:LEU:HD21 | 1:6:89:VAL:HG13 | 2.00 | 0.44 |
| 2:A:126:VAL:HG11 | 2:A:201:ILE:HD13 | 1.99 | 0.44 |
| 3:D:101:GLU:HA | 3:D:105:LEU:HD22 | 2.00 | 0.44 |
| 2:F:148:SER:HB3 | 2:F:154:LEU:HD21 | 1.99 | 0.44 |
| 2:I:55:VAL:CG1 | 2:I:71:CYS:HB2 | 2.47 | 0.44 |
| 2:I:144:THR:CG2 | 2:I:146:VAL:H | 2.24 | 0.44 |
| 1:O:55:GLN:HG2 | 1:O:64:ASP:HA | 1.99 | 0.44 |
| 2:P:176:GLN:HE21 | 1:R:130:ARG:HH12 | 1.66 | 0.44 |
| 2:S:119:THR:O | 2:S:210:LYS:HE3 | 2.17 | 0.44 |
| 2:Y:74:ILE:HB | 2:Y:76:GLN:CD | 2.38 | 0.44 |
| 2:Y:95:LYS:HB3 | 2:Y:109:MET:HB3 | 2.00 | 0.44 |
| 3:2:55:ARG:CD | 3:2:114:TYR:HD1 | 2.31 | 0.43 |
| 3:2:104:LEU:HD13 | 3:2:119:VAL:CG1 | 2.48 | 0.43 |
| 1:3:59:TYR:HB3 | 1:3:60:ARG:H | 1.75 | 0.43 |
| 2:4:52:VAL:O | 2:4:98:ALA:HA | 2.18 | 0.43 |
| 2:4:181:GLY:HA2 | 1:6:173:TYR:CZ | 2.52 | 0.43 |
| 3:5:52:ILE:HG13 | 3:5:53:VAL:N | 2.33 | 0.43 |
| 3:5:107:GLN:NE2 | 3:5:109:ASP:HB2 | 2.29 | 0.43 |
| 2:F:130:PRO:HA | 2:F:135:ILE:HD13 | 2.00 | 0.43 |
| 1:H:184:TRP:CE3 | 1:H:213:GLY:HA2 | 2.53 | 0.43 |
| 2:I:162:ASP:HB2 | 2:I:206:PRO:HD2 | 1.99 | 0.43 |
| 3:J:84:SER:O | 3:J:88:GLN:HG3 | 2.18 | 0.43 |
| 2:M:51:THR:HG23 | 2:M:99:VAL:O | 2.18 | 0.43 |
| 1:O:45:PHE:O | 1:O:47:LYS:N | 2.51 | 0.43 |
| 2:P:126:VAL:HB | 2:P:215:TYR:CE2 | 2.52 | 0.43 |
| 2:S:114:SER:CB | 2:S:117:GLN:HG3 | 2.47 | 0.43 |
| 1:U:42:VAL:HG22 | 1:U:52:PHE:HZ | 1.82 | 0.43 |
| 1:U:90:ARG:HD2 | 1:U:97:HIS:HB2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:7:169:LEU:HD12 | 2:7:169:LEU:HA | 1.88 | 0.43 |
| 3:8:79:LEU:HD22 | 3:8:144:ASN:HB3 | 1.99 | 0.43 |
| 2:B:56:GLU:HB2 | 2:B:95:LYS:HD2 | 2.00 | 0.43 |
| 2:B:126:VAL:HB | 2:B:215:TYR:CE2 | 2.52 | 0.43 |
| 3:D:46:ASN:HB3 | 3:D:125:LEU:HD21 | 2.01 | 0.43 |
| 2:F:129:ILE:HD12 | 2:M:40:THR:HG21 | 1.99 | 0.43 |
| 2:M:169:LEU:HA | 2:M:169:LEU:HD12 | 1.78 | 0.43 |
| 2:P:135:ILE:HG22 | 2:P:188:PHE:HB2 | 1.99 | 0.43 |
| 3:Z:98:PHE:CD1 | 3:Z:149:LYS:HG2 | 2.52 | 0.43 |
| 3:Z:99:THR:O | 3:Z:103:VAL:HG13 | 2.19 | 0.43 |
| 3:5:40:CYS:O | 3:5:40:CYS:SG | 2.76 | 0.43 |
| 2:A:215:TYR:HE2 | 2:A:217:CYS:SG | 2.41 | 0.43 |
| 1:E:158:TYR:HB3 | 1:E:189:ILE:HG12 | 1.99 | 0.43 |
| 3:G:78:LYS:HA | 3:G:81:ARG:NH1 | 2.33 | 0.43 |
| 1:K:60:ARG:NH1 | 2:M:64:LYS:HD2 | 2.32 | 0.43 |
| 2:M:86:ARG:HE | 2:M:147:LEU:HD21 | 1.84 | 0.43 |
| 1:O:135:GLN:HG2 | 1:O:144:THR:HG22 | 1.99 | 0.43 |
| 3:Q:134:ILE:HD13 | 3:Q:138:ASP:HB3 | 2.00 | 0.43 |
| 1:C:43:PRO:O | 1:C:45:PHE:N | 2.51 | 0.43 |
| 3:D:112:GLN:HB2 | 3:D:113:PRO:HA | 2.01 | 0.43 |
| 1:K:93:LEU:HD12 | 1:K:94:ALA:N | 2.34 | 0.43 |
| 1:O:88:ARG:HD3 | 1:O:100:TRP:CE3 | 2.54 | 0.43 |
| 2:1:59:LYS:HE3 | 2:1:59:LYS:HB2 | 1.75 | 0.43 |
| 2:4:34:ASN:OD1 | 2:4:121:ILE:HA | 2.19 | 0.43 |
| 3:5:51:TYR:HB3 | 1:6:148:ILE:HG13 | 2.00 | 0.43 |
| 3:8:47:PHE:CD2 | 3:8:175:ARG:HG3 | 2.53 | 0.43 |
| 2:B:217:CYS:HB3 | 2:B:219:VAL:HG13 | 2.00 | 0.43 |
| 3:G:96:LEU:HD22 | 3:G:174:LEU:HD21 | 2.01 | 0.43 |
| 1:H:93:LEU:HD23 | 1:H:94:ALA:H | 1.82 | 0.43 |
| 1:H:116:PRO:HD3 | 14:H:405:HOH:O | 2.18 | 0.43 |
| 2:M:180:GLU:OE1 | 1:O:173:TYR:HB3 | 2.18 | 0.43 |
| 3:T:117:GLU:OE2 | 1:U:80:SER:HA | 2.19 | 0.43 |
| 3:2:92:MET:HB3 | 3:2:174:LEU:HG | 2.00 | 0.43 |
| 3:8:112:GLN:HG2 | 3:8:113:PRO:HA | 2.00 | 0.43 |
| 3:J:59:LEU:HD13 | 3:J:114:TYR:HB2 | 2.01 | 0.43 |
| 3:L:43:HIS:ND1 | 3:L:45:ARG:HG2 | 2.33 | 0.43 |
| 1:R:88:ARG:HD2 | 1:R:100:TRP:CG | 2.54 | 0.43 |
| 1:R:133:ALA:HB3 | 1:R:144:THR:HB | 2.00 | 0.43 |
| 3:T:59:LEU:CD1 | 3:T:167:LEU:HD23 | 2.48 | 0.43 |
| 1:X:115:PRO:HA | 1:X:116:PRO:HD3 | 1.88 | 0.43 |
| 2:4:55:VAL:HB | 2:4:71:CYS:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:40:CYS:HB2 | 3:G:132:CYS:HB2 | 1.65 | 0.43 |
| 2:I:85:THR:HB | 2:I:92:TYR:CE2 | 2.54 | 0.43 |
| 2:I:144:THR:HG23 | 2:I:146:VAL:N | 2.22 | 0.43 |
| 3:L:100:LEU:O | 3:L:105:LEU:HD23 | 2.19 | 0.43 |
| 2:M:119:THR:O | 2:M:210:LYS:HE3 | 2.19 | 0.43 |
| 2:M:187:GLU:O | 2:M:189:LEU:HD12 | 2.19 | 0.43 |
| 3:Q:59:LEU:HD11 | 3:Q:111:PHE:HB3 | 2.01 | 0.43 |
| 2:S:36:GLU:OE1 | 2:S:122:LYS:NZ | 2.45 | 0.43 |
| 1:U:136:ILE:HD12 | 1:U:143:TRP:HB3 | 2.00 | 0.43 |
| 1:X:206:GLU:OE1 | 1:X:206:GLU:N | 2.49 | 0.43 |
| 2:Y:68:LYS:HE2 | 2:Y:84:GLU:OE2 | 2.18 | 0.43 |
| 3:Z:74:LEU:HB2 | 3:Z:166:GLU:OE1 | 2.19 | 0.43 |
| 3:2:41:LYS:HG2 | 3:2:42:LEU:N | 2.31 | 0.43 |
| 3:2:104:LEU:HD12 | 3:2:105:LEU:N | 2.33 | 0.43 |
| 2:I:139:VAL:HG11 | 2:I:165:TYR:CE1 | 2.54 | 0.43 |
| 2:I:156:LEU:HD23 | 2:I:156:LEU:HA | 1.78 | 0.43 |
| 3:J:112:GLN:HB2 | 3:J:113:PRO:HA | 2.01 | 0.43 |
| 1:K:88:ARG:HD2 | 1:K:100:TRP:CG | 2.54 | 0.43 |
| 2:M:29:LYS:O | 2:M:39:LEU:HD12 | 2.19 | 0.43 |
| 2:M:42:ASP:OD1 | 2:M:43:GLY:N | 2.52 | 0.43 |
| 2:M:208:LEU:CD1 | 12:M:305:GOL:H11 | 2.49 | 0.43 |
| 1:O:158:TYR:HA | 1:O:188:CYS:O | 2.19 | 0.43 |
| 3:W:134:ILE:HG22 | 3:W:136:GLY:N | 2.34 | 0.43 |
| 2:Y:146:VAL:HG22 | 2:Y:154:LEU:CD2 | 2.48 | 0.43 |
| 1:O:21:ILE:HD13 | 1:O:21:ILE:HG21 | 1.72 | 0.43 |
| 3:2:99:THR:O | 3:2:104:LEU:HG | 2.19 | 0.43 |
| 2:4:148:SER:HB2 | 2:4:154:LEU:HD21 | 2.01 | 0.43 |
| 2:I:178:HIS:CD2 | 1:K:130:ARG:HD2 | 2.54 | 0.43 |
| 3:Q:40:CYS:HB3 | 3:Q:132:CYS:HB2 | 1.60 | 0.43 |
| 3:Q:79:LEU:HD21 | 3:Q:95:VAL:HG21 | 2.00 | 0.43 |
| 3:Q:121:PHE:HD1 | 1:R:82:TYR:CE2 | 2.37 | 0.43 |
| 3:Q:134:ILE:HG13 | 3:Q:135:SER:N | 2.34 | 0.43 |
| 1:U:182:GLU:O | 1:U:185:THR:HG22 | 2.19 | 0.43 |
| 2:1:60:TYR:OH | 3:2:162:LYS:HD2 | 2.19 | 0.43 |
| 3:2:83:VAL:HG23 | 3:2:83:VAL:O | 2.19 | 0.43 |
| 1:3:88:ARG:HD2 | 1:3:100:TRP:CD2 | 2.54 | 0.43 |
| 1:3:149:TYR:HD2 | 1:3:195:LEU:HD21 | 1.84 | 0.43 |
| 2:4:171:VAL:HG13 | 2:4:175:TYR:O | 2.18 | 0.43 |
| 2:4:198:LEU:HD21 | 1:E:49:GLN:HA | 2.00 | 0.43 |
| 3:8:155:LEU:HD12 | 3:8:155:LEU:HA | 1.83 | 0.43 |
| 1:9:192:GLN:HB3 | 1:9:204:TRP:CE3 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:130:PRO:HA | 2:B:135:ILE:HD13 | 2.01 | 0.43 |
| 1:C:31:SER:HA | 1:C:35:LYS:O | 2.19 | 0.43 |
| 3:G:69:ASN:OD1 | 3:G:72:VAL:HG22 | 2.19 | 0.43 |
| 3:G:74:LEU:HB2 | 3:G:166:GLU:OE1 | 2.19 | 0.43 |
| 3:J:52:ILE:HD12 | 3:J:52:ILE:HA | 1.90 | 0.43 |
| 1:R:123:LEU:CD1 | 1:R:124:ALA:H | 2.22 | 0.43 |
| 3:T:134:ILE:O | 3:T:134:ILE:HG13 | 2.12 | 0.43 |
| 2:V:167:LEU:HD11 | 2:V:186:TYR:CB | 2.48 | 0.43 |
| 3:2:67:ASP:OD1 | 3:2:162:LYS:HE2 | 2.19 | 0.42 |
| 3:2:104:LEU:HD13 | 3:2:119:VAL:HG13 | 2.01 | 0.42 |
| 3:2:110:ARG:CD | 3:2:111:PHE:H | 2.31 | 0.42 |
| 1:3:136:ILE:HG22 | 1:3:145:LEU:HD12 | 2.00 | 0.42 |
| 2:B:83:MET:HE3 | 2:B:86:ARG:HG3 | 2.00 | 0.42 |
| 3:G:149:LYS:HG2 | 3:G:149:LYS:H | 1.60 | 0.42 |
| 2:I:119:THR:O | 2:I:210:LYS:HE3 | 2.19 | 0.42 |
| 3:J:165:GLY:HA3 | 14:J:305:HOH:O | 2.19 | 0.42 |
| 3:Q:87:ASP:HB3 | 3:Q:141:ILE:HD11 | 2.01 | 0.42 |
| 3:Q:98:PHE:HE1 | 3:Q:153:LYS:NZ | 2.17 | 0.42 |
| 1:R:175:SER:HB2 | 14:R:307:HOH:O | 2.19 | 0.42 |
| 2:1:99:VAL:HG22 | 2:1:105:PRO:HB3 | 2.01 | 0.42 |
| 3:2:98:PHE:CE1 | 3:2:149:LYS:HG2 | 2.53 | 0.42 |
| 1:6:106:CYS:SG | 1:6:109:GLU:OE1 | 2.75 | 0.42 |
| 3:D:149:LYS:HA | 3:D:152:VAL:HG12 | 2.02 | 0.42 |
| 1:H:47:LYS:NZ | 1:H:49:GLN:H | 2.16 | 0.42 |
| 2:I:132:VAL:HG23 | 2:I:133:ARG:N | 2.33 | 0.42 |
| 1:O:65:HIS:CE1 | 1:O:78:HIS:CD2 | 3.07 | 0.42 |
| 1:R:136:ILE:HD11 | 1:R:148:ILE:HD11 | 2.00 | 0.42 |
| 3:T:160:GLU:O | 3:T:164:ILE:HG13 | 2.19 | 0.42 |
| 2:Y:91:PHE:CE2 | 2:Y:114:SER:HB2 | 2.53 | 0.42 |
| 3:Z:105:LEU:HB2 | 3:Z:106:PRO:HD3 | 2.01 | 0.42 |
| 2:1:162:ASP:HB2 | 2:1:206:PRO:HD2 | 2.02 | 0.42 |
| 2:4:35:PHE:CE2 | 2:4:159:ILE:HD13 | 2.53 | 0.42 |
| 2:4:41:TRP:CE3 | 2:4:96:VAL:HG21 | 2.55 | 0.42 |
| 3:D:69:ASN:CG | 3:D:72:VAL:HG22 | 2.39 | 0.42 |
| 1:H:47:LYS:HD2 | 1:H:47:LYS:HA | 1.62 | 0.42 |
| 1:K:200:ARG:HE | 1:K:200:ARG:HB2 | 1.51 | 0.42 |
| 3:L:74:LEU:HB2 | 3:L:166:GLU:OE1 | 2.19 | 0.42 |
