



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:56 PM BST

PDB ID : 2WIN
Title : C3 convertase (C3bBb) stabilized by SCIN
Authors : Wu, J.; Janssen, B.J.; Gros, P.
Deposited on : 2009-05-13
Resolution : 3.90 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 : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

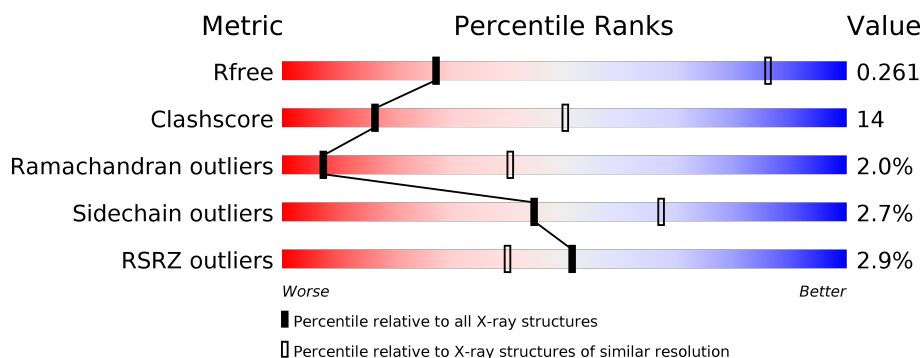
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1002 (4.14-3.66) |
| Clashscore | 141614 | 1004 (4.12-3.68) |
| Ramachandran outliers | 138981 | 1021 (4.14-3.66) |
| Sidechain outliers | 138945 | 1014 (4.14-3.66) |
| RSRZ outliers | 127900 | 1275 (4.20-3.60) |

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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 645 | <div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div> |
| 1 | C | 645 | <div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div> |
| 1 | E | 645 | <div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div> |
| 1 | G | 645 | <div> <div>9%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>..</div> </div> </div> |
| 2 | B | 915 | <div> <div>%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>...</div> </div> </div> |
| 2 | D | 915 | <div> <div>%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>...</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | F | 915 | |
| 2 | H | 915 | |
| 3 | I | 507 | |
| 3 | J | 507 | |
| 3 | K | 507 | |
| 3 | L | 507 | |
| 4 | M | 92 | |
| 4 | N | 92 | |
| 4 | P | 92 | |
| 4 | Q | 92 | |
| 5 | O | 4 | |
| 5 | R | 4 | |
| 5 | T | 4 | |
| 5 | U | 4 | |
| 6 | S | 5 | |
| 6 | W | 5 | |
| 7 | V | 6 | |
| 8 | X | 4 | |
| 9 | Y | 3 | |
| 9 | a | 3 | |
| 10 | Z | 2 | |
| 11 | b | 5 | |
| 12 | c | 3 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 10 | NAG | Z | 1 | X | - | - | - |
| 11 | NAG | b | 1 | X | - | - | - |
| 11 | MAN | b | 3 | X | - | - | - |
| 11 | MAN | b | 4 | X | - | - | - |
| 11 | MAN | b | 5 | X | - | - | - |
| 16 | NAG | K | 1749 | X | - | - | - |
| 16 | NAG | L | 1746 | X | - | - | - |
| 5 | NAG | O | 1 | X | - | - | - |
| 6 | BMA | W | 5 | - | - | - | X |
| 7 | NAG | V | 1 | X | - | - | - |
| 8 | MAN | X | 3 | X | - | - | - |
| 8 | MAN | X | 4 | X | - | - | - |
| 9 | MAN | Y | 3 | X | - | - | - |
| 9 | MAN | a | 3 | X | - | - | - |

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 67989 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 COMPLEMENT C3 BETA CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4958 | 3157 | 841 | 945 | 15 | | | |
| 1 | C | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4958 | 3157 | 841 | 945 | 15 | | | |
| 1 | E | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4958 | 3157 | 841 | 945 | 15 | | | |
| 1 | G | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4958 | 3157 | 841 | 945 | 15 | | | |

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | B | 901 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7177 | 4545 | 1209 | 1386 | 37 | | | |
| 2 | D | 901 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7166 | 4537 | 1208 | 1384 | 37 | | | |
| 2 | F | 900 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7172 | 4545 | 1206 | 1384 | 37 | | | |
| 2 | H | 900 | Total | C | N | O | S | 2313 | 0 | 0 |
| | | | 7175 | 4547 | 1209 | 1382 | 37 | | | |

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | I | 507 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4004 | 2543 | 685 | 756 | 20 | | | |
| 3 | J | 507 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4004 | 2543 | 685 | 756 | 20 | | | |
| 3 | K | 507 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4004 | 2543 | 685 | 756 | 20 | | | |
| 3 | L | 507 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4004 | 2543 | 685 | 756 | 20 | | | |

- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

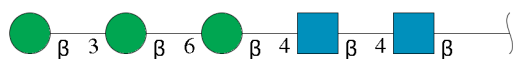
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | M | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 682 | 432 | 111 | 137 | 2 | | | |
| 4 | N | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 682 | 432 | 111 | 137 | 2 | | | |
| 4 | P | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 682 | 432 | 111 | 137 | 2 | | | |
| 4 | Q | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 682 | 432 | 111 | 137 | 2 | | | |

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



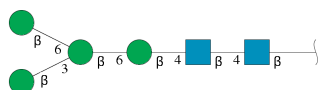
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5 | O | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | R | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | T | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | U | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |

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



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6 | S | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 61 | 34 | 2 | 25 | | | |
| 6 | W | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 61 | 34 | 2 | 25 | | | |

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 7 | V | 6 | Total | C | N | O | 0 | 0 | 0 |
| | | | 72 | 40 | 2 | 30 | | | |

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 8 | X | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |

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



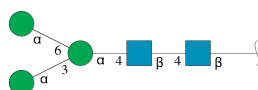
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 9 | Y | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 9 | a | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |

- 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 | Z | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



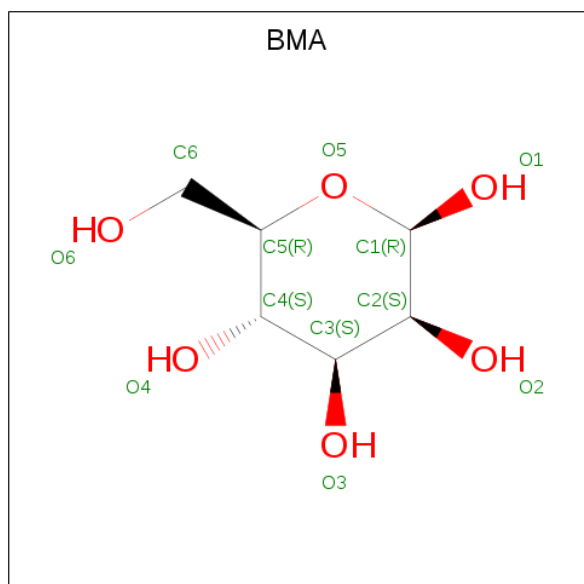
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 11 | b | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 61 | 34 | 2 | 25 | | | |

- Molecule 12 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.