| 3:L:96:LEU:HA | 3:L:99:THR:HG22 | 2.01 | 0.42 |
| 2:M:51:THR:OG1 | 2:M:100:SER:HA | 2.19 | 0.42 |
| 2:Y:41:TRP:CE2 | 2:Y:77:LYS:HA | 2.54 | 0.42 |
| 2:1:29:LYS:O | 2:1:39:LEU:HD12 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:5:39:ARG:HE | 3:5:39:ARG:HA | 1.83 | 0.42 |
| 3:8:49:SER:HB3 | 3:8:52:ILE:HG12 | 2.01 | 0.42 |
| 3:8:142:GLN:HA | 3:8:145:VAL:HG12 | 2.02 | 0.42 |
| 2:A:200:SER:HA | 2:A:215:TYR:O | 2.19 | 0.42 |
| 1:C:113:ILE:HB | 1:C:202:GLY:CA | 2.50 | 0.42 |
| 3:J:149:LYS:O | 3:J:153:LYS:HD3 | 2.19 | 0.42 |
| 1:K:142:THR:H | 1:K:142:THR:HG23 | 1.52 | 0.42 |
| 3:T:91:LEU:O | 3:T:95:VAL:HG23 | 2.19 | 0.42 |
| 2:V:95:LYS:HB3 | 2:V:109:MET:HB3 | 2.01 | 0.42 |
| 3:2:93:LYS:NZ | 3:2:129:LEU:O | 2.41 | 0.42 |
| 2:4:195:THR:HB | 2:4:197:PHE:CE1 | 2.54 | 0.42 |
| 3:5:43:HIS:CE1 | 3:5:45:ARG:HG3 | 2.55 | 0.42 |
| 3:5:51:TYR:CB | 1:6:148:ILE:HG13 | 2.48 | 0.42 |
| 2:A:166:ARG:HA | 2:A:180:GLU:HG2 | 2.02 | 0.42 |
| 3:D:80:PHE:O | 3:D:83:VAL:HG22 | 2.19 | 0.42 |
| 2:F:91:PHE:HD2 | 2:F:112:ARG:HG2 | 1.84 | 0.42 |
| 2:P:58:LYS:HD2 | 2:P:62:GLU:O | 2.19 | 0.42 |
| 2:P:153:GLN:H | 2:P:153:GLN:HG2 | 1.63 | 0.42 |
| 1:R:34:PHE:CE2 | 1:R:148:ILE:HD13 | 2.54 | 0.42 |
| 1:R:90:ARG:CD | 1:R:97:HIS:HB2 | 2.49 | 0.42 |
| 1:X:22:PRO:HG2 | 1:X:43:PRO:HB2 | 2.01 | 0.42 |
| 3:Z:52:ILE:HD12 | 3:Z:52:ILE:HA | 1.85 | 0.42 |
| 1:6:57:GLU:OE2 | 1:6:86:THR:N | 2.40 | 0.42 |
| 3:8:91:LEU:O | 3:8:95:VAL:HG23 | 2.20 | 0.42 |
| 2:I:62:GLU:HB2 | 14:I:403:HOH:O | 2.20 | 0.42 |
| 2:I:127:THR:HA | 14:I:404:HOH:O | 2.19 | 0.42 |
| 2:I:131:LYS:HB2 | 2:I:134:SER:O | 2.19 | 0.42 |
| 2:S:130:PRO:HA | 2:S:135:ILE:HD13 | 2.02 | 0.42 |
| 2:V:167:LEU:N | 2:V:167:LEU:HD23 | 2.34 | 0.42 |
| 3:W:48:GLN:NE2 | 1:X:150:ASP:OD2 | 2.49 | 0.42 |
| 1:9:90:ARG:HD2 | 1:9:97:HIS:HB3 | 2.02 | 0.42 |
| 1:9:113:ILE:HG23 | 1:9:145:LEU:HD23 | 2.02 | 0.42 |
| 1:E:55:GLN:HG2 | 1:E:64:ASP:HA | 2.01 | 0.42 |
| 2:F:91:PHE:CE2 | 2:F:114:SER:HB2 | 2.54 | 0.42 |
| 3:N:115:MET:O | 3:N:119:VAL:HG23 | 2.20 | 0.42 |
| 2:P:91:PHE:CD2 | 2:P:114:SER:HB2 | 2.55 | 0.42 |
| 2:Y:160:PHE:CD1 | 2:Y:205:THR:HG21 | 2.54 | 0.42 |
| 1:0:81:LYS:HE2 | 1:0:138:ASN:ND2 | 2.34 | 0.42 |
| 3:2:115:MET:HE3 | 3:2:115:MET:HB3 | 1.47 | 0.42 |
| 1:3:78:HIS:HA | 1:3:138:ASN:ND2 | 2.35 | 0.42 |
| 1:9:144:THR:HG22 | 1:9:147:ASN:OD1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:59:LEU:HD23 | 3:G:118:VAL:HG11 | 2.02 | 0.42 |
| 3:G:77:GLU:CD | 3:G:81:ARG:HH12 | 2.20 | 0.42 |
| 3:Q:52:ILE:HD12 | 3:Q:52:ILE:HA | 1.70 | 0.42 |
| 2:V:128:CYS:HB3 | 2:V:219:VAL:HG11 | 2.01 | 0.42 |
| 3:W:152:VAL:HG23 | 3:W:159:GLY:O | 2.18 | 0.42 |
| 2:7:25:LEU:HD21 | 2:7:28:VAL:HG21 | 2.00 | 0.42 |
| 2:B:167:LEU:HD23 | 2:B:167:LEU:H | 1.84 | 0.42 |
| 1:C:181:LEU:HB3 | 1:C:187:TYR:CE1 | 2.55 | 0.42 |
| 1:H:163:THR:HG22 | 1:H:164:ASN:H | 1.85 | 0.42 |
| 3:L:88:GLN:O | 3:L:92:MET:HG2 | 2.20 | 0.42 |
| 3:W:73:ARG:HB3 | 3:W:78:LYS:HZ2 | 1.85 | 0.42 |
| 2:Y:165:TYR:O | 2:Y:180:GLU:HA | 2.20 | 0.42 |
| 3:Z:42:LEU:HG | 3:Z:129:LEU:HD21 | 2.02 | 0.42 |
| 1:6:120:ILE:HD11 | 1:6:189:ILE:HD11 | 2.00 | 0.42 |
| 1:6:155:ARG:HD2 | 1:6:192:GLN:OE1 | 2.20 | 0.42 |
| 1:9:198:GLN:HE21 | 1:9:198:GLN:HB2 | 1.65 | 0.42 |
| 2:A:86:ARG:HH21 | 2:A:147:LEU:HD21 | 1.84 | 0.42 |
| 1:C:153:ALA:HB2 | 1:C:196:LEU:HD11 | 2.02 | 0.42 |
| 1:K:146:LYS:NZ | 1:K:174:ASP:OD1 | 2.46 | 0.42 |
| 3:N:114:TYR:O | 3:N:118:VAL:HG23 | 2.20 | 0.42 |
| 2:P:169:LEU:HD12 | 2:P:169:LEU:HA | 1.82 | 0.42 |
| 2:S:164:PHE:HE1 | 2:S:206:PRO:HG3 | 1.85 | 0.42 |
| 3:T:42:LEU:O | 3:T:179:VAL:HG23 | 2.19 | 0.42 |
| 3:T:51:TYR:OH | 3:T:117:GLU:HG2 | 2.19 | 0.42 |
| 3:T:52:ILE:HD13 | 1:U:82:TYR:CZ | 2.55 | 0.42 |
| 2:V:58:LYS:HE3 | 2:V:65:TRP:HE1 | 1.84 | 0.42 |
| 2:Y:177:MET:CE | 2:Y:188:PHE:HB3 | 2.50 | 0.42 |
| 2:1:91:PHE:CD2 | 2:1:114:SER:HB2 | 2.55 | 0.41 |
| 1:3:149:TYR:HB3 | 1:3:195:LEU:HD11 | 2.01 | 0.41 |
| 2:M:28:VAL:O | 2:M:28:VAL:HG13 | 2.20 | 0.41 |
| 3:Q:90:TYR:O | 3:Q:93:LYS:HB3 | 2.19 | 0.41 |
| 1:R:172:PRO:HG2 | 1:R:173:TYR:CE2 | 2.55 | 0.41 |
| 2:S:41:TRP:O | 2:S:77:LYS:HB3 | 2.20 | 0.41 |
| 2:S:156:LEU:HD23 | 14:S:410:HOH:O | 2.19 | 0.41 |
| 2:V:129:ILE:HB | 2:V:136:GLN:HB3 | 2.01 | 0.41 |
| 1:X:185:THR:H | 1:X:212:THR:CG2 | 2.25 | 0.41 |
| 2:Y:83:MET:SD | 2:Y:86:ARG:NH1 | 2.92 | 0.41 |
| 3:Z:134:ILE:HA | 3:Z:134:ILE:HD13 | 1.71 | 0.41 |
| 3:Z:142:GLN:HA | 3:Z:145:VAL:HG22 | 2.02 | 0.41 |
| 3:2:113:PRO:HG2 | 3:2:114:TYR:CD2 | 2.55 | 0.41 |
| 1:3:32:VAL:HG22 | 1:3:112:ILE:HB | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:5:77:GLU:O | 3:5:81:ARG:HG3 | 2.19 | 0.41 |
| 1:6:185:THR:H | 1:6:212:THR:CG2 | 2.28 | 0.41 |
| 2:7:63:ARG:HD3 | 2:7:63:ARG:C | 2.41 | 0.41 |
| 2:7:148:SER:OG | 2:7:149:GLU:N | 2.52 | 0.41 |
| 1:9:198:GLN:O | 1:9:200:ARG:HG3 | 2.20 | 0.41 |
| 1:C:90:ARG:CZ | 1:C:92:GLU:OE2 | 2.68 | 0.41 |
| 2:I:169:LEU:HD12 | 2:I:169:LEU:HA | 1.83 | 0.41 |
| 2:I:189:LEU:O | 1:K:123:LEU:HD21 | 2.20 | 0.41 |
| 3:N:45:ARG:O | 1:O:150:ASP:HB2 | 2.20 | 0.41 |
| 2:P:68:LYS:HG2 | 2:P:79:CYS:SG | 2.61 | 0.41 |
| 2:P:190:GLY:HA3 | 1:R:123:LEU:HD11 | 2.00 | 0.41 |
| 2:S:177:MET:HE2 | 2:S:188:PHE:HD1 | 1.85 | 0.41 |
| 3:T:124:LYS:HD2 | 1:U:82:TYR:CD2 | 2.55 | 0.41 |
| 1:0:20:MET:CG | 1:0:21:ILE:H | 2.33 | 0.41 |
| 2:4:139:VAL:HG11 | 2:4:165:TYR:CZ | 2.56 | 0.41 |
| 1:9:113:ILE:HB | 1:9:202:GLY:HA2 | 2.02 | 0.41 |
| 2:B:164:PHE:HE1 | 2:B:206:PRO:HG3 | 1.86 | 0.41 |
| 3:J:44:VAL:HB | 3:J:179:VAL:HG11 | 2.01 | 0.41 |
| 3:N:42:LEU:HD21 | 3:N:129:LEU:HG | 2.01 | 0.41 |
| 1:O:146:LYS:NZ | 1:O:174:ASP:OD1 | 2.51 | 0.41 |
| 1:R:51:THR:O | 1:R:92:GLU:HG2 | 2.20 | 0.41 |
| 1:U:120:ILE:HD12 | 1:U:129:LEU:HD22 | 2.01 | 0.41 |
| 1:X:79:LEU:HB3 | 1:X:85:TYR:CE2 | 2.55 | 0.41 |
| 1:3:59:TYR:HD1 | 1:3:59:TYR:HA | 1.71 | 0.41 |
| 2:4:91:PHE:HA | 2:4:113:PHE:O | 2.20 | 0.41 |
| 1:6:88:ARG:HD2 | 1:6:100:TRP:CD2 | 2.56 | 0.41 |
| 2:7:24:LEU:HD23 | 2:7:24:LEU:HA | 1.64 | 0.41 |
| 3:D:59:LEU:HD12 | 3:D:59:LEU:HA | 1.71 | 0.41 |
| 1:H:23:PRO:HB2 | 1:H:101:VAL:CG2 | 2.51 | 0.41 |
| 3:J:83:VAL:HG11 | 3:J:91:LEU:HD22 | 2.02 | 0.41 |
| 2:P:41:TRP:CE2 | 2:P:77:LYS:HA | 2.55 | 0.41 |
| 2:P:134:SER:HA | 2:P:191:LEU:HD12 | 2.01 | 0.41 |
| 2:S:50:ASP:OD2 | 2:S:101:ALA:HB2 | 2.20 | 0.41 |
| 1:U:93:LEU:HD23 | 1:U:93:LEU:HA | 1.87 | 0.41 |
| 2:V:55:VAL:HG22 | 2:V:68:LYS:HB3 | 2.02 | 0.41 |
| 3:W:47:PHE:CE2 | 3:W:174:LEU:HB3 | 2.53 | 0.41 |
| 1:0:40:TRP:HZ2 | 1:0:71:SER:O | 2.03 | 0.41 |
| 1:0:160:LYS:HB2 | 1:0:160:LYS:HE3 | 1.65 | 0.41 |
| 1:3:51:THR:OG1 | 1:3:68:ARG:HA | 2.21 | 0.41 |
| 2:4:42:ASP:OD1 | 2:4:43:GLY:N | 2.52 | 0.41 |
| 1:9:198:GLN:HB3 | 1:9:200:ARG:HE | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:144:THR:HG21 | 2:A:159:ILE:HD11 | 2.03 | 0.41 |
| 1:H:115:PRO:HA | 1:H:116:PRO:HD3 | 1.87 | 0.41 |
| 2:I:86:ARG:NH2 | 2:I:145:PRO:O | 2.53 | 0.41 |
| 1:K:45:PHE:CZ | 1:K:47:LYS:HB2 | 2.56 | 0.41 |
| 2:V:139:VAL:O | 2:V:184:ARG:HD3 | 2.18 | 0.41 |
| 2:Y:162:ASP:HB2 | 2:Y:206:PRO:HD2 | 2.01 | 0.41 |
| 1:O:141:GLU:HB2 | 1:O:143:TRP:NE1 | 2.36 | 0.41 |
| 2:1:60:TYR:OH | 3:2:166:GLU:OE2 | 2.26 | 0.41 |
| 2:A:55:VAL:O | 2:A:72:GLN:NE2 | 2.53 | 0.41 |
| 2:I:49:SER:O | 2:I:50:ASP:HB2 | 2.20 | 0.41 |
| 1:K:152:TRP:CZ2 | 1:K:193:GLY:HA3 | 2.56 | 0.41 |
| 3:L:103:VAL:HG11 | 3:L:163:ALA:CB | 2.49 | 0.41 |
| 2:Y:134:SER:HB2 | 2:Y:188:PHE:O | 2.20 | 0.41 |
| 2:Y:217:CYS:HB3 | 2:Y:219:VAL:HG13 | 2.01 | 0.41 |
| 3:2:55:ARG:HB2 | 3:2:55:ARG:CZ | 2.51 | 0.41 |
| 3:2:124:LYS:O | 3:2:128:LYS:HG3 | 2.20 | 0.41 |
| 1:3:123:LEU:HD23 | 1:3:123:LEU:HA | 1.86 | 0.41 |
| 3:5:105:LEU:HD23 | 3:5:105:LEU:HA | 1.96 | 0.41 |
| 2:A:216:VAL:CG1 | 1:H:46:PRO:HB2 | 2.51 | 0.41 |
| 2:B:91:PHE:CD2 | 2:B:114:SER:HB2 | 2.54 | 0.41 |
| 1:C:88:ARG:HD2 | 1:C:100:TRP:CG | 2.56 | 0.41 |
| 2:I:55:VAL:CG1 | 2:I:68:LYS:HB3 | 2.50 | 0.41 |
| 1:K:88:ARG:HD2 | 1:K:100:TRP:CD2 | 2.56 | 0.41 |
| 1:K:184:TRP:CD1 | 1:K:213:GLY:HA2 | 2.55 | 0.41 |
| 1:U:56:TYR:HB3 | 1:U:87:VAL:HG12 | 2.01 | 0.41 |
| 2:1:37:ASN:OD1 | 2:1:85:THR:OG1 | 2.37 | 0.41 |
| 1:3:137:GLU:C | 1:3:139:GLU:H | 2.24 | 0.41 |
| 2:7:44:GLY:C | 2:7:46:ALA:H | 2.24 | 0.41 |
| 1:E:45:PHE:HA | 1:E:46:PRO:HD3 | 1.87 | 0.41 |
| 3:L:90:TYR:CD1 | 3:L:134:ILE:HG13 | 2.56 | 0.41 |
| 2:M:192:THR:O | 2:M:195:THR:OG1 | 2.39 | 0.41 |
| 3:Q:59:LEU:CD1 | 3:Q:111:PHE:HB3 | 2.50 | 0.41 |
| 3:Q:86:LYS:HD2 | 3:Q:86:LYS:HA | 1.59 | 0.41 |
| 3:W:162:LYS:O | 3:W:166:GLU:HG3 | 2.21 | 0.41 |
| 1:O:50:LEU:HD12 | 1:O:50:LEU:HA | 1.83 | 0.41 |
| 1:O:80:SER:O | 1:O:107:PRO:HG2 | 2.21 | 0.41 |
| 3:2:100:LEU:HA | 3:2:104:LEU:HG | 2.03 | 0.41 |
| 3:2:153:LYS:HE2 | 3:2:153:LYS:HB3 | 1.90 | 0.41 |
| 1:3:113:ILE:HB | 1:3:202:GLY:HA2 | 2.02 | 0.41 |
| 1:3:197:ASP:OD1 | 1:3:198:GLN:N | 2.54 | 0.41 |
| 3:5:39:ARG:HA | 3:5:39:ARG:NE | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:6:113:ILE:HB | 1:6:202:GLY:HA2 | 2.03 | 0.41 |
| 2:7:39:LEU:HD21 | 2:7:96:VAL:HG13 | 2.03 | 0.41 |
| 2:7:217:CYS:HB3 | 2:7:219:VAL:HG13 | 2.02 | 0.41 |
| 3:8:96:LEU:CD1 | 3:8:122:LEU:HD22 | 2.51 | 0.41 |
| 3:8:99:THR:O | 3:8:103:VAL:HG22 | 2.21 | 0.41 |
| 3:8:152:VAL:HG12 | 3:8:159:GLY:O | 2.20 | 0.41 |
| 1:9:23:PRO:HB3 | 1:9:99:GLU:CG | 2.50 | 0.41 |
| 1:9:40:TRP:CE2 | 1:9:72:THR:HA | 2.56 | 0.41 |
| 2:A:121:ILE:HB | 2:A:212:SER:HB3 | 2.03 | 0.41 |
| 2:A:164:PHE:HE1 | 2:A:206:PRO:HG3 | 1.86 | 0.41 |
| 2:B:54:SER:O | 2:B:96:VAL:HA | 2.21 | 0.41 |
| 2:B:154:LEU:N | 14:B:401:HOH:O | 2.20 | 0.41 |
| 3:D:74:LEU:HB2 | 3:D:166:GLU:OE1 | 2.21 | 0.41 |
| 2:F:68:LYS:HG2 | 2:F:79:CYS:SG | 2.61 | 0.41 |
| 3:G:89:CYS:HB2 | 3:G:177:ALA:O | 2.20 | 0.41 |
| 3:G:100:LEU:HD23 | 3:G:104:LEU:HD12 | 2.02 | 0.41 |
| 1:H:157:GLN:HA | 1:H:167:PHE:O | 2.21 | 0.41 |
| 3:Q:124:LYS:HE3 | 1:R:106:CYS:SG | 2.60 | 0.41 |
| 2:S:168:GLU:HG2 | 2:S:200:SER:HB3 | 2.02 | 0.41 |
| 3:T:90:TYR:CD2 | 3:T:134:ILE:HB | 2.56 | 0.41 |
| 2:V:42:ASP:HA | 2:V:77:LYS:HD3 | 2.02 | 0.41 |
| 2:Y:66:LEU:HB3 | 14:Y:415:HOH:O | 2.21 | 0.41 |
| 3:Z:125:LEU:HD23 | 3:Z:125:LEU:HA | 1.92 | 0.41 |
| 2:1:215:TYR:HE2 | 2:1:217:CYS:SG | 2.44 | 0.41 |
| 3:5:59:LEU:HG | 3:5:114:TYR:HB2 | 2.03 | 0.41 |
| 1:9:46:PRO:HG2 | 1:9:50:LEU:HD11 | 2.03 | 0.41 |
| 2:B:143:LEU:HD23 | 2:B:143:LEU:HA | 1.94 | 0.41 |
| 2:B:192:THR:O | 2:B:195:THR:OG1 | 2.39 | 0.41 |
| 3:D:66:ALA:N | 14:D:302:HOH:O | 2.53 | 0.41 |
| 3:D:142:GLN:HA | 3:D:145:VAL:HG22 | 2.02 | 0.41 |
| 3:D:154:LYS:HG3 | 3:D:155:LEU:CD1 | 2.51 | 0.41 |
| 3:G:118:VAL:O | 3:G:122:LEU:HD13 | 2.21 | 0.41 |
| 1:K:126:SER:O | 1:K:127:LEU:HD12 | 2.21 | 0.41 |
| 2:P:167:LEU:HD23 | 2:P:167:LEU:N | 2.36 | 0.41 |
| 2:S:94:ALA:O | 2:S:110:THR:HG23 | 2.21 | 0.41 |
| 1:X:136:ILE:CG2 | 1:X:145:LEU:HD12 | 2.50 | 0.41 |
| 1:0:21:ILE:CG1 | 1:0:98:SER:HB2 | 2.51 | 0.40 |
| 1:0:98:SER:OG | 1:0:99:GLU:N | 2.54 | 0.40 |
| 2:4:32:SER:HB2 | 2:4:113:PHE:CZ | 2.55 | 0.40 |
| 2:4:88:HIS:HA | 2:4:115:SER:OG | 2.22 | 0.40 |
| 1:6:115:PRO:HA | 1:6:116:PRO:HD3 | 1.92 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:8:90:TYR:CD1 | 3:8:93:LYS:HD3 | 2.57 | 0.40 |
| 2:B:139:VAL:O | 2:B:184:ARG:HD3 | 2.21 | 0.40 |
| 3:D:70:THR:H | 3:D:70:THR:HG23 | 1.63 | 0.40 |
| 2:F:218:ARG:HH22 | 1:U:93:LEU:CD1 | 2.34 | 0.40 |
| 2:I:205:THR:OG1 | 2:I:210:LYS:HB2 | 2.21 | 0.40 |
| 3:J:107:GLN:OE1 | 3:J:110:ARG:HD2 | 2.20 | 0.40 |
| 1:K:55:GLN:NE2 | 1:K:64:ASP:OD1 | 2.53 | 0.40 |
| 3:N:100:LEU:O | 3:N:105:LEU:HD23 | 2.21 | 0.40 |
| 1:0:182:GLU:O | 1:0:185:THR:OG1 | 2.40 | 0.40 |
| 3:2:69:ASN:OD1 | 3:2:72:VAL:HG23 | 2.21 | 0.40 |
| 1:6:81:LYS:NZ | 1:6:139:GLU:OE2 | 2.37 | 0.40 |
| 3:8:78:LYS:HG3 | 3:8:81:ARG:NH2 | 2.36 | 0.40 |
| 2:A:95:LYS:HB3 | 2:A:109:MET:HB3 | 2.03 | 0.40 |
| 2:B:216:VAL:CG1 | 1:X:46:PRO:HB2 | 2.51 | 0.40 |
| 3:D:69:ASN:HB3 | 3:D:162:LYS:NZ | 2.35 | 0.40 |
| 2:I:24:LEU:HA | 2:I:24:LEU:HD13 | 1.83 | 0.40 |
| 2:I:55:VAL:HG12 | 2:I:71:CYS:O | 2.21 | 0.40 |
| 2:I:217:CYS:HB3 | 2:I:219:VAL:HG13 | 2.02 | 0.40 |
| 2:P:139:VAL:CG2 | 2:P:184:ARG:HA | 2.51 | 0.40 |
| 1:X:80:SER:O | 1:X:107:PRO:HG2 | 2.21 | 0.40 |
| 2:Y:24:LEU:HD13 | 2:Y:24:LEU:N | 2.37 | 0.40 |
| 1:0:150:ASP:OD1 | 3:Z:45:ARG:HG3 | 2.21 | 0.40 |
| 1:0:193:GLY:O | 1:0:202:GLY:N | 2.47 | 0.40 |
| 2:4:117:GLN:HG3 | 2:4:118:HIS:ND1 | 2.37 | 0.40 |
| 3:8:96:LEU:HD11 | 3:8:122:LEU:HD22 | 2.03 | 0.40 |
| 3:8:112:GLN:HG2 | 14:8:302:HOH:O | 2.21 | 0.40 |
| 1:E:40:TRP:O | 1:E:72:THR:HB | 2.21 | 0.40 |
| 2:F:60:TYR:OH | 3:G:162:LYS:HD2 | 2.22 | 0.40 |
| 3:G:98:PHE:HA | 3:G:101:GLU:HG2 | 2.03 | 0.40 |
| 3:G:128:LYS:NZ | 14:G:303:HOH:O | 2.54 | 0.40 |
| 1:K:125:GLU:HG3 | 1:K:181:LEU:O | 2.21 | 0.40 |
| 1:X:136:ILE:HG12 | 1:X:143:TRP:O | 2.21 | 0.40 |
| 2:B:103:GLY:N | 2:B:104:PRO:CD | 2.84 | 0.40 |
| 1:C:88:ARG:HD2 | 1:C:100:TRP:CD2 | 2.56 | 0.40 |
| 3:D:168:ASP:OD1 | 3:D:169:LEU:N | 2.54 | 0.40 |
| 3:J:90:TYR:HH | 3:J:133:HIS:CD2 | 2.40 | 0.40 |
| 3:N:79:LEU:HG | 3:N:91:LEU:HD21 | 2.03 | 0.40 |
| 3:Q:117:GLU:OE1 | 14:Q:302:HOH:O | 2.22 | 0.40 |
| 1:R:48:THR:O | 1:R:49:GLN:C | 2.59 | 0.40 |
| 2:S:68:LYS:HG2 | 2:S:79:CYS:SG | 2.61 | 0.40 |
| 2:V:170:HIS:HD1 | 2:V:176:GLN:HG2 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:0:135:GLN:NE2 | 1:0:142:THR:HA | 2.36 | 0.40 |
| 1:0:185:THR:O | 1:0:212:THR:HG23 | 2.22 | 0.40 |
| 2:I:58:LYS:NZ | 2:I:65:TRP:HE1 | 2.19 | 0.40 |
| 1:O:152:TRP:CH2 | 1:O:193:GLY:HA3 | 2.57 | 0.40 |
| 2:S:56:GLU:HG3 | 2:S:95:LYS:HG3 | 2.03 | 0.40 |
| 1:U:139:GLU:HG2 | 1:U:143:TRP:HD1 | 1.85 | 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 | 0 | 191/204 (94%) | 178 (93%) | 12 (6%) | 1 (0%) | 29 | 52 |
| 1 | 3 | 193/204 (95%) | 176 (91%) | 14 (7%) | 3 (2%) | 9 | 19 |
| 1 | 6 | 193/204 (95%) | 178 (92%) | 13 (7%) | 2 (1%) | 15 | 32 |
| 1 | 9 | 182/204 (89%) | 168 (92%) | 11 (6%) | 3 (2%) | 9 | 19 |
| 1 | C | 193/204 (95%) | 183 (95%) | 7 (4%) | 3 (2%) | 9 | 19 |
| 1 | E | 193/204 (95%) | 184 (95%) | 7 (4%) | 2 (1%) | 15 | 32 |
| 1 | H | 193/204 (95%) | 184 (95%) | 8 (4%) | 1 (0%) | 29 | 52 |
| 1 | K | 193/204 (95%) | 178 (92%) | 11 (6%) | 4 (2%) | 7 | 13 |
| 1 | O | 194/204 (95%) | 179 (92%) | 11 (6%) | 4 (2%) | 7 | 13 |
| 1 | R | 193/204 (95%) | 182 (94%) | 7 (4%) | 4 (2%) | 7 | 13 |
| 1 | U | 193/204 (95%) | 176 (91%) | 16 (8%) | 1 (0%) | 29 | 52 |
| 1 | X | 195/204 (96%) | 184 (94%) | 8 (4%) | 3 (2%) | 10 | 21 |
| 2 | 1 | 199/204 (98%) | 191 (96%) | 7 (4%) | 1 (0%) | 29 | 52 |
| 2 | 4 | 199/204 (98%) | 193 (97%) | 5 (2%) | 1 (0%) | 29 | 52 |
| 2 | 7 | 199/204 (98%) | 194 (98%) | 5 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2 | A | 199/204 (98%) | 192 (96%) | 6 (3%) | 1 (0%) | 29 | 52 |
| 2 | B | 199/204 (98%) | 190 (96%) | 6 (3%) | 3 (2%) | 10 | 21 |
| 2 | F | 199/204 (98%) | 192 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | I | 199/204 (98%) | 192 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | M | 199/204 (98%) | 192 (96%) | 6 (3%) | 1 (0%) | 29 | 52 |
| 2 | P | 199/204 (98%) | 192 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | S | 199/204 (98%) | 194 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | V | 199/204 (98%) | 195 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | Y | 199/204 (98%) | 192 (96%) | 7 (4%) | 0 | 100 | 100 |
| 3 | 2 | 138/149 (93%) | 133 (96%) | 5 (4%) | 0 | 100 | 100 |
| 3 | 5 | 139/149 (93%) | 135 (97%) | 4 (3%) | 0 | 100 | 100 |
| 3 | 8 | 138/149 (93%) | 130 (94%) | 8 (6%) | 0 | 100 | 100 |
| 3 | D | 139/149 (93%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 3 | G | 139/149 (93%) | 134 (96%) | 5 (4%) | 0 | 100 | 100 |