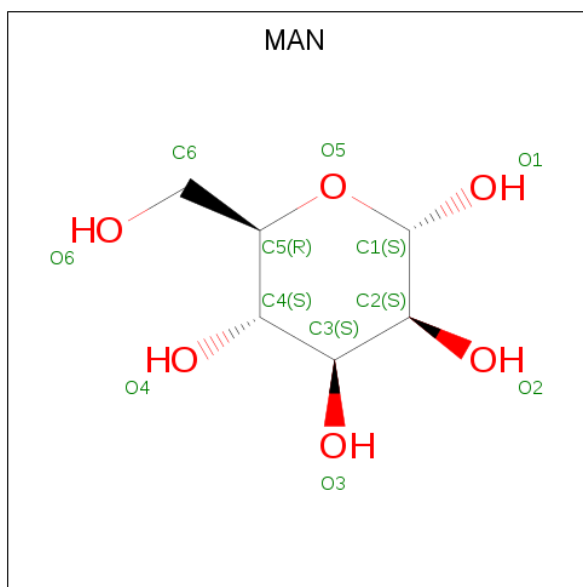
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 12 | c | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |

- Molecule 13 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 13 | B | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 13 | K | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |

- Molecule 14 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

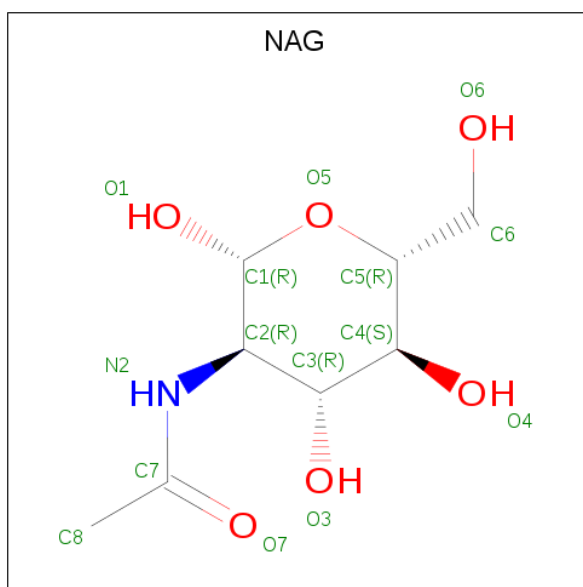


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 14 | G | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 15 | I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 15 | L | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 15 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 16 | K | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 16 | L | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

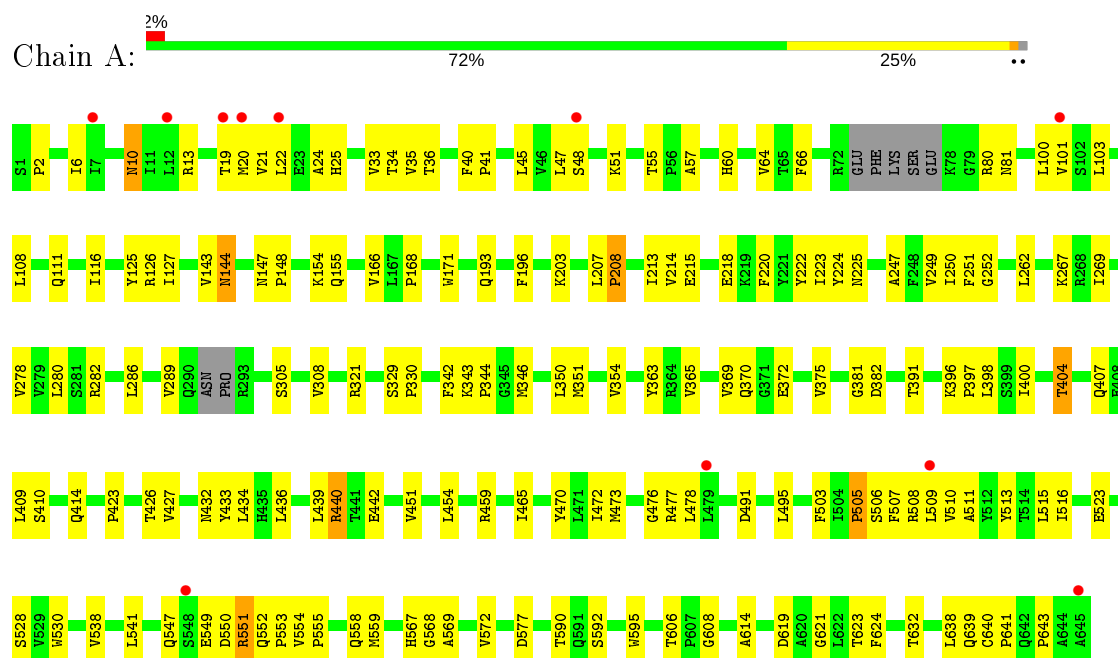
- Molecule 17 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 17 | B | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 17 | I | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 17 | J | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 17 | K | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 17 | L | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

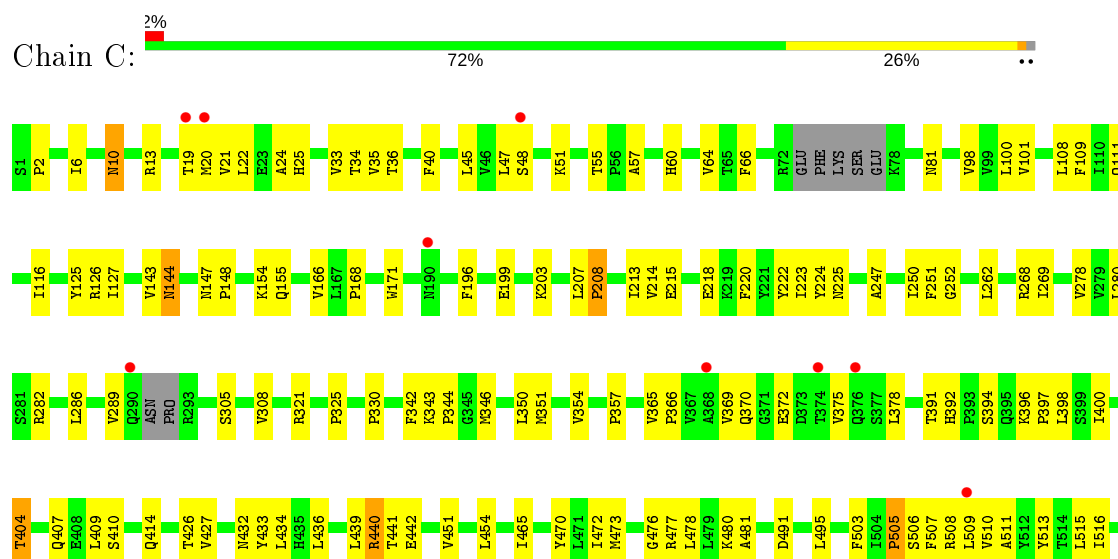
3 Residue-property plots [i](#)

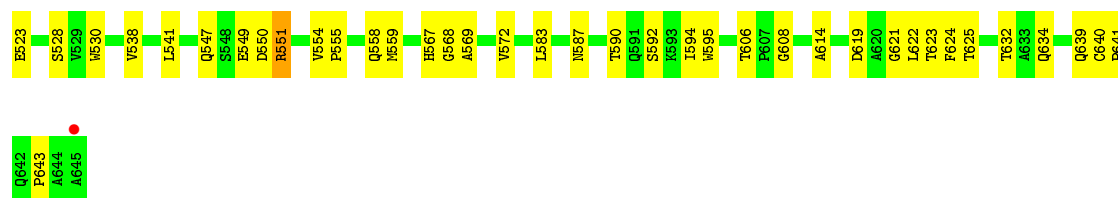
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: COMPLEMENT C3 BETA CHAIN