| 3 | J | 138/149 (93%) | 133 (96%) | 5 (4%) | 0 | 100 | 100 |
| 3 | L | 139/149 (93%) | 135 (97%) | 3 (2%) | 1 (1%) | 22 | 43 |
| 3 | N | 138/149 (93%) | 135 (98%) | 3 (2%) | 0 | 100 | 100 |
| 3 | Q | 140/149 (94%) | 135 (96%) | 3 (2%) | 2 (1%) | 11 | 22 |
| 3 | T | 140/149 (94%) | 136 (97%) | 4 (3%) | 0 | 100 | 100 |
| 3 | W | 139/149 (93%) | 133 (96%) | 5 (4%) | 1 (1%) | 22 | 43 |
| 3 | Z | 139/149 (93%) | 134 (96%) | 5 (4%) | 0 | 100 | 100 |
| All | All | 6360/6684 (95%) | 6065 (95%) | 253 (4%) | 42 (1%) | 22 | 43 |

All (42) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 6 | 142 | THR |
| 1 | E | 46 | PRO |
| 1 | K | 142 | THR |
| 1 | O | 125 | GLU |
| 1 | X | 125 | GLU |
| 1 | 3 | 49 | GLN |
| 2 | 4 | 103 | GLY |
| 2 | A | 103 | GLY |
| 1 | C | 49 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 180 | ASN |
| 2 | M | 47 | SER |
| 1 | O | 199 | GLN |
| 1 | 3 | 199 | GLN |
| 1 | 6 | 180 | ASN |
| 1 | 9 | 46 | PRO |
| 1 | C | 125 | GLU |
| 1 | O | 44 | ALA |
| 1 | U | 199 | GLN |
| 1 | X | 180 | ASN |
| 1 | 3 | 138 | ASN |
| 1 | 9 | 47 | LYS |
| 1 | 9 | 199 | GLN |
| 2 | B | 49 | SER |
| 1 | E | 199 | GLN |
| 1 | H | 199 | GLN |
| 1 | K | 43 | PRO |
| 1 | K | 199 | GLN |
| 1 | O | 49 | GLN |
| 1 | R | 161 | GLN |
| 1 | R | 199 | GLN |
| 1 | 0 | 180 | ASN |
| 2 | 1 | 49 | SER |
| 2 | B | 102 | GLY |
| 1 | C | 199 | GLN |
| 1 | R | 94 | ALA |
| 1 | R | 125 | GLU |
| 3 | W | 84 | SER |
| 1 | X | 199 | GLN |
| 3 | L | 84 | SER |
| 3 | Q | 84 | SER |
| 2 | B | 103 | GLY |
| 3 | Q | 136 | GLY |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | 0 | 174/188 (93%) | 168 (97%) | 6 (3%) | 37 | 63 |
| 1 | 3 | 176/188 (94%) | 149 (85%) | 27 (15%) | 2 | 4 |
| 1 | 6 | 178/188 (95%) | 152 (85%) | 26 (15%) | 3 | 5 |
| 1 | 9 | 167/188 (89%) | 144 (86%) | 23 (14%) | 3 | 6 |
| 1 | C | 180/188 (96%) | 171 (95%) | 9 (5%) | 24 | 47 |
| 1 | E | 175/188 (93%) | 166 (95%) | 9 (5%) | 24 | 46 |
| 1 | H | 178/188 (95%) | 162 (91%) | 16 (9%) | 9 | 18 |
| 1 | K | 177/188 (94%) | 158 (89%) | 19 (11%) | 6 | 12 |
| 1 | O | 178/188 (95%) | 163 (92%) | 15 (8%) | 11 | 21 |
| 1 | R | 179/188 (95%) | 163 (91%) | 16 (9%) | 9 | 19 |
| 1 | U | 177/188 (94%) | 160 (90%) | 17 (10%) | 8 | 16 |
| 1 | X | 179/188 (95%) | 160 (89%) | 19 (11%) | 6 | 12 |
| 2 | 1 | 182/185 (98%) | 166 (91%) | 16 (9%) | 10 | 19 |
| 2 | 4 | 181/185 (98%) | 167 (92%) | 14 (8%) | 13 | 25 |
| 2 | 7 | 180/185 (97%) | 166 (92%) | 14 (8%) | 12 | 25 |
| 2 | A | 180/185 (97%) | 167 (93%) | 13 (7%) | 14 | 29 |
| 2 | B | 181/185 (98%) | 166 (92%) | 15 (8%) | 11 | 22 |
| 2 | F | 181/185 (98%) | 167 (92%) | 14 (8%) | 13 | 25 |
| 2 | I | 182/185 (98%) | 168 (92%) | 14 (8%) | 13 | 25 |
| 2 | M | 181/185 (98%) | 170 (94%) | 11 (6%) | 18 | 38 |
| 2 | P | 184/185 (100%) | 170 (92%) | 14 (8%) | 13 | 26 |
| 2 | S | 183/185 (99%) | 169 (92%) | 14 (8%) | 13 | 25 |
| 2 | V | 182/185 (98%) | 167 (92%) | 15 (8%) | 11 | 22 |
| 2 | Y | 182/185 (98%) | 161 (88%) | 21 (12%) | 5 | 10 |
| 3 | 2 | 121/135 (90%) | 106 (88%) | 15 (12%) | 4 | 8 |
| 3 | 5 | 126/135 (93%) | 115 (91%) | 11 (9%) | 10 | 20 |
| 3 | 8 | 123/135 (91%) | 98 (80%) | 25 (20%) | 1 | 2 |
| 3 | D | 128/135 (95%) | 120 (94%) | 8 (6%) | 18 | 36 |
| 3 | G | 125/135 (93%) | 107 (86%) | 18 (14%) | 3 | 5 |
| 3 | J | 126/135 (93%) | 110 (87%) | 16 (13%) | 4 | 8 |
| 3 | L | 126/135 (93%) | 116 (92%) | 10 (8%) | 12 | 24 |
| 3 | N | 120/135 (89%) | 108 (90%) | 12 (10%) | 7 | 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3 | Q | 125/135 (93%) | 118 (94%) | 7 (6%) | 21 | 42 |
| 3 | T | 128/135 (95%) | 113 (88%) | 15 (12%) | 5 | 10 |
| 3 | W | 126/135 (93%) | 111 (88%) | 15 (12%) | 5 | 9 |
| 3 | Z | 127/135 (94%) | 114 (90%) | 13 (10%) | 7 | 14 |
| All | All | 5798/6096 (95%) | 5256 (91%) | 542 (9%) | 9 | 17 |

All (542) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 81 | LYS |
| 1 | 0 | 93 | LEU |
| 1 | 0 | 142 | THR |
| 1 | 0 | 150 | ASP |
| 1 | 0 | 165 | GLU |
| 1 | 0 | 186 | THR |
| 2 | 1 | 30 | PHE |
| 2 | 1 | 48 | THR |
| 2 | 1 | 64 | LYS |
| 2 | 1 | 75 | THR |
| 2 | 1 | 86 | ARG |
| 2 | 1 | 97 | THR |
| 2 | 1 | 106 | VAL |
| 2 | 1 | 110 | THR |
| 2 | 1 | 117 | GLN |
| 2 | 1 | 122 | LYS |
| 2 | 1 | 142 | THR |
| 2 | 1 | 167 | LEU |
| 2 | 1 | 171 | VAL |
| 2 | 1 | 195 | THR |
| 2 | 1 | 204 | LEU |
| 2 | 1 | 207 | ILE |
| 3 | 2 | 41 | LYS |
| 3 | 2 | 43 | HIS |
| 3 | 2 | 52 | ILE |
| 3 | 2 | 65 | LEU |
| 3 | 2 | 70 | THR |
| 3 | 2 | 71 | ASP |
| 3 | 2 | 81 | ARG |
| 3 | 2 | 86 | LYS |
| 3 | 2 | 93 | LYS |
| 3 | 2 | 103 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 2 | 105 | LEU |
| 3 | 2 | 110 | ARG |
| 3 | 2 | 123 | THR |
| 3 | 2 | 154 | LYS |
| 3 | 2 | 174 | LEU |
| 1 | 3 | 42 | VAL |
| 1 | 3 | 48 | THR |
| 1 | 3 | 51 | THR |
| 1 | 3 | 53 | THR |
| 1 | 3 | 59 | TYR |
| 1 | 3 | 78 | HIS |
| 1 | 3 | 80 | SER |
| 1 | 3 | 81 | LYS |
| 1 | 3 | 90 | ARG |
| 1 | 3 | 93 | LEU |
| 1 | 3 | 95 | ASP |
| 1 | 3 | 96 | GLU |
| 1 | 3 | 103 | VAL |
| 1 | 3 | 104 | THR |
| 1 | 3 | 108 | VAL |
| 1 | 3 | 123 | LEU |
| 1 | 3 | 137 | GLU |
| 1 | 3 | 144 | THR |
| 1 | 3 | 149 | TYR |
| 1 | 3 | 160 | LYS |
| 1 | 3 | 161 | GLN |
| 1 | 3 | 166 | LYS |
| 1 | 3 | 181 | LEU |
| 1 | 3 | 185 | THR |
| 1 | 3 | 189 | ILE |
| 1 | 3 | 195 | LEU |
| 1 | 3 | 214 | ASN |
| 2 | 4 | 28 | VAL |
| 2 | 4 | 48 | THR |
| 2 | 4 | 63 | ARG |
| 2 | 4 | 64 | LYS |
| 2 | 4 | 142 | THR |
| 2 | 4 | 167 | LEU |
| 2 | 4 | 171 | VAL |
| 2 | 4 | 174 | THR |
| 2 | 4 | 179 | LEU |
| 2 | 4 | 189 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 4 | 191 | LEU |
| 2 | 4 | 192 | THR |
| 2 | 4 | 195 | THR |
| 2 | 4 | 202 | THR |
| 3 | 5 | 44 | VAL |
| 3 | 5 | 53 | VAL |
| 3 | 5 | 59 | LEU |
| 3 | 5 | 65 | LEU |
| 3 | 5 | 70 | THR |
| 3 | 5 | 86 | LYS |
| 3 | 5 | 87 | ASP |
| 3 | 5 | 93 | LYS |
| 3 | 5 | 103 | VAL |
| 3 | 5 | 123 | THR |
| 3 | 5 | 151 | THR |
| 1 | 6 | 20 | MET |
| 1 | 6 | 21 | ILE |
| 1 | 6 | 42 | VAL |
| 1 | 6 | 51 | THR |
| 1 | 6 | 53 | THR |
| 1 | 6 | 55 | GLN |
| 1 | 6 | 56 | TYR |
| 1 | 6 | 57 | GLU |
| 1 | 6 | 60 | ARG |
| 1 | 6 | 63 | GLN |
| 1 | 6 | 93 | LEU |
| 1 | 6 | 123 | LEU |
| 1 | 6 | 136 | ILE |
| 1 | 6 | 138 | ASN |
| 1 | 6 | 141 | GLU |
| 1 | 6 | 142 | THR |
| 1 | 6 | 144 | THR |
| 1 | 6 | 148 | ILE |
| 1 | 6 | 150 | ASP |
| 1 | 6 | 160 | LYS |
| 1 | 6 | 181 | LEU |
| 1 | 6 | 182 | GLU |
| 1 | 6 | 185 | THR |
| 1 | 6 | 186 | THR |
| 1 | 6 | 189 | ILE |
| 1 | 6 | 199 | GLN |
| 2 | 7 | 57 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 7 | 63 | ARG |
| 2 | 7 | 64 | LYS |
| 2 | 7 | 75 | THR |
| 2 | 7 | 117 | GLN |
| 2 | 7 | 138 | LEU |
| 2 | 7 | 142 | THR |
| 2 | 7 | 147 | LEU |
| 2 | 7 | 154 | LEU |
| 2 | 7 | 157 | GLU |
| 2 | 7 | 167 | LEU |
| 2 | 7 | 174 | THR |
| 2 | 7 | 183 | GLN |
| 2 | 7 | 195 | THR |
| 3 | 8 | 41 | LYS |
| 3 | 8 | 42 | LEU |
| 3 | 8 | 44 | VAL |
| 3 | 8 | 45 | ARG |
| 3 | 8 | 53 | VAL |
| 3 | 8 | 59 | LEU |
| 3 | 8 | 62 | GLU |
| 3 | 8 | 65 | LEU |
| 3 | 8 | 71 | ASP |
| 3 | 8 | 86 | LYS |
| 3 | 8 | 103 | VAL |
| 3 | 8 | 104 | LEU |
| 3 | 8 | 112 | GLN |
| 3 | 8 | 119 | VAL |
| 3 | 8 | 123 | THR |
| 3 | 8 | 124 | LYS |
| 3 | 8 | 132 | CYS |
| 3 | 8 | 141 | ILE |
| 3 | 8 | 142 | GLN |
| 3 | 8 | 149 | LYS |
| 3 | 8 | 152 | VAL |
| 3 | 8 | 157 | GLU |
| 3 | 8 | 167 | LEU |
| 3 | 8 | 178 | CYS |
| 3 | 8 | 179 | VAL |
| 1 | 9 | 49 | GLN |
| 1 | 9 | 50 | LEU |
| 1 | 9 | 53 | THR |
| 1 | 9 | 58 | SER |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 9 | 72 | THR |
| 1 | 9 | 86 | THR |
| 1 | 9 | 97 | HIS |
| 1 | 9 | 100 | TRP |
| 1 | 9 | 123 | LEU |
| 1 | 9 | 129 | LEU |
| 1 | 9 | 138 | ASN |
| 1 | 9 | 142 | THR |
| 1 | 9 | 148 | ILE |
| 1 | 9 | 151 | SER |
| 1 | 9 | 158 | TYR |
| 1 | 9 | 170 | VAL |
| 1 | 9 | 177 | VAL |
| 1 | 9 | 182 | GLU |
| 1 | 9 | 185 | THR |
| 1 | 9 | 189 | ILE |
| 1 | 9 | 196 | LEU |
| 1 | 9 | 198 | GLN |
| 1 | 9 | 201 | THR |
| 2 | A | 28 | VAL |
| 2 | A | 50 | ASP |
| 2 | A | 75 | THR |
| 2 | A | 83 | MET |
| 2 | A | 99 | VAL |
| 2 | A | 100 | SER |
| 2 | A | 106 | VAL |
| 2 | A | 117 | GLN |
| 2 | A | 142 | THR |
| 2 | A | 144 | THR |
| 2 | A | 146 | VAL |
| 2 | A | 195 | THR |
| 2 | A | 216 | VAL |
| 2 | B | 40 | THR |
| 2 | B | 75 | THR |
| 2 | B | 86 | ARG |
| 2 | B | 95 | LYS |
| 2 | B | 96 | VAL |
| 2 | B | 97 | THR |
| 2 | B | 99 | VAL |
| 2 | B | 117 | GLN |
| 2 | B | 142 | THR |
| 2 | B | 144 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 154 | LEU |
| 2 | B | 167 | LEU |
| 2 | B | 174 | THR |
| 2 | B | 205 | THR |
| 2 | B | 216 | VAL |
| 1 | C | 20 | MET |
| 1 | C | 48 | THR |
| 1 | C | 60 | ARG |
| 1 | C | 67 | LYS |
| 1 | C | 87 | VAL |
| 1 | C | 96 | GLU |
| 1 | C | 104 | THR |
| 1 | C | 129 | LEU |
| 1 | C | 144 | THR |
| 3 | D | 52 | ILE |
| 3 | D | 70 | THR |
| 3 | D | 86 | LYS |
| 3 | D | 105 | LEU |
| 3 | D | 134 | ILE |
| 3 | D | 151 | THR |
| 3 | D | 172 | MET |
| 3 | D | 174 | LEU |
| 1 | E | 20 | MET |
| 1 | E | 49 | GLN |
| 1 | E | 81 | LYS |
| 1 | E | 141 | GLU |
| 1 | E | 142 | THR |
| 1 | E | 144 | THR |
| 1 | E | 150 | ASP |
| 1 | E | 196 | LEU |
| 1 | E | 212 | THR |
| 2 | F | 25 | LEU |
| 2 | F | 30 | PHE |
| 2 | F | 49 | SER |
| 2 | F | 63 | ARG |
| 2 | F | 66 | LEU |
| 2 | F | 83 | MET |
| 2 | F | 99 | VAL |
| 2 | F | 117 | GLN |
| 2 | F | 129 | ILE |
| 2 | F | 142 | THR |
| 2 | F | 147 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 180 | GLU |
| 2 | F | 195 | THR |
| 2 | F | 204 | LEU |
| 3 | G | 52 | ILE |
| 3 | G | 65 | LEU |
| 3 | G | 70 | THR |
| 3 | G | 78 | LYS |
| 3 | G | 91 | LEU |
| 3 | G | 99 | THR |
| 3 | G | 103 | VAL |
| 3 | G | 110 | ARG |
| 3 | G | 118 | VAL |
| 3 | G | 119 | VAL |
| 3 | G | 143 | LYS |
| 3 | G | 148 | LEU |
| 3 | G | 151 | THR |
| 3 | G | 152 | VAL |
| 3 | G | 167 | LEU |
| 3 | G | 172 | MET |
| 3 | G | 173 | SER |
| 3 | G | 174 | LEU |
| 1 | H | 51 | THR |
| 1 | H | 80 | SER |
| 1 | H | 81 | LYS |
| 1 | H | 93 | LEU |
| 1 | H | 103 | VAL |
| 1 | H | 104 | THR |
| 1 | H | 120 | ILE |
| 1 | H | 123 | LEU |
| 1 | H | 127 | LEU |
| 1 | H | 130 | ARG |
| 1 | H | 136 | ILE |
| 1 | H | 141 | GLU |
| 1 | H | 144 | THR |
| 1 | H | 148 | ILE |
| 1 | H | 158 | TYR |
| 1 | H | 163 | THR |
| 2 | I | 28 | VAL |
| 2 | I | 30 | PHE |
| 2 | I | 40 | THR |
| 2 | I | 58 | LYS |
| 2 | I | 74 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I | 97 | THR |
| 2 | I | 106 | VAL |
| 2 | I | 117 | GLN |
| 2 | I | 142 | THR |
| 2 | I | 144 | THR |
| 2 | I | 157 | GLU |
| 2 | I | 171 | VAL |
| 2 | I | 174 | THR |
| 2 | I | 179 | LEU |
| 3 | J | 52 | ILE |
| 3 | J | 53 | VAL |
| 3 | J | 58 | MET |
| 3 | J | 65 | LEU |
| 3 | J | 70 | THR |
| 3 | J | 71 | ASP |
| 3 | J | 74 | LEU |
| 3 | J | 86 | LYS |
| 3 | J | 95 | VAL |
| 3 | J | 105 | LEU |
| 3 | J | 133 | HIS |
| 3 | J | 134 | ILE |
| 3 | J | 151 | THR |
| 3 | J | 157 | GLU |
| 3 | J | 172 | MET |
| 3 | J | 174 | LEU |
| 1 | K | 25 | GLU |
| 1 | K | 47 | LYS |
| 1 | K | 51 | THR |
| 1 | K | 53 | THR |
| 1 | K | 55 | GLN |
| 1 | K | 61 | SER |
| 1 | K | 87 | VAL |
| 1 | K | 93 | LEU |
| 1 | K | 101 | VAL |
| 1 | K | 119 | GLN |
| 1 | K | 129 | LEU |
| 1 | K | 158 | TYR |
| 1 | K | 164 | ASN |
| 1 | K | 165 | GLU |
| 1 | K | 177 | VAL |
| 1 | K | 185 | THR |
| 1 | K | 198 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 200 | ARG |
| 1 | K | 214 | ASN |
| 3 | L | 52 | ILE |
| 3 | L | 70 | THR |
| 3 | L | 71 | ASP |
| 3 | L | 77 | GLU |
| 3 | L | 79 | LEU |
| 3 | L | 119 | VAL |
| 3 | L | 134 | ILE |
| 3 | L | 141 | ILE |
| 3 | L | 150 | GLU |
| 3 | L | 174 | LEU |
| 2 | M | 30 | PHE |
| 2 | M | 83 | MET |
| 2 | M | 97 | THR |
| 2 | M | 99 | VAL |
| 2 | M | 115 | SER |
| 2 | M | 117 | GLN |
| 2 | M | 147 | LEU |
| 2 | M | 155 | THR |
| 2 | M | 174 | THR |
| 2 | M | 183 | GLN |
| 2 | M | 195 | THR |
| 3 | N | 41 | LYS |
| 3 | N | 45 | ARG |
| 3 | N | 65 | LEU |
| 3 | N | 70 | THR |
| 3 | N | 71 | ASP |
| 3 | N | 84 | SER |
| 3 | N | 103 | VAL |
| 3 | N | 112 | GLN |
| 3 | N | 123 | THR |
| 3 | N | 142 | GLN |
| 3 | N | 174 | LEU |
| 3 | N | 179 | VAL |
| 1 | O | 20 | MET |
| 1 | O | 21 | ILE |
| 1 | O | 27 | VAL |
| 1 | O | 32 | VAL |
| 1 | O | 42 | VAL |
| 1 | O | 47 | LYS |
| 1 | O | 49 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 53 | THR |
| 1 | O | 81 | LYS |
| 1 | O | 123 | LEU |
| 1 | O | 129 | LEU |
| 1 | O | 136 | ILE |
| 1 | O | 142 | THR |
| 1 | O | 164 | ASN |
| 1 | O | 214 | ASN |
| 2 | P | 24 | LEU |
| 2 | P | 28 | VAL |
| 2 | P | 40 | THR |
| 2 | P | 117 | GLN |
| 2 | P | 132 | VAL |
| 2 | P | 154 | LEU |
| 2 | P | 167 | LEU |
| 2 | P | 168 | GLU |
| 2 | P | 174 | THR |
| 2 | P | 183 | GLN |
| 2 | P | 192 | THR |
| 2 | P | 195 | THR |
| 2 | P | 198 | LEU |
| 2 | P | 216 | VAL |
| 3 | Q | 52 | ILE |
| 3 | Q | 58 | MET |
| 3 | Q | 70 | THR |
| 3 | Q | 78 | LYS |
| 3 | Q | 83 | VAL |
| 3 | Q | 134 | ILE |
| 3 | Q | 172 | MET |
| 1 | R | 32 | VAL |
| 1 | R | 51 | THR |
| 1 | R | 56 | TYR |
| 1 | R | 58 | SER |
| 1 | R | 90 | ARG |
| 1 | R | 93 | LEU |
| 1 | R | 104 | THR |
| 1 | R | 123 | LEU |
| 1 | R | 142 | THR |
| 1 | R | 148 | ILE |
| 1 | R | 161 | GLN |
| 1 | R | 170 | VAL |
| 1 | R | 185 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 200 | ARG |
| 1 | R | 208 | ILE |
| 1 | R | 212 | THR |
| 2 | S | 40 | THR |
| 2 | S | 48 | THR |
| 2 | S | 56 | GLU |
| 2 | S | 74 | ILE |
| 2 | S | 75 | THR |
| 2 | S | 117 | GLN |
| 2 | S | 144 | THR |
| 2 | S | 167 | LEU |
| 2 | S | 174 | THR |
| 2 | S | 180 | GLU |
| 2 | S | 183 | GLN |
| 2 | S | 196 | GLU |
| 2 | S | 198 | LEU |
| 2 | S | 201 | ILE |
| 3 | T | 39 | ARG |
| 3 | T | 44 | VAL |
| 3 | T | 58 | MET |
| 3 | T | 59 | LEU |
| 3 | T | 65 | LEU |
| 3 | T | 71 | ASP |
| 3 | T | 93 | LYS |
| 3 | T | 134 | ILE |
| 3 | T | 151 | THR |
| 3 | T | 153 | LYS |
| 3 | T | 167 | LEU |
| 3 | T | 172 | MET |
| 3 | T | 173 | SER |
| 3 | T | 174 | LEU |
| 3 | T | 179 | VAL |
| 1 | U | 28 | ARG |
| 1 | U | 32 | VAL |
| 1 | U | 56 | TYR |
| 1 | U | 58 | SER |
| 1 | U | 61 | SER |
| 1 | U | 81 | LYS |
| 1 | U | 86 | THR |
| 1 | U | 93 | LEU |
| 1 | U | 96 | GLU |
| 1 | U | 105 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | U | 118 | MET |
| 1 | U | 148 | ILE |
| 1 | U | 161 | GLN |
| 1 | U | 169 | VAL |
| 1 | U | 186 | THR |
| 1 | U | 200 | ARG |
| 1 | U | 214 | ASN |
| 2 | V | 30 | PHE |
| 2 | V | 40 | THR |
| 2 | V | 48 | THR |
| 2 | V | 52 | VAL |
| 2 | V | 72 | GLN |
| 2 | V | 76 | GLN |
| 2 | V | 95 | LYS |
| 2 | V | 106 | VAL |
| 2 | V | 117 | GLN |
| 2 | V | 142 | THR |
| 2 | V | 147 | LEU |
| 2 | V | 167 | LEU |
| 2 | V | 174 | THR |
| 2 | V | 195 | THR |
| 2 | V | 204 | LEU |
| 3 | W | 44 | VAL |
| 3 | W | 52 | ILE |
| 3 | W | 70 | THR |
| 3 | W | 71 | ASP |
| 3 | W | 78 | LYS |
| 3 | W | 101 | GLU |
| 3 | W | 110 | ARG |
| 3 | W | 118 | VAL |
| 3 | W | 119 | VAL |
| 3 | W | 132 | CYS |
| 3 | W | 134 | ILE |
| 3 | W | 151 | THR |
| 3 | W | 153 | LYS |
| 3 | W | 167 | LEU |
| 3 | W | 174 | LEU |
| 1 | X | 51 | THR |
| 1 | X | 61 | SER |
| 1 | X | 67 | LYS |
| 1 | X | 80 | SER |
| 1 | X | 86 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 92 | GLU |
| 1 | X | 104 | THR |
| 1 | X | 123 | LEU |
| 1 | X | 142 | THR |
| 1 | X | 144 | THR |
| 1 | X | 150 | ASP |
| 1 | X | 158 | TYR |
| 1 | X | 163 | THR |
| 1 | X | 166 | LYS |