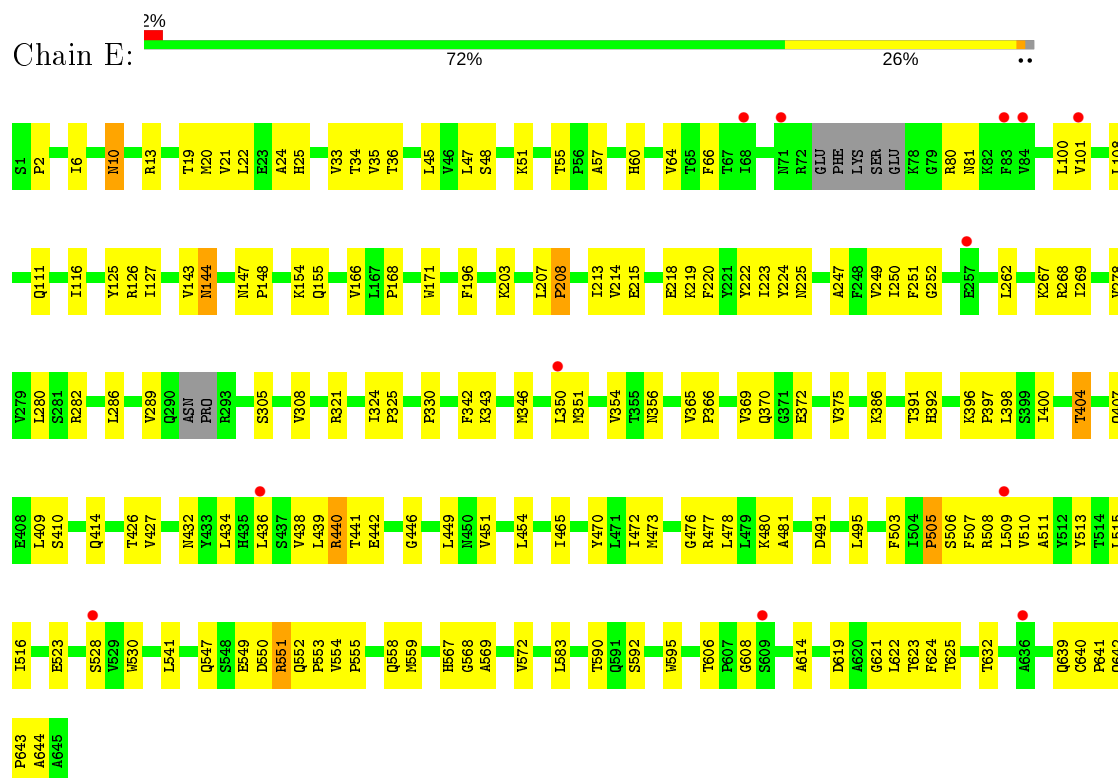


• Molecule 1: COMPLEMENT C3 BETA CHAIN

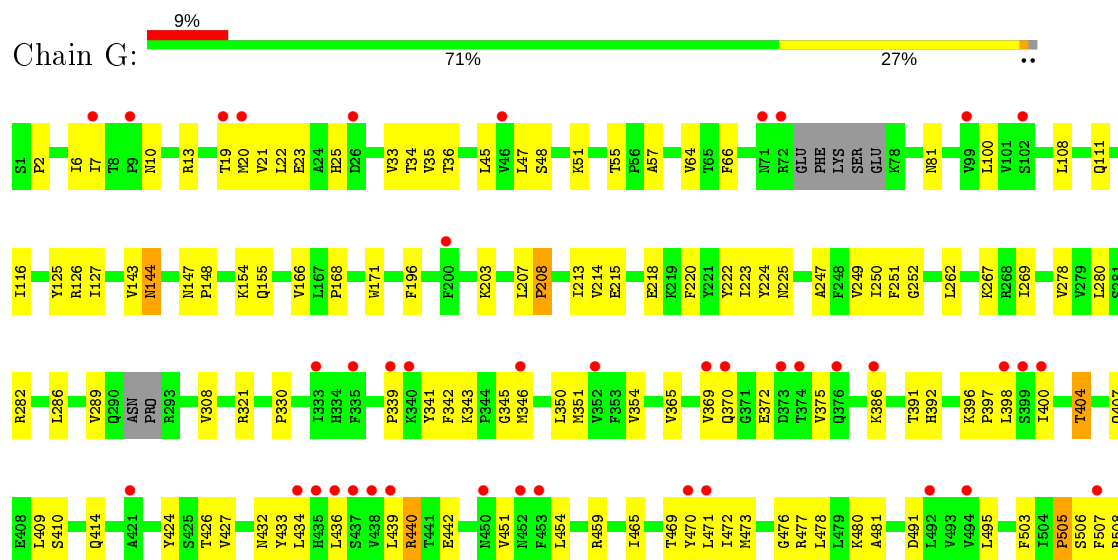


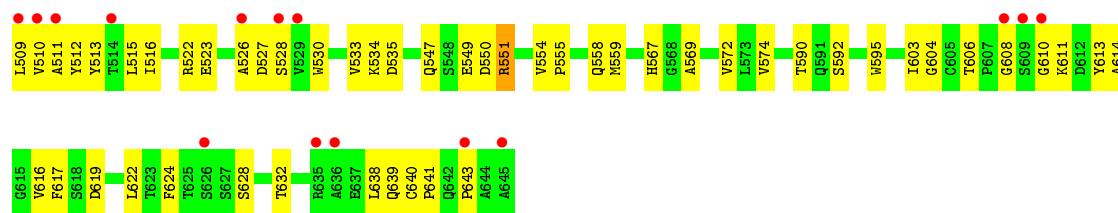


• Molecule 1: COMPLEMENT C3 BETA CHAIN

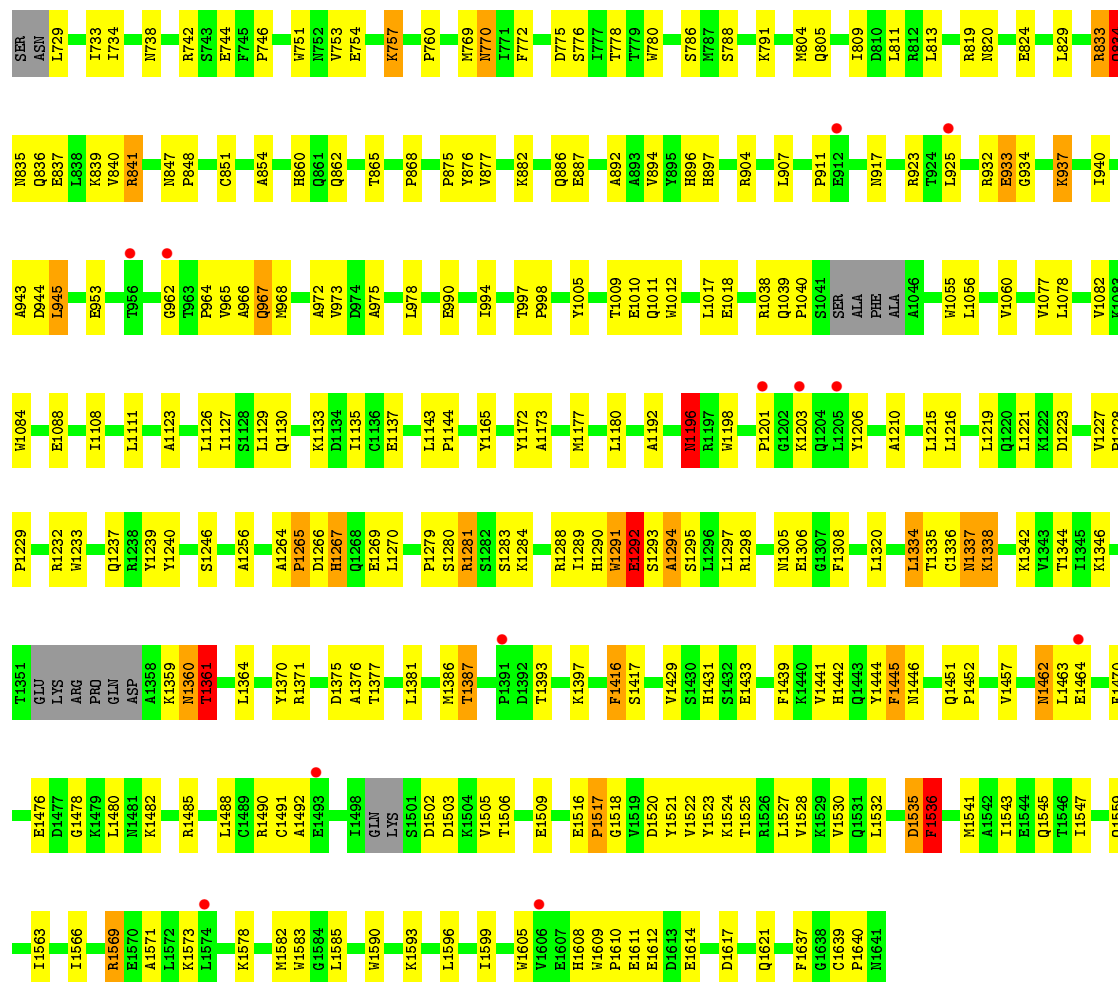


• Molecule 1: COMPLEMENT C3 BETA CHAIN