| 1 | X | 170 | VAL |
| 1 | X | 181 | LEU |
| 1 | X | 182 | GLU |
| 1 | X | 198 | GLN |
| 1 | X | 214 | ASN |
| 2 | Y | 24 | LEU |
| 2 | Y | 48 | THR |
| 2 | Y | 49 | SER |
| 2 | Y | 55 | VAL |
| 2 | Y | 58 | LYS |
| 2 | Y | 64 | LYS |
| 2 | Y | 86 | ARG |
| 2 | Y | 97 | THR |
| 2 | Y | 99 | VAL |
| 2 | Y | 127 | THR |
| 2 | Y | 142 | THR |
| 2 | Y | 146 | VAL |
| 2 | Y | 154 | LEU |
| 2 | Y | 166 | ARG |
| 2 | Y | 167 | LEU |
| 2 | Y | 179 | LEU |
| 2 | Y | 180 | GLU |
| 2 | Y | 183 | GLN |
| 2 | Y | 192 | THR |
| 2 | Y | 195 | THR |
| 2 | Y | 204 | LEU |
| 3 | Z | 52 | ILE |
| 3 | Z | 58 | MET |
| 3 | Z | 65 | LEU |
| 3 | Z | 71 | ASP |
| 3 | Z | 77 | GLU |
| 3 | Z | 96 | LEU |
| 3 | Z | 103 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Z | 105 | LEU |
| 3 | Z | 123 | THR |
| 3 | Z | 134 | ILE |
| 3 | Z | 151 | THR |
| 3 | Z | 167 | LEU |
| 3 | Z | 174 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 65 | HIS |
| 1 | 0 | 102 | GLN |
| 2 | 1 | 178 | HIS |
| 2 | 4 | 118 | HIS |
| 3 | 5 | 107 | GLN |
| 1 | 6 | 65 | HIS |
| 1 | 6 | 199 | GLN |
| 2 | 7 | 118 | HIS |
| 2 | 7 | 170 | HIS |
| 1 | 9 | 128 | HIS |
| 3 | D | 48 | GLN |
| 1 | H | 190 | GLN |
| 1 | K | 102 | GLN |
| 1 | K | 198 | GLN |
| 3 | L | 48 | GLN |
| 3 | L | 68 | GLN |
| 2 | S | 176 | GLN |
| 1 | U | 39 | GLN |
| 1 | X | 190 | GLN |
| 3 | Z | 94 | GLN |
| 3 | Z | 107 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

67 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$ |
| 4 | NAG | a | 1 | 2,4 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.94 | 2 (11%) |
| 4 | NAG | a | 2 | 4 | 14,14,15 | 0.88 | 1 (7%) | 17,19,21 | 1.56 | 2 (11%) |
| 4 | BMA | a | 3 | 4 | 11,11,12 | 1.11 | 1 (9%) | 15,15,17 | 1.93 | 4 (26%) |
| 4 | FUC | a | 4 | 4 | 10,10,11 | 1.34 | 2 (20%) | 14,14,16 | 1.19 | 1 (7%) |
| 5 | NAG | b | 1 | 3,5 | 14,14,15 | 0.51 | 0 | 17,19,21 | 0.83 | 1 (5%) |
| 5 | NAG | b | 2 | 5 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.80 | 0 |
| 5 | FUC | b | 3 | 5 | 10,10,11 | 1.94 | 3 (30%) | 14,14,16 | 1.33 | 2 (14%) |
| 4 | NAG | c | 1 | 2,4 | 14,14,15 | 0.47 | 0 | 17,19,21 | 1.17 | 1 (5%) |
| 4 | NAG | c | 2 | 4 | 14,14,15 | 1.07 | 1 (7%) | 17,19,21 | 1.46 | 4 (23%) |
| 4 | BMA | c | 3 | 4 | 11,11,12 | 1.47 | 2 (18%) | 15,15,17 | 1.42 | 2 (13%) |
| 4 | FUC | c | 4 | 4 | 10,10,11 | 1.42 | 1 (10%) | 14,14,16 | 1.19 | 2 (14%) |
| 6 | NAG | d | 1 | 3,6 | 14,14,15 | 0.66 | 0 | 17,19,21 | 0.90 | 0 |
| 6 | FUC | d | 2 | 6 | 10,10,11 | 1.57 | 2 (20%) | 14,14,16 | 1.22 | 2 (14%) |
| 5 | NAG | e | 1 | 2,5 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.99 | 1 (5%) |
| 5 | NAG | e | 2 | 5 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.97 | 1 (5%) |
| 5 | FUC | e | 3 | 5 | 10,10,11 | 1.26 | 1 (10%) | 14,14,16 | 1.10 | 0 |
| 7 | NAG | f | 1 | 3,7 | 14,14,15 | 1.06 | 1 (7%) | 17,19,21 | 0.89 | 1 (5%) |
| 7 | FUC | f | 2 | 7 | 10,10,11 | 0.87 | 0 | 14,14,16 | 0.83 | 0 |
| 8 | NAG | g | 1 | 2,8 | 14,14,15 | 0.60 | 0 | 17,19,21 | 0.73 | 0 |
| 8 | NAG | g | 2 | 8 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.52 | 0 |
| 8 | BMA | g | 3 | 8 | 11,11,12 | 1.37 | 2 (18%) | 15,15,17 | 0.82 | 0 |
| 9 | NAG | h | 1 | 3,9 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.63 | 0 |
| 9 | NAG | h | 2 | 9 | 14,14,15 | 0.63 | 0 | 17,19,21 | 1.49 | 2 (11%) |
| 9 | BMA | h | 3 | 9 | 11,11,12 | 0.64 | 0 | 15,15,17 | 1.45 | 2 (13%) |
| 9 | FUC | h | 4 | 9 | 10,10,11 | 1.32 | 2 (20%) | 14,14,16 | 1.37 | 2 (14%) |
| 9 | FUC | h | 5 | 9 | 10,10,11 | 1.38 | 2 (20%) | 14,14,16 | 1.58 | 4 (28%) |
| 5 | NAG | i | 1 | 2,5 | 14,14,15 | 0.71 | 1 (7%) | 17,19,21 | 0.62 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | NAG | i | 2 | 5 | 14,14,15 | 0.58 | 0 | 17,19,21 | 0.67 | 0 |
| 5 | FUC | i | 3 | 5 | 10,10,11 | 1.30 | 1 (10%) | 14,14,16 | 1.56 | 2 (14%) |
| 5 | NAG | j | 1 | 3,5 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.73 | 0 |
| 5 | NAG | j | 2 | 5 | 14,14,15 | 0.43 | 0 | 17,19,21 | 0.67 | 0 |
| 5 | FUC | j | 3 | 5 | 10,10,11 | 1.38 | 2 (20%) | 14,14,16 | 1.89 | 5 (35%) |
| 9 | NAG | k | 1 | 2,9 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.69 | 0 |
| 9 | NAG | k | 2 | 9 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.48 | 0 |
| 9 | BMA | k | 3 | 9 | 11,11,12 | 1.30 | 2 (18%) | 15,15,17 | 0.90 | 0 |
| 9 | FUC | k | 4 | 9 | 10,10,11 | 1.04 | 2 (20%) | 14,14,16 | 1.01 | 0 |
| 9 | FUC | k | 5 | 9 | 10,10,11 | 1.12 | 1 (10%) | 14,14,16 | 0.94 | 1 (7%) |
| 5 | NAG | l | 1 | 3,5 | 14,14,15 | 0.90 | 1 (7%) | 17,19,21 | 1.09 | 1 (5%) |
| 5 | NAG | l | 2 | 5 | 14,14,15 | 0.87 | 1 (7%) | 17,19,21 | 0.88 | 0 |
| 5 | FUC | l | 3 | 5 | 10,10,11 | 1.45 | 3 (30%) | 14,14,16 | 2.28 | 4 (28%) |
| 5 | NAG | m | 1 | 3,5 | 14,14,15 | 0.44 | 0 | 17,19,21 | 1.22 | 3 (17%) |
| 5 | NAG | m | 2 | 5 | 14,14,15 | 0.37 | 0 | 17,19,21 | 0.65 | 0 |
| 5 | FUC | m | 3 | 5 | 10,10,11 | 2.31 | 3 (30%) | 14,14,16 | 2.17 | 5 (35%) |
| 4 | NAG | n | 1 | 2,4 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.52 | 0 |
| 4 | NAG | n | 2 | 4 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.49 | 0 |
| 4 | BMA | n | 3 | 4 | 11,11,12 | 1.13 | 1 (9%) | 15,15,17 | 0.84 | 0 |
| 4 | FUC | n | 4 | 4 | 10,10,11 | 1.12 | 1 (10%) | 14,14,16 | 1.05 | 1 (7%) |
| 6 | NAG | o | 1 | 3,6 | 14,14,15 | 0.88 | 2 (14%) | 17,19,21 | 1.11 | 1 (5%) |
| 6 | FUC | o | 2 | 6 | 10,10,11 | 1.23 | 1 (10%) | 14,14,16 | 1.33 | 2 (14%) |
| 6 | NAG | p | 1 | 2,6 | 14,14,15 | 0.83 | 1 (7%) | 17,19,21 | 0.51 | 0 |
| 6 | FUC | p | 2 | 6 | 10,10,11 | 1.42 | 2 (20%) | 14,14,16 | 1.66 | 1 (7%) |
| 10 | NAG | q | 1 | 3,10 | 14,14,15 | 0.64 | 1 (7%) | 17,19,21 | 0.99 | 1 (5%) |
| 10 | NAG | q | 2 | 10 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.58 | 0 |
| 6 | NAG | r | 1 | 2,6 | 14,14,15 | 0.89 | 1 (7%) | 17,19,21 | 0.70 | 0 |
| 6 | FUC | r | 2 | 6 | 10,10,11 | 1.70 | 3 (30%) | 14,14,16 | 1.46 | 2 (14%) |
| 5 | NAG | s | 1 | 3,5 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.64 | 0 |
| 5 | NAG | s | 2 | 5 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.52 | 0 |
| 5 | FUC | s | 3 | 5 | 10,10,11 | 1.11 | 1 (10%) | 14,14,16 | 0.76 | 0 |
| 6 | NAG | t | 1 | 2,6 | 14,14,15 | 0.83 | 1 (7%) | 17,19,21 | 0.68 | 0 |
| 6 | FUC | t | 2 | 6 | 10,10,11 | 0.84 | 0 | 14,14,16 | 1.13 | 2 (14%) |
| 6 | NAG | u | 1 | 3,6 | 14,14,15 | 0.83 | 1 (7%) | 17,19,21 | 0.46 | 0 |
| 6 | FUC | u | 2 | 6 | 10,10,11 | 1.70 | 3 (30%) | 14,14,16 | 1.36 | 0 |
| 6 | NAG | v | 1 | 2,6 | 14,14,15 | 0.77 | 0 | 17,19,21 | 0.72 | 0 |
| 6 | FUC | v | 2 | 6 | 10,10,11 | 1.07 | 1 (10%) | 14,14,16 | 1.96 | 4 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 11 | NAG | w | 1 | 3,11 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.76 | 1 (5%) |
| 11 | FUC | w | 2 | 11 | 10,10,11 | 0.56 | 0 | 14,14,16 | 0.92 | 0 |
| 11 | FUC | w | 3 | 11 | 10,10,11 | 1.23 | 1 (10%) | 14,14,16 | 1.26 | 2 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4 | NAG | a | 1 | 2,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | a | 2 | 4 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | BMA | a | 3 | 4 | - | 2/2/19/22 | 0/1/1/1 |
| 4 | FUC | a | 4 | 4 | - | - | 0/1/1/1 |
| 5 | NAG | b | 1 | 3,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | b | 2 | 5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | FUC | b | 3 | 5 | - | - | 0/1/1/1 |
| 4 | NAG | c | 1 | 2,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | c | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | BMA | c | 3 | 4 | - | 2/2/19/22 | 0/1/1/1 |
| 4 | FUC | c | 4 | 4 | - | - | 0/1/1/1 |
| 6 | NAG | d | 1 | 3,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | FUC | d | 2 | 6 | - | - | 0/1/1/1 |
| 5 | NAG | e | 1 | 2,5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | e | 2 | 5 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | FUC | e | 3 | 5 | - | - | 0/1/1/1 |
| 7 | NAG | f | 1 | 3,7 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | FUC | f | 2 | 7 | - | - | 0/1/1/1 |
| 8 | NAG | g | 1 | 2,8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | NAG | g | 2 | 8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | BMA | g | 3 | 8 | - | 0/2/19/22 | 0/1/1/1 |
| 9 | NAG | h | 1 | 3,9 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | h | 2 | 9 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | BMA | h | 3 | 9 | - | 1/2/19/22 | 0/1/1/1 |
| 9 | FUC | h | 4 | 9 | - | - | 0/1/1/1 |
| 9 | FUC | h | 5 | 9 | - | - | 0/1/1/1 |
| 5 | NAG | i | 1 | 2,5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | i | 2 | 5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | FUC | i | 3 | 5 | - | - | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5 | NAG | j | 1 | 3,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | j | 2 | 5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | FUC | j | 3 | 5 | - | - | 0/1/1/1 |
| 9 | NAG | k | 1 | 2,9 | - | 0/6/23/26 | 0/1/1/1 |
| 9 | NAG | k | 2 | 9 | - | 1/6/23/26 | 0/1/1/1 |
| 9 | BMA | k | 3 | 9 | - | 0/2/19/22 | 0/1/1/1 |
| 9 | FUC | k | 4 | 9 | - | - | 0/1/1/1 |
| 9 | FUC | k | 5 | 9 | - | - | 0/1/1/1 |
| 5 | NAG | l | 1 | 3,5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | l | 2 | 5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | FUC | l | 3 | 5 | - | - | 0/1/1/1 |
| 5 | NAG | m | 1 | 3,5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | m | 2 | 5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | FUC | m | 3 | 5 | - | - | 0/1/1/1 |
| 4 | NAG | n | 1 | 2,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | n | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | BMA | n | 3 | 4 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | FUC | n | 4 | 4 | - | - | 0/1/1/1 |
| 6 | NAG | o | 1 | 3,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | FUC | o | 2 | 6 | - | - | 0/1/1/1 |
| 6 | NAG | p | 1 | 2,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | FUC | p | 2 | 6 | - | - | 0/1/1/1 |
| 10 | NAG | q | 1 | 3,10 | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NAG | q | 2 | 10 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | r | 1 | 2,6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | FUC | r | 2 | 6 | - | - | 0/1/1/1 |
| 5 | NAG | s | 1 | 3,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | s | 2 | 5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | FUC | s | 3 | 5 | - | - | 0/1/1/1 |
| 6 | NAG | t | 1 | 2,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | FUC | t | 2 | 6 | - | - | 0/1/1/1 |
| 6 | NAG | u | 1 | 3,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | FUC | u | 2 | 6 | - | - | 0/1/1/1 |
| 6 | NAG | v | 1 | 2,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | FUC | v | 2 | 6 | - | - | 0/1/1/1 |
| 11 | NAG | w | 1 | 3,11 | - | 0/6/23/26 | 0/1/1/1 |
| 11 | FUC | w | 2 | 11 | - | - | 0/1/1/1 |
| 11 | FUC | w | 3 | 11 | - | - | 0/1/1/1 |

All (59) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5 | m | 3 | FUC | C1-C2 | 4.87 | 1.63 | 1.52 |
| 5 | b | 3 | FUC | C2-C3 | 4.16 | 1.58 | 1.52 |
| 7 | f | 1 | NAG | O5-C1 | 3.77 | 1.49 | 1.43 |
| 5 | m | 3 | FUC | O5-C1 | 3.64 | 1.49 | 1.43 |
| 4 | c | 4 | FUC | O5-C1 | -3.62 | 1.37 | 1.43 |
| 6 | r | 2 | FUC | C2-C3 | 3.46 | 1.57 | 1.52 |
| 5 | i | 3 | FUC | C4-C5 | 3.31 | 1.60 | 1.52 |
| 6 | u | 2 | FUC | C2-C3 | 3.29 | 1.57 | 1.52 |
| 5 | e | 3 | FUC | C1-C2 | 3.27 | 1.59 | 1.52 |
| 4 | c | 3 | BMA | C1-C2 | 3.26 | 1.59 | 1.52 |
| 6 | p | 2 | FUC | C1-C2 | 3.20 | 1.59 | 1.52 |
| 9 | h | 4 | FUC | O5-C5 | 3.10 | 1.50 | 1.43 |
| 5 | l | 2 | NAG | C1-C2 | 3.00 | 1.56 | 1.52 |
| 5 | l | 1 | NAG | O5-C1 | 2.99 | 1.48 | 1.43 |
| 4 | c | 2 | NAG | C1-C2 | 2.97 | 1.56 | 1.52 |
| 6 | u | 2 | FUC | C1-C2 | 2.94 | 1.58 | 1.52 |
| 4 | a | 4 | FUC | C1-C2 | 2.93 | 1.58 | 1.52 |
| 4 | c | 3 | BMA | C2-C3 | 2.83 | 1.56 | 1.52 |
| 9 | k | 5 | FUC | O5-C1 | -2.80 | 1.39 | 1.43 |
| 6 | r | 2 | FUC | C1-C2 | 2.80 | 1.58 | 1.52 |
| 5 | l | 3 | FUC | C4-C5 | 2.79 | 1.59 | 1.52 |
| 5 | m | 3 | FUC | O5-C5 | 2.78 | 1.49 | 1.43 |
| 4 | a | 3 | BMA | C1-C2 | 2.78 | 1.58 | 1.52 |
| 8 | g | 3 | BMA | C4-C5 | 2.74 | 1.58 | 1.53 |
| 9 | h | 5 | FUC | C1-C2 | 2.73 | 1.58 | 1.52 |
| 6 | d | 2 | FUC | C4-C3 | 2.71 | 1.59 | 1.52 |
| 5 | j | 3 | FUC | C1-C2 | 2.62 | 1.58 | 1.52 |
| 9 | k | 3 | BMA | C1-C2 | 2.62 | 1.58 | 1.52 |
| 4 | n | 4 | FUC | C2-C3 | 2.60 | 1.56 | 1.52 |
| 8 | g | 3 | BMA | C4-C3 | 2.59 | 1.58 | 1.52 |
| 6 | d | 2 | FUC | C4-C5 | 2.57 | 1.58 | 1.52 |
| 6 | p | 2 | FUC | C2-C3 | 2.52 | 1.56 | 1.52 |
| 5 | b | 3 | FUC | O5-C5 | 2.48 | 1.48 | 1.43 |
| 5 | i | 1 | NAG | C1-C2 | 2.48 | 1.56 | 1.52 |
| 4 | a | 2 | NAG | O5-C1 | -2.46 | 1.39 | 1.43 |
| 6 | o | 2 | FUC | C2-C3 | 2.43 | 1.56 | 1.52 |
| 6 | p | 1 | NAG | O5-C1 | 2.43 | 1.47 | 1.43 |
| 11 | w | 3 | FUC | C1-C2 | 2.42 | 1.57 | 1.52 |
| 5 | b | 3 | FUC | C4-C5 | 2.41 | 1.58 | 1.52 |
| 6 | v | 2 | FUC | C1-C2 | 2.37 | 1.57 | 1.52 |
| 5 | s | 3 | FUC | C2-C3 | 2.34 | 1.56 | 1.52 |
| 6 | u | 1 | NAG | O5-C1 | 2.34 | 1.47 | 1.43 |
| 10 | q | 1 | NAG | O5-C1 | 2.32 | 1.47 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6 | r | 1 | NAG | C1-C2 | 2.30 | 1.55 | 1.52 |
| 9 | h | 5 | FUC | O5-C5 | 2.29 | 1.48 | 1.43 |
| 5 | l | 3 | FUC | O5-C5 | 2.24 | 1.48 | 1.43 |
| 5 | j | 3 | FUC | O5-C5 | 2.24 | 1.48 | 1.43 |
| 9 | h | 4 | FUC | C1-C2 | 2.23 | 1.57 | 1.52 |
| 9 | k | 4 | FUC | C1-C2 | 2.20 | 1.57 | 1.52 |
| 6 | r | 2 | FUC | O5-C5 | 2.17 | 1.48 | 1.43 |
| 6 | o | 1 | NAG | C1-C2 | 2.15 | 1.55 | 1.52 |
| 6 | t | 1 | NAG | O5-C1 | 2.15 | 1.47 | 1.43 |
| 6 | u | 2 | FUC | O5-C1 | -2.11 | 1.40 | 1.43 |
| 4 | n | 3 | BMA | C4-C5 | 2.10 | 1.57 | 1.53 |
| 5 | l | 3 | FUC | C2-C3 | 2.07 | 1.55 | 1.52 |
| 6 | o | 1 | NAG | O5-C1 | 2.05 | 1.47 | 1.43 |
| 4 | a | 4 | FUC | O5-C1 | -2.05 | 1.40 | 1.43 |
| 9 | k | 3 | BMA | C2-C3 | 2.03 | 1.55 | 1.52 |
| 9 | k | 4 | FUC | O5-C5 | 2.01 | 1.47 | 1.43 |

All (74) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4 | a | 3 | BMA | C1-O5-C5 | 5.07 | 119.06 | 112.19 |
| 6 | p | 2 | FUC | C1-C2-C3 | 5.01 | 115.83 | 109.67 |
| 4 | a | 2 | NAG | C2-N2-C7 | 4.81 | 129.75 | 122.90 |
| 6 | v | 2 | FUC | O5-C1-C2 | 4.72 | 118.05 | 110.77 |
| 5 | l | 3 | FUC | O5-C5-C4 | 4.63 | 117.82 | 109.52 |
| 5 | m | 3 | FUC | O5-C5-C4 | 4.57 | 117.73 | 109.52 |
| 5 | j | 3 | FUC | C1-O5-C5 | 4.44 | 122.83 | 112.78 |
| 5 | l | 3 | FUC | C3-C4-C5 | 4.36 | 116.57 | 109.77 |
| 9 | h | 2 | NAG | C1-O5-C5 | 4.31 | 118.03 | 112.19 |
| 5 | m | 3 | FUC | C1-O5-C5 | 4.22 | 122.35 | 112.78 |
| 4 | c | 1 | NAG | O4-C4-C5 | -3.96 | 99.45 | 109.30 |
| 4 | c | 2 | NAG | C1-O5-C5 | -3.86 | 106.96 | 112.19 |
| 6 | r | 2 | FUC | C1-C2-C3 | 3.84 | 114.38 | 109.67 |
| 5 | i | 3 | FUC | C1-C2-C3 | -3.73 | 105.08 | 109.67 |
| 5 | e | 2 | NAG | C1-O5-C5 | 3.66 | 117.15 | 112.19 |
| 4 | c | 3 | BMA | C1-O5-C5 | 3.49 | 116.93 | 112.19 |
| 6 | o | 1 | NAG | O3-C3-C2 | 3.45 | 116.60 | 109.47 |
| 9 | h | 3 | BMA | C1-O5-C5 | 3.39 | 116.78 | 112.19 |
| 5 | l | 3 | FUC | O3-C3-C4 | -3.38 | 102.53 | 110.35 |
| 9 | h | 5 | FUC | C2-C3-C4 | -3.13 | 105.47 | 110.89 |
| 11 | w | 3 | FUC | C1-C2-C3 | 3.13 | 113.51 | 109.67 |
| 4 | a | 4 | FUC | O2-C2-C1 | 3.10 | 115.49 | 109.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9 | h | 2 | NAG | O4-C4-C5 | 3.06 | 116.89 | 109.30 |