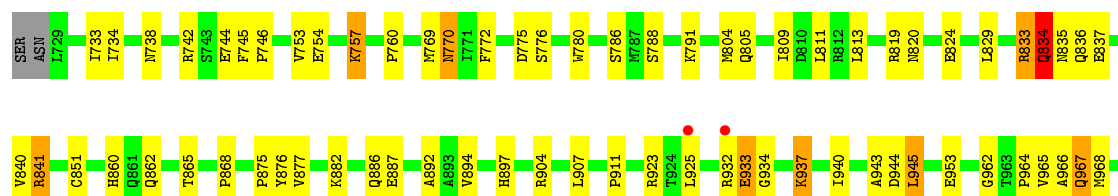


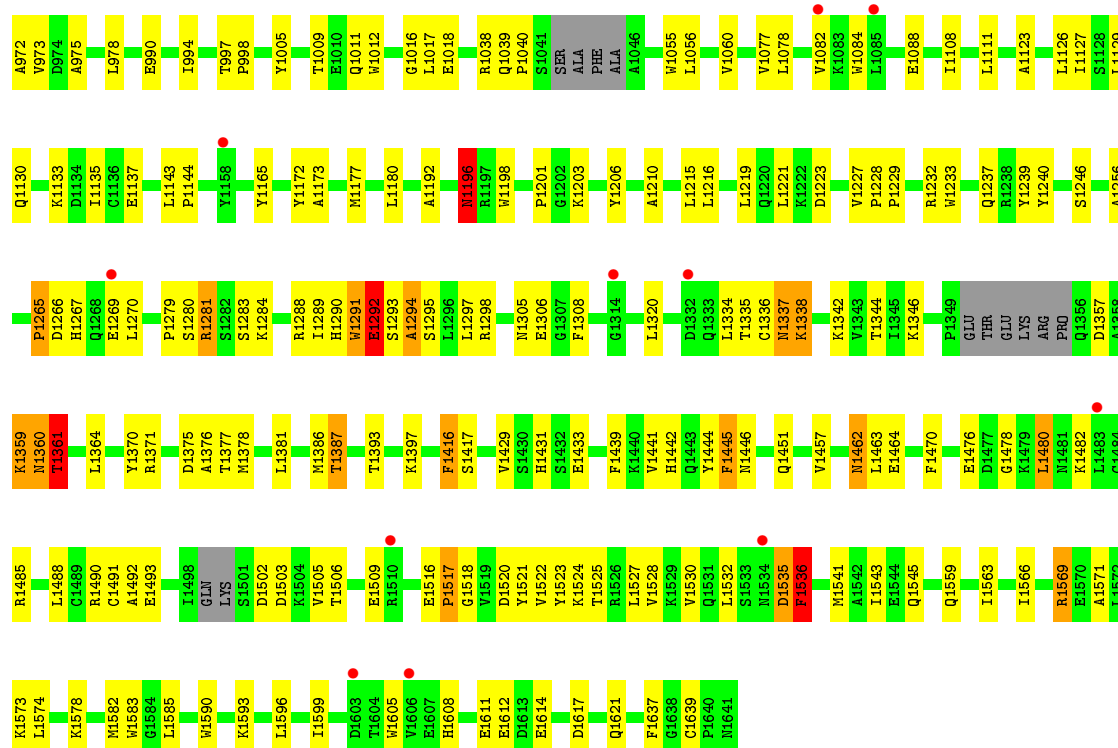


● Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

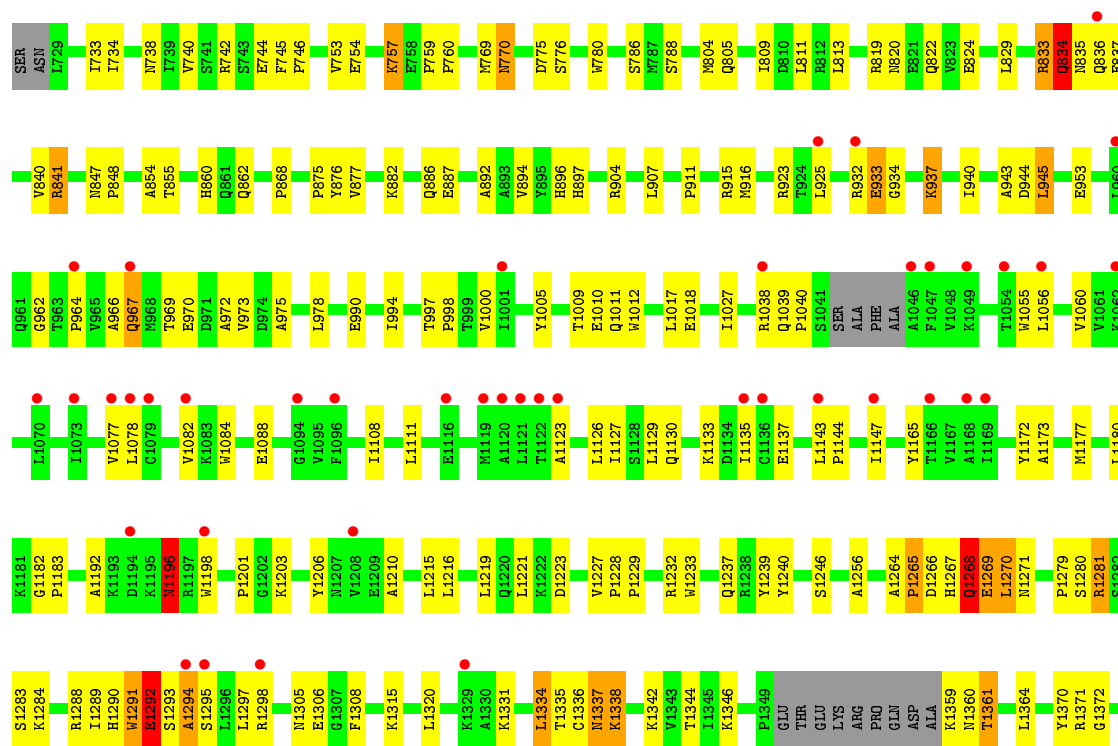


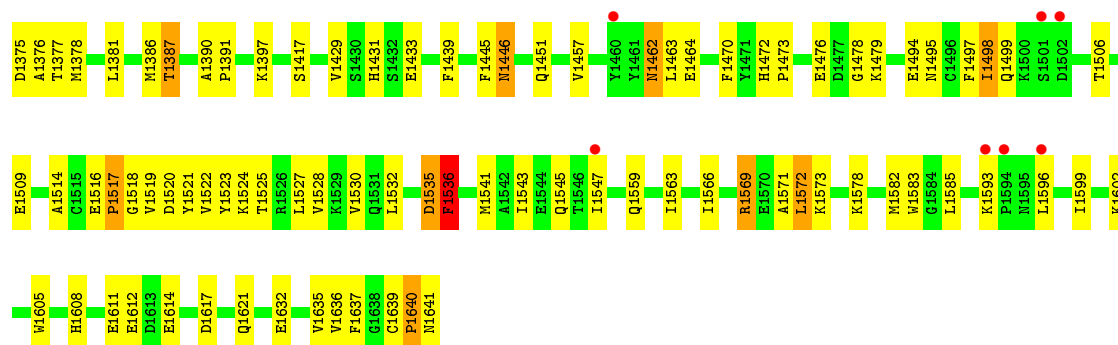
● Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



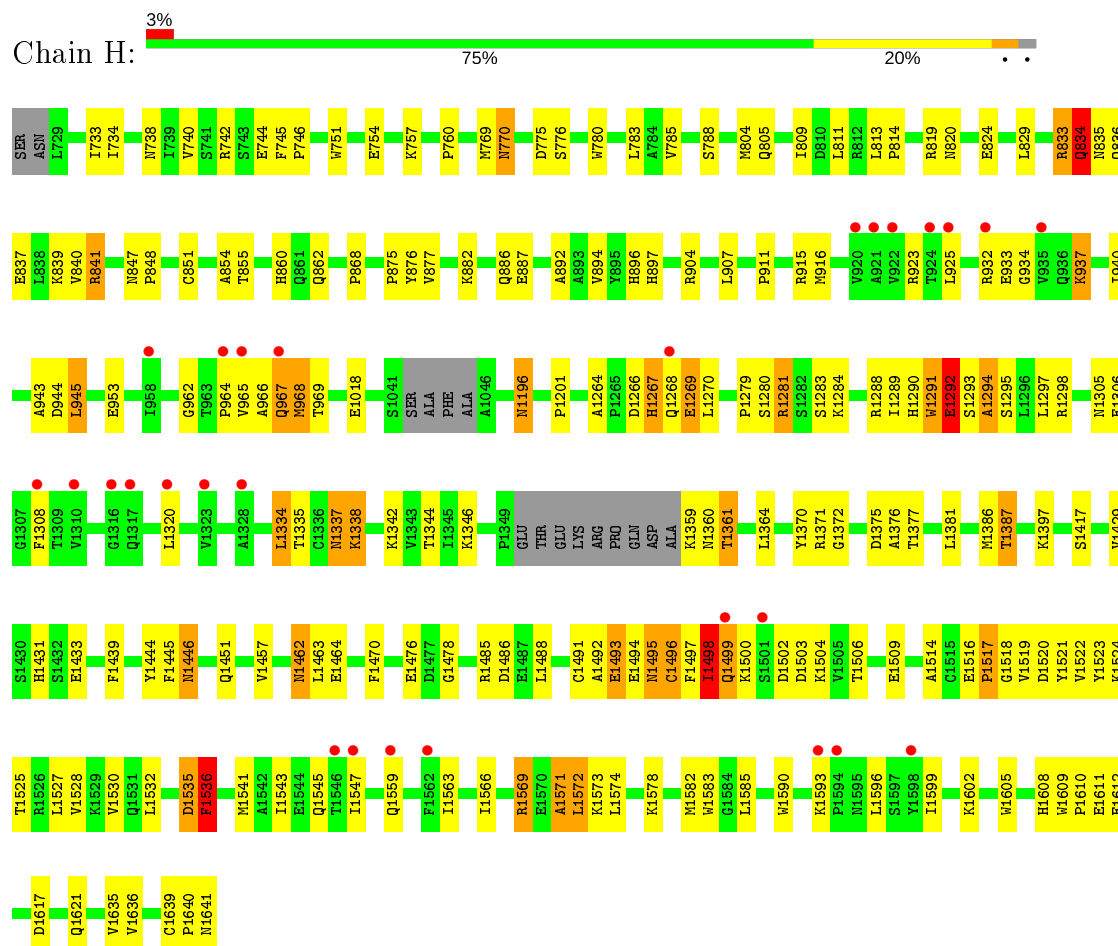


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

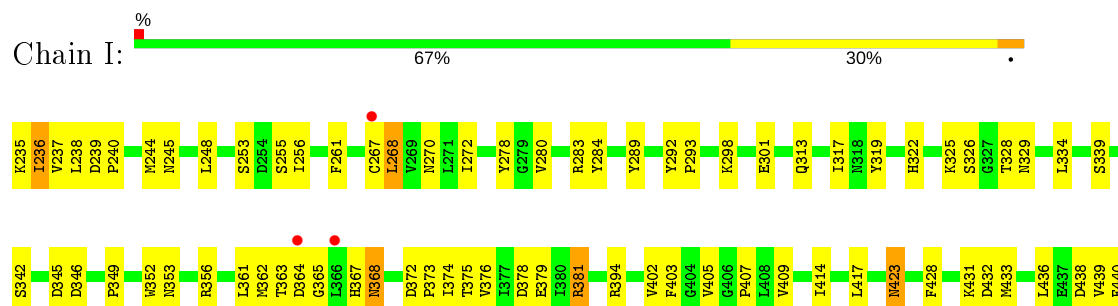


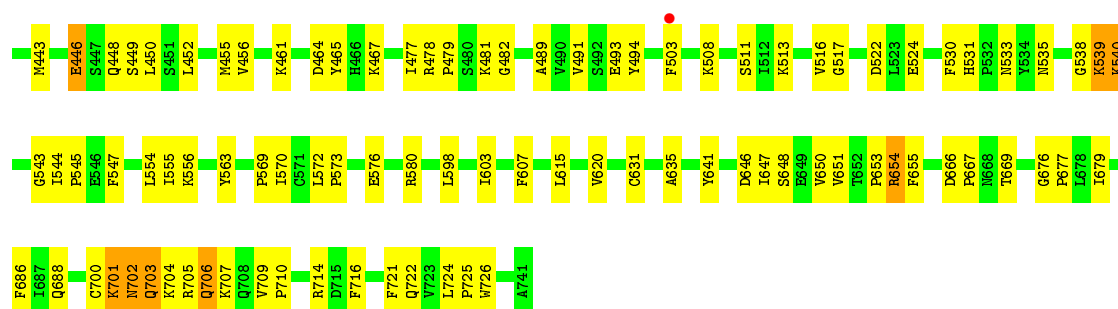


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

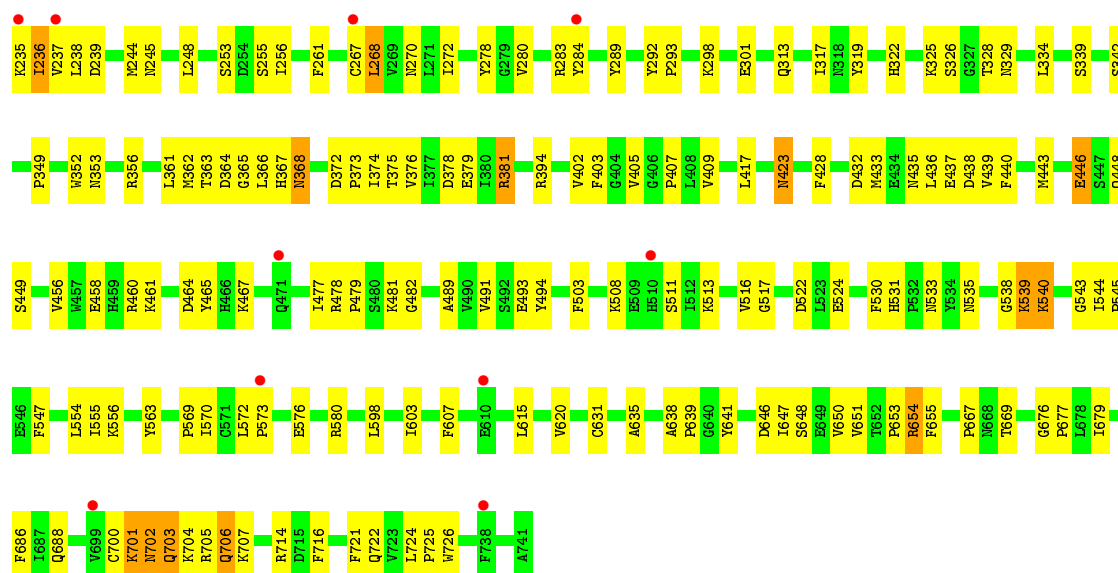


• Molecule 3: COMPLEMENT FACTOR B

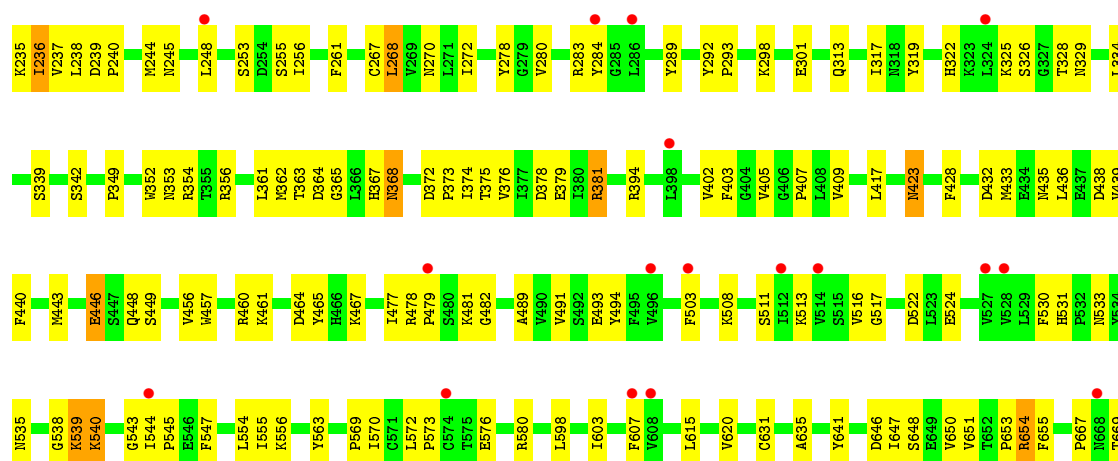


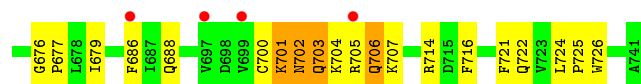


• Molecule 3: COMPLEMENT FACTOR B

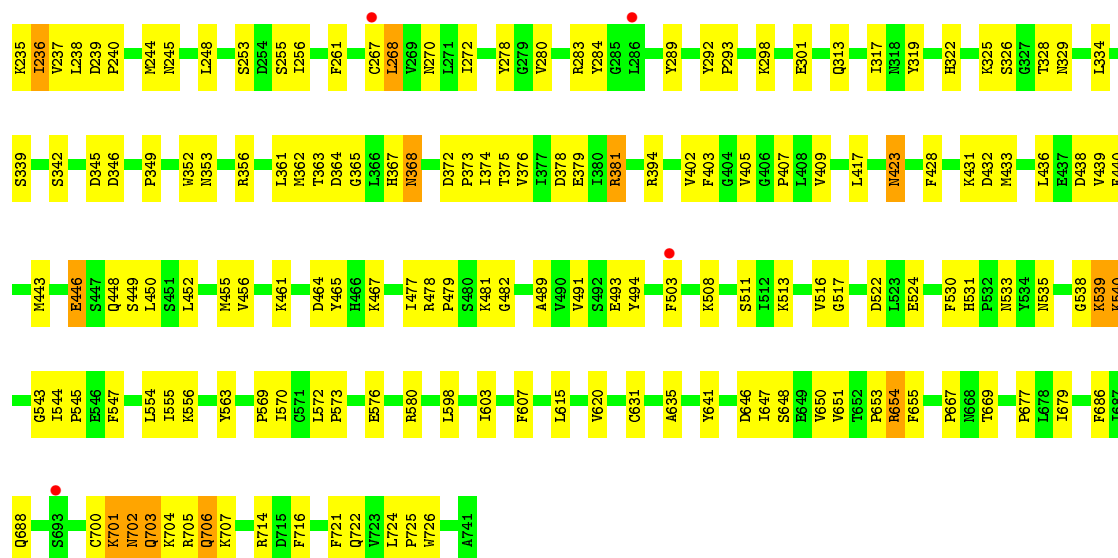


• Molecule 3: COMPLEMENT FACTOR B





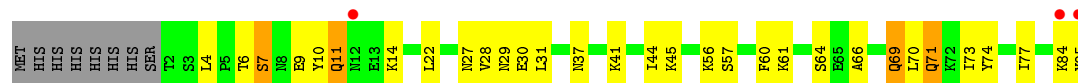
• Molecule 3: COMPLEMENT FACTOR B



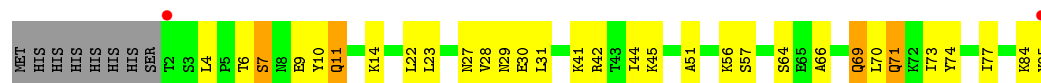
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

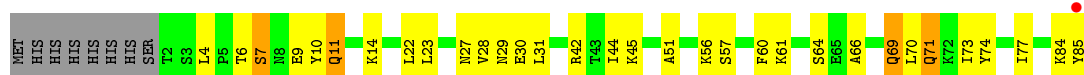


• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

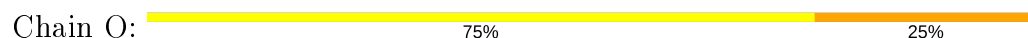


• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR





- Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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





- Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



- Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain Y:



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

Chain a:



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

Chain Z:

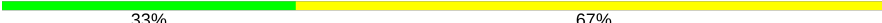


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 


MAG1
MAG2
BMA3

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 228.63Å 121.49Å 280.78Å 90.00° 91.64° 90.00° | Depositor |
| Resolution (Å) | 39.67 – 3.90 39.68 – 3.90 | Depositor EDS |
| % Data completeness (in resolution range) | 97.6 (39.67-3.90) 89.7 (39.68-3.90) | Depositor EDS |
| R_{merge} | 0.13 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.95 (at 3.87Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, R_{free} | 0.253 , 0.268 0.247 , 0.261 | Depositor DCC |
| R_{free} test set | 2089 reflections (1.52%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 125.3 | Xtriage |
| Anisotropy | 0.223 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 76.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$ | Xtriage |
| Estimated twinning fraction | 0.128 for h,-k,-l | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 67989 | wwPDB-VP |
| Average B, all atoms (Å ²) | 158.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.20 | 0/5056 | 0.37 | 0/6870 |
| 1 | C | 0.20 | 0/5056 | 0.37 | 0/6870 |
| 1 | E | 0.20 | 0/5056 | 0.37 | 0/6870 |
| 1 | G | 0.21 | 0/5056 | 0.38 | 0/6870 |
| 2 | B | 0.21 | 0/7317 | 0.36 | 0/9907 |
| 2 | D | 0.21 | 0/7306 | 0.36 | 0/9894 |
| 2 | F | 0.21 | 0/7314 | 0.36 | 0/9905 |
| 2 | H | 0.22 | 0/7315 | 0.36 | 0/9902 |
| 3 | I | 0.20 | 0/4092 | 0.37 | 0/5543 |
| 3 | J | 0.20 | 0/4092 | 0.37 | 0/5543 |
| 3 | K | 0.20 | 0/4092 | 0.37 | 0/5543 |
| 3 | L | 0.20 | 0/4092 | 0.37 | 0/5543 |
| 4 | M | 0.21 | 0/690 | 0.33 | 0/923 |
| 4 | N | 0.21 | 0/690 | 0.32 | 0/923 |
| 4 | P | 0.21 | 0/690 | 0.33 | 0/923 |
| 4 | Q | 0.21 | 0/690 | 0.33 | 0/923 |
| All | All | 0.21 | 0/68604 | 0.36 | 0/92952 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4958 | 0 | 5017 | 127 | 0 |
| 1 | C | 4958 | 0 | 5017 | 128 | 0 |
| 1 | E | 4958 | 0 | 5017 | 130 | 0 |
| 1 | G | 4958 | 0 | 5016 | 144 | 0 |
| 2 | B | 7177 | 0 | 7085 | 201 | 0 |
| 2 | D | 7166 | 0 | 7062 | 193 | 0 |
| 2 | F | 7172 | 0 | 7080 | 220 | 0 |
| 2 | H | 7175 | 0 | 7087 | 195 | 0 |
| 3 | I | 4004 | 0 | 3966 | 128 | 0 |
| 3 | J | 4004 | 0 | 3967 | 129 | 0 |
| 3 | K | 4004 | 0 | 3965 | 125 | 0 |
| 3 | L | 4004 | 0 | 3966 | 126 | 0 |
| 4 | M | 682 | 0 | 697 | 35 | 0 |
| 4 | N | 682 | 0 | 697 | 38 | 0 |
| 4 | P | 682 | 0 | 697 | 33 | 0 |
| 4 | Q | 682 | 0 | 697 | 38 | 0 |
| 5 | O | 50 | 0 | 43 | 1 | 0 |
| 5 | R | 50 | 0 | 42 | 1 | 0 |
| 5 | T | 50 | 0 | 43 | 1 | 0 |
| 5 | U | 50 | 0 | 43 | 3 | 0 |
| 6 | S | 61 | 0 | 52 | 1 | 0 |
| 6 | W | 61 | 0 | 52 | 5 | 0 |
| 7 | V | 72 | 0 | 61 | 2 | 0 |
| 8 | X | 50 | 0 | 43 | 2 | 0 |
| 9 | Y | 39 | 0 | 34 | 2 | 0 |
| 9 | a | 39 | 0 | 34 | 0 | 0 |
| 10 | Z | 28 | 0 | 25 | 0 | 0 |
| 11 | b | 61 | 0 | 52 | 0 | 0 |
| 12 | c | 39 | 0 | 34 | 0 | 0 |
| 13 | B | 11 | 0 | 10 | 0 | 0 |
| 13 | K | 11 | 0 | 10 | 0 | 0 |
| 14 | G | 11 | 0 | 10 | 1 | 0 |
| 15 | I | 1 | 0 | 0 | 0 | 0 |
| 15 | J | 1 | 0 | 0 | 0 | 0 |
| 15 | K | 1 | 0 | 0 | 0 | 0 |
| 15 | L | 1 | 0 | 0 | 0 | 0 |
| 16 | K | 14 | 0 | 13 | 3 | 0 |
| 16 | L | 14 | 0 | 13 | 0 | 0 |
| 17 | B | 1 | 0 | 0 | 0 | 0 |
| 17 | I | 2 | 0 | 0 | 0 | 0 |
| 17 | J | 2 | 0 | 0 | 1 | 0 |
| 17 | K | 2 | 0 | 0 | 0 | 0 |
| 17 | L | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 67989 | 0 | 67647 | 1863 | 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 (1863) 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:G:426:THR:HG21 | 1:G:432:ASN:H | 1.20 | 1.07 |
| 2:H:1494:GLU:HB3 | 2:H:1602:LYS:HB3 | 1.36 | 1.04 |
| 2:D:1569:ARG:HB2 | 2:D:1569:ARG:HH11 | 1.32 | 0.94 |
| 2:F:1569:ARG:HB2 | 2:F:1569:ARG:HH11 | 1.32 | 0.94 |
| 2:H:1569:ARG:HB2 | 2:H:1569:ARG:HH11 | 1.32 | 0.94 |
| 2:B:1569:ARG:HH11 | 2:B:1569:ARG:HB2 | 1.32 | 0.94 |
| 2:H:1268:GLN:HG3 | 2:H:1269:GLU:H | 1.34 | 0.92 |
| 1:G:505:PRO:HG3 | 1:G:595:TRP:CE3 | 2.08 | 0.88 |
| 3:L:267:CYS:HB2 | 3:L:433:MET:HE1 | 1.54 | 0.87 |
| 2:F:1359:LYS:HD2 | 4:M:4:LEU:HD11 | 1.58 | 0.86 |
| 1:A:549:GLU:HG2 | 1:A:550:ASP:H | 1.44 | 0.83 |
| 1:G:477:ARG:HH11 | 1:G:477:ARG:HG2 | 1.44 | 0.83 |
| 1:C:549:GLU:HG2 | 1:C:550:ASP:H | 1.44 | 0.82 |
| 1:E:477:ARG:HH11 | 1:E:477:ARG:HG2 | 1.44 | 0.82 |
| 2:H:1497:PHE:HE2 | 2:H:1571:ALA:HB1 | 1.43 | 0.82 |
| 1:E:547:GLN:HE22 | 1:E:559:MET:HA | 1.44 | 0.82 |
| 1:G:549:GLU:HG2 | 1:G:550:ASP:H | 1.44 | 0.82 |
| 3:J:381:ARG:HH21 | 3:J:381:ARG:HG2 | 1.45 | 0.82 |
| 1:E:549:GLU:HG2 | 1:E:550:ASP:H | 1.44 | 0.82 |
| 4:Q:6:THR:H | 4:Q:9:GLU:HB3 | 1.45 | 0.82 |
| 4:N:6:THR:H | 4:N:9:GLU:HB3 | 1.45 | 0.81 |
| 4:P:6:THR:H | 4:P:9:GLU:HB3 | 1.45 | 0.81 |
| 1:A:547:GLN:HE22 | 1:A:559:MET:HA | 1.44 | 0.81 |
| 2:H:1485:ARG:HD3 | 2:H:1536:PHE:CZ | 2.16 | 0.81 |