| 5 | e | 1 | NAG | O4-C4-C3 | -3.01 | 103.39 | 110.35 |
| 5 | m | 3 | FUC | C1-C2-C3 | 2.99 | 113.34 | 109.67 |
| 5 | l | 3 | FUC | C1-O5-C5 | 2.87 | 119.29 | 112.78 |
| 9 | h | 5 | FUC | O5-C5-C4 | 2.85 | 114.63 | 109.52 |
| 9 | h | 5 | FUC | O2-C2-C1 | 2.82 | 114.92 | 109.15 |
| 5 | l | 1 | NAG | O4-C4-C3 | 2.76 | 116.73 | 110.35 |
| 4 | a | 3 | BMA | C1-C2-C3 | 2.74 | 113.04 | 109.67 |
| 5 | b | 3 | FUC | O5-C5-C4 | 2.73 | 114.43 | 109.52 |
| 4 | c | 3 | BMA | C1-C2-C3 | 2.72 | 113.01 | 109.67 |
| 4 | c | 4 | FUC | C1-C2-C3 | -2.71 | 106.34 | 109.67 |
| 5 | j | 3 | FUC | O5-C5-C4 | 2.68 | 114.32 | 109.52 |
| 4 | a | 3 | BMA | O5-C1-C2 | 2.67 | 114.89 | 110.77 |
| 5 | j | 3 | FUC | O2-C2-C1 | 2.64 | 114.55 | 109.15 |
| 6 | v | 2 | FUC | O5-C5-C6 | -2.62 | 101.69 | 107.33 |
| 4 | c | 4 | FUC | O2-C2-C1 | 2.60 | 114.48 | 109.15 |
| 6 | o | 2 | FUC | C1-O5-C5 | 2.59 | 118.66 | 112.78 |
| 9 | h | 4 | FUC | C1-O5-C5 | 2.55 | 118.56 | 112.78 |
| 9 | h | 4 | FUC | O5-C5-C4 | 2.54 | 114.08 | 109.52 |
| 9 | h | 5 | FUC | C1-O5-C5 | 2.47 | 118.39 | 112.78 |
| 4 | n | 4 | FUC | C1-C2-C3 | 2.45 | 112.68 | 109.67 |
| 6 | v | 2 | FUC | O3-C3-C2 | -2.43 | 105.34 | 109.99 |
| 4 | a | 3 | BMA | O2-C2-C3 | -2.42 | 105.28 | 110.14 |
| 5 | j | 3 | FUC | C2-C3-C4 | -2.42 | 106.71 | 110.89 |
| 4 | a | 1 | NAG | O4-C4-C3 | -2.41 | 104.77 | 110.35 |
| 6 | r | 2 | FUC | O5-C5-C4 | 2.41 | 113.85 | 109.52 |
| 9 | h | 3 | BMA | O5-C1-C2 | 2.41 | 114.49 | 110.77 |
| 6 | t | 2 | FUC | C1-O5-C5 | 2.41 | 118.24 | 112.78 |
| 6 | d | 2 | FUC | O5-C5-C4 | 2.37 | 113.77 | 109.52 |
| 5 | j | 3 | FUC | O5-C1-C2 | 2.37 | 114.42 | 110.77 |
| 6 | o | 2 | FUC | O5-C5-C4 | 2.35 | 113.75 | 109.52 |
| 4 | c | 2 | NAG | O4-C4-C5 | -2.35 | 103.45 | 109.30 |
| 6 | v | 2 | FUC | C1-O5-C5 | 2.34 | 118.08 | 112.78 |
| 5 | m | 3 | FUC | O5-C1-C2 | 2.31 | 114.34 | 110.77 |
| 5 | b | 1 | NAG | C1-C2-N2 | 2.30 | 114.42 | 110.49 |
| 4 | a | 1 | NAG | O4-C4-C5 | -2.30 | 103.58 | 109.30 |
| 4 | c | 2 | NAG | C4-C3-C2 | 2.29 | 114.38 | 111.02 |
| 4 | a | 2 | NAG | O4-C4-C5 | 2.28 | 114.97 | 109.30 |
| 9 | k | 5 | FUC | O2-C2-C1 | 2.24 | 113.73 | 109.15 |
| 11 | w | 3 | FUC | C1-O5-C5 | 2.24 | 117.85 | 112.78 |
| 6 | t | 2 | FUC | O5-C5-C4 | 2.24 | 113.53 | 109.52 |
| 5 | i | 3 | FUC | O5-C5-C4 | 2.17 | 113.41 | 109.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11 | w | 1 | NAG | C1-O5-C5 | 2.16 | 115.12 | 112.19 |
| 5 | m | 1 | NAG | C6-C5-C4 | 2.15 | 118.03 | 113.00 |
| 6 | d | 2 | FUC | C1-O5-C5 | 2.13 | 117.62 | 112.78 |
| 7 | f | 1 | NAG | C1-O5-C5 | 2.13 | 115.08 | 112.19 |
| 5 | b | 3 | FUC | C1-O5-C5 | 2.12 | 117.59 | 112.78 |
| 5 | m | 1 | NAG | O3-C3-C4 | 2.10 | 115.20 | 110.35 |
| 10 | q | 1 | NAG | C1-C2-N2 | 2.09 | 114.07 | 110.49 |
| 5 | m | 3 | FUC | C6-C5-C4 | -2.06 | 109.26 | 113.07 |
| 4 | c | 2 | NAG | C2-N2-C7 | 2.06 | 125.84 | 122.90 |
| 5 | m | 1 | NAG | C1-O5-C5 | 2.04 | 114.96 | 112.19 |

There are no chirality outliers.

All (68) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 5 | l | 2 | NAG | C1-C2-N2-C7 |
| 5 | m | 1 | NAG | C4-C5-C6-O6 |
| 6 | r | 1 | NAG | C1-C2-N2-C7 |
| 5 | b | 2 | NAG | O5-C5-C6-O6 |
| 4 | a | 2 | NAG | O5-C5-C6-O6 |
| 4 | n | 2 | NAG | O5-C5-C6-O6 |
| 6 | d | 1 | NAG | O5-C5-C6-O6 |
| 6 | o | 1 | NAG | O5-C5-C6-O6 |
| 4 | c | 3 | BMA | O5-C5-C6-O6 |
| 6 | u | 1 | NAG | O5-C5-C6-O6 |
| 10 | q | 1 | NAG | O5-C5-C6-O6 |
| 5 | l | 1 | NAG | O5-C5-C6-O6 |
| 4 | a | 3 | BMA | O5-C5-C6-O6 |
| 5 | i | 2 | NAG | O5-C5-C6-O6 |
| 5 | b | 2 | NAG | C4-C5-C6-O6 |
| 9 | h | 2 | NAG | C4-C5-C6-O6 |
| 5 | m | 1 | NAG | O5-C5-C6-O6 |
| 9 | h | 2 | NAG | O5-C5-C6-O6 |
| 4 | c | 3 | BMA | C4-C5-C6-O6 |
| 5 | e | 1 | NAG | O5-C5-C6-O6 |
| 5 | m | 2 | NAG | O5-C5-C6-O6 |
| 6 | p | 1 | NAG | O5-C5-C6-O6 |
| 4 | n | 2 | NAG | C4-C5-C6-O6 |
| 6 | d | 1 | NAG | C4-C5-C6-O6 |
| 6 | u | 1 | NAG | C4-C5-C6-O6 |
| 4 | a | 2 | NAG | C8-C7-N2-C2 |
| 4 | a | 2 | NAG | O7-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 5 | e | 1 | NAG | C4-C5-C6-O6 |
| 6 | o | 1 | NAG | C4-C5-C6-O6 |
| 10 | q | 1 | NAG | C4-C5-C6-O6 |
| 4 | a | 1 | NAG | O5-C5-C6-O6 |
| 5 | j | 2 | NAG | O5-C5-C6-O6 |
| 6 | r | 1 | NAG | O5-C5-C6-O6 |
| 9 | h | 1 | NAG | O5-C5-C6-O6 |
| 5 | l | 1 | NAG | C4-C5-C6-O6 |
| 4 | a | 1 | NAG | C4-C5-C6-O6 |
| 9 | h | 1 | NAG | C4-C5-C6-O6 |
| 6 | p | 1 | NAG | C4-C5-C6-O6 |
| 6 | r | 1 | NAG | C4-C5-C6-O6 |
| 5 | s | 2 | NAG | O5-C5-C6-O6 |
| 4 | a | 2 | NAG | C4-C5-C6-O6 |
| 9 | h | 3 | BMA | O5-C5-C6-O6 |
| 5 | s | 2 | NAG | C4-C5-C6-O6 |
| 4 | c | 1 | NAG | C4-C5-C6-O6 |
| 4 | c | 2 | NAG | O5-C5-C6-O6 |
| 5 | j | 2 | NAG | C4-C5-C6-O6 |
| 5 | e | 2 | NAG | O5-C5-C6-O6 |
| 5 | l | 1 | NAG | C1-C2-N2-C7 |
| 4 | c | 1 | NAG | O5-C5-C6-O6 |
| 5 | i | 2 | NAG | C4-C5-C6-O6 |
| 9 | k | 2 | NAG | O5-C5-C6-O6 |
| 5 | m | 2 | NAG | C4-C5-C6-O6 |
| 4 | a | 3 | BMA | C4-C5-C6-O6 |
| 5 | b | 2 | NAG | C3-C2-N2-C7 |
| 5 | l | 2 | NAG | C3-C2-N2-C7 |
| 6 | r | 1 | NAG | C3-C2-N2-C7 |
| 6 | t | 1 | NAG | C3-C2-N2-C7 |
| 10 | q | 2 | NAG | C3-C2-N2-C7 |
| 4 | a | 2 | NAG | C1-C2-N2-C7 |
| 4 | c | 2 | NAG | C1-C2-N2-C7 |
| 5 | b | 2 | NAG | C1-C2-N2-C7 |
| 4 | a | 2 | NAG | C3-C2-N2-C7 |
| 5 | i | 1 | NAG | C3-C2-N2-C7 |
| 5 | l | 1 | NAG | C3-C2-N2-C7 |
| 5 | m | 2 | NAG | C3-C2-N2-C7 |
| 6 | t | 1 | NAG | C4-C5-C6-O6 |
| 5 | i | 1 | NAG | C1-C2-N2-C7 |
| 5 | m | 2 | NAG | C1-C2-N2-C7 |

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

8 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$ |
| 12 | GOL | H | 301 | - | 5,5,5 | 1.23 | 1 (20%) | 5,5,5 | 0.76 | 0 |
| 12 | GOL | Y | 303 | - | 5,5,5 | 1.06 | 0 | 5,5,5 | 0.73 | 0 |
| 12 | GOL | J | 204 | - | 5,5,5 | 1.06 | 0 | 5,5,5 | 0.89 | 0 |
| 12 | GOL | O | 401 | - | 5,5,5 | 0.89 | 0 | 5,5,5 | 0.98 | 0 |
| 12 | GOL | K | 301 | - | 5,5,5 | 0.97 | 0 | 5,5,5 | 0.99 | 0 |
| 12 | GOL | M | 305 | - | 5,5,5 | 1.63 | 1 (20%) | 5,5,5 | 0.81 | 0 |
| 12 | GOL | A | 304 | - | 5,5,5 | 1.24 | 0 | 5,5,5 | 0.94 | 0 |
| 13 | NAG | B | 301 | 2 | 14,14,15 | 0.92 | 1 (7%) | 17,19,21 | 0.57 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 12 | GOL | H | 301 | - | - | 2/4/4/4 | - |
| 12 | GOL | Y | 303 | - | - | 2/4/4/4 | - |
| 12 | GOL | J | 204 | - | - | 2/4/4/4 | - |
| 12 | GOL | O | 401 | - | - | 2/4/4/4 | - |
| 12 | GOL | K | 301 | - | - | 2/4/4/4 | - |
| 12 | GOL | M | 305 | - | - | 4/4/4/4 | - |
| 12 | GOL | A | 304 | - | - | 4/4/4/4 | - |
| 13 | NAG | B | 301 | 2 | - | 2/6/23/26 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 12 | M | 305 | GOL | C3-C2 | 2.81 | 1.63 | 1.51 |
| 13 | B | 301 | NAG | O5-C1 | 2.76 | 1.48 | 1.43 |
| 12 | H | 301 | GOL | C1-C2 | 2.44 | 1.61 | 1.51 |

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 12 | A | 304 | GOL | C1-C2-C3-O3 |
| 12 | H | 301 | GOL | C1-C2-C3-O3 |
| 12 | Y | 303 | GOL | O1-C1-C2-O2 |
| 13 | B | 301 | NAG | C4-C5-C6-O6 |
| 13 | B | 301 | NAG | O5-C5-C6-O6 |
| 12 | J | 204 | GOL | C1-C2-C3-O3 |
| 12 | K | 301 | GOL | C1-C2-C3-O3 |
| 12 | M | 305 | GOL | O1-C1-C2-C3 |
| 12 | M | 305 | GOL | C1-C2-C3-O3 |
| 12 | O | 401 | GOL | C1-C2-C3-O3 |
| 12 | Y | 303 | GOL | O1-C1-C2-C3 |
| 12 | A | 304 | GOL | O2-C2-C3-O3 |
| 12 | H | 301 | GOL | O2-C2-C3-O3 |
| 12 | M | 305 | GOL | O1-C1-C2-O2 |
| 12 | J | 204 | GOL | O2-C2-C3-O3 |
| 12 | M | 305 | GOL | O2-C2-C3-O3 |
| 12 | O | 401 | GOL | O2-C2-C3-O3 |
| 12 | A | 304 | GOL | O1-C1-C2-O2 |
| 12 | K | 301 | GOL | O2-C2-C3-O3 |
| 12 | A | 304 | GOL | O1-C1-C2-C3 |

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | Y | 303 | GOL | 1 | 0 |
| 12 | M | 305 | GOL | 2 | 0 |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.