| 1:G:547:GLN:HE22 | 1:G:559:MET:HA | 1.44 | 0.81 |
| 3:K:381:ARG:HG2 | 3:K:381:ARG:HH21 | 1.45 | 0.81 |
| 1:C:547:GLN:HE22 | 1:C:559:MET:HA | 1.44 | 0.81 |
| 4:M:6:THR:H | 4:M:9:GLU:HB3 | 1.45 | 0.81 |
| 1:A:477:ARG:HG2 | 1:A:477:ARG:HH11 | 1.44 | 0.80 |
| 1:C:477:ARG:HH11 | 1:C:477:ARG:HG2 | 1.44 | 0.80 |
| 1:G:508:ARG:CZ | 1:G:604:GLY:HA3 | 2.12 | 0.80 |
| 3:L:381:ARG:HG2 | 3:L:381:ARG:HH21 | 1.45 | 0.80 |
| 2:B:819:ARG:HG2 | 2:B:819:ARG:HH11 | 1.46 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:819:ARG:HG2 | 2:D:819:ARG:HH11 | 1.46 | 0.80 |
| 3:I:381:ARG:HH21 | 3:I:381:ARG:HG2 | 1.45 | 0.80 |
| 1:C:45:LEU:HD11 | 1:C:48:SER:HB3 | 1.64 | 0.79 |
| 2:H:833:ARG:HH11 | 2:H:833:ARG:HG2 | 1.48 | 0.79 |
| 2:D:833:ARG:HG2 | 2:D:833:ARG:HH11 | 1.48 | 0.79 |
| 2:H:1488:LEU:HG | 2:H:1590:TRP:HH2 | 1.47 | 0.79 |
| 2:F:819:ARG:HH11 | 2:F:819:ARG:HG2 | 1.46 | 0.79 |
| 2:H:819:ARG:HG2 | 2:H:819:ARG:HH11 | 1.46 | 0.79 |
| 2:D:1532:LEU:HD11 | 2:D:1569:ARG:HD3 | 1.65 | 0.78 |
| 3:I:244:MET:HG3 | 3:I:356:ARG:HB2 | 1.65 | 0.78 |
| 1:G:45:LEU:HD11 | 1:G:48:SER:HB3 | 1.64 | 0.78 |
| 2:H:1532:LEU:HD11 | 2:H:1569:ARG:HD3 | 1.65 | 0.78 |
| 2:F:1532:LEU:HD11 | 2:F:1569:ARG:HD3 | 1.65 | 0.78 |
| 1:E:45:LEU:HD11 | 1:E:48:SER:HB3 | 1.64 | 0.78 |
| 1:A:45:LEU:HD11 | 1:A:48:SER:HB3 | 1.64 | 0.78 |
| 2:B:1532:LEU:HD11 | 2:B:1569:ARG:HD3 | 1.65 | 0.78 |
| 2:F:833:ARG:HG2 | 2:F:833:ARG:HH11 | 1.48 | 0.78 |
| 2:H:966:ALA:O | 2:H:967:GLN:HB2 | 1.83 | 0.78 |
| 2:F:738:ASN:HD22 | 4:P:45:LYS:HE2 | 1.47 | 0.78 |
| 2:B:833:ARG:HG2 | 2:B:833:ARG:HH11 | 1.48 | 0.77 |
| 2:H:738:ASN:HD22 | 4:Q:45:LYS:HE2 | 1.49 | 0.77 |
| 2:F:932:ARG:NH1 | 3:L:339:SER:HB2 | 1.99 | 0.77 |
| 2:F:841:ARG:HH11 | 2:F:841:ARG:HG2 | 1.50 | 0.77 |
| 3:J:244:MET:HG3 | 3:J:356:ARG:HB2 | 1.65 | 0.77 |
| 3:K:244:MET:HG3 | 3:K:356:ARG:HB2 | 1.65 | 0.77 |
| 3:L:244:MET:HG3 | 3:L:356:ARG:HB2 | 1.65 | 0.77 |
| 2:F:742:ARG:HB3 | 2:F:775:ASP:HB3 | 1.67 | 0.77 |
| 1:G:506:SER:HB2 | 1:G:530:TRP:HE1 | 1.50 | 0.77 |
| 2:B:841:ARG:HG2 | 2:B:841:ARG:HH11 | 1.50 | 0.76 |
| 2:F:740:VAL:HB | 4:P:42:ARG:HB2 | 1.68 | 0.76 |
| 1:A:506:SER:HB2 | 1:A:530:TRP:HE1 | 1.50 | 0.76 |
| 1:E:506:SER:HB2 | 1:E:530:TRP:HE1 | 1.50 | 0.76 |
| 3:I:705:ARG:O | 3:I:706:GLN:HB2 | 1.86 | 0.75 |
| 3:L:705:ARG:O | 3:L:706:GLN:HB2 | 1.86 | 0.75 |
| 3:K:354:ARG:HB2 | 16:K:1749:NAG:H81 | 1.67 | 0.75 |
| 2:D:841:ARG:HH11 | 2:D:841:ARG:HG2 | 1.50 | 0.75 |
| 2:H:1498:ILE:HD12 | 2:H:1605:TRP:HA | 1.65 | 0.75 |
| 3:J:705:ARG:O | 3:J:706:GLN:HB2 | 1.86 | 0.75 |
| 2:F:1569:ARG:CB | 2:F:1569:ARG:HH11 | 2.00 | 0.75 |
| 2:H:841:ARG:HG2 | 2:H:841:ARG:HH11 | 1.50 | 0.75 |
| 1:C:440:ARG:HG3 | 1:C:440:ARG:O | 1.85 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:506:SER:HB2 | 1:C:530:TRP:HE1 | 1.50 | 0.75 |
| 3:L:446:GLU:O | 3:L:450:LEU:HG | 1.86 | 0.74 |
| 2:B:1569:ARG:HH11 | 2:B:1569:ARG:CB | 2.00 | 0.74 |
| 1:C:404:THR:HG23 | 1:C:414:GLN:HE21 | 1.53 | 0.74 |
| 3:L:489:ALA:HB2 | 3:L:677:PRO:HG3 | 1.70 | 0.74 |
| 1:E:440:ARG:HG3 | 1:E:440:ARG:O | 1.85 | 0.74 |
| 3:K:705:ARG:O | 3:K:706:GLN:HB2 | 1.86 | 0.74 |
| 2:H:1569:ARG:HH11 | 2:H:1569:ARG:CB | 2.00 | 0.74 |
| 3:I:464:ASP:HB3 | 3:I:615:LEU:HB2 | 1.70 | 0.74 |
| 1:A:440:ARG:O | 1:A:440:ARG:HG3 | 1.86 | 0.74 |
| 1:G:440:ARG:O | 1:G:440:ARG:HG3 | 1.85 | 0.74 |
| 2:H:877:VAL:HG22 | 2:H:1451:GLN:HE21 | 1.53 | 0.74 |
| 3:K:464:ASP:HB3 | 3:K:615:LEU:HB2 | 1.70 | 0.74 |
| 1:A:404:THR:HG23 | 1:A:414:GLN:HE21 | 1.53 | 0.74 |
| 1:E:223:ILE:HD12 | 1:E:223:ILE:H | 1.53 | 0.74 |
| 2:H:740:VAL:HB | 4:Q:42:ARG:HB2 | 1.69 | 0.74 |
| 2:F:834:GLN:NE2 | 2:F:835:ASN:H | 1.86 | 0.73 |
| 2:D:1569:ARG:HH11 | 2:D:1569:ARG:CB | 2.00 | 0.73 |
| 1:G:223:ILE:HD12 | 1:G:223:ILE:H | 1.53 | 0.73 |
| 3:I:248:LEU:HD22 | 3:I:268:LEU:HD22 | 1.71 | 0.73 |
| 2:B:834:GLN:NE2 | 2:B:835:ASN:H | 1.86 | 0.73 |
| 1:E:404:THR:HG23 | 1:E:414:GLN:HE21 | 1.53 | 0.73 |
| 2:H:742:ARG:HB3 | 2:H:775:ASP:HB3 | 1.71 | 0.73 |
| 1:C:223:ILE:H | 1:C:223:ILE:HD12 | 1.53 | 0.73 |
| 1:G:404:THR:HG23 | 1:G:414:GLN:HE21 | 1.52 | 0.73 |
| 1:A:223:ILE:H | 1:A:223:ILE:HD12 | 1.53 | 0.73 |
| 3:L:248:LEU:HD22 | 3:L:268:LEU:HD22 | 1.71 | 0.73 |
| 2:B:966:ALA:O | 2:B:967:GLN:HB2 | 1.88 | 0.73 |
| 3:I:489:ALA:HB2 | 3:I:677:PRO:HG3 | 1.70 | 0.73 |
| 2:D:834:GLN:NE2 | 2:D:835:ASN:H | 1.86 | 0.73 |
| 2:F:966:ALA:O | 2:F:967:GLN:HB2 | 1.89 | 0.73 |
| 2:D:966:ALA:O | 2:D:967:GLN:HB2 | 1.88 | 0.73 |
| 2:D:742:ARG:HB3 | 2:D:775:ASP:HB3 | 1.71 | 0.72 |
| 3:L:464:ASP:HB3 | 3:L:615:LEU:HB2 | 1.70 | 0.72 |
| 1:G:424:TYR:O | 1:G:433:TYR:HE1 | 1.73 | 0.72 |
| 2:F:1269:GLU:HG3 | 2:F:1315:LYS:HB3 | 1.70 | 0.72 |
| 2:H:1497:PHE:CE2 | 2:H:1571:ALA:HB1 | 2.24 | 0.72 |
| 3:K:489:ALA:HB2 | 3:K:677:PRO:HG3 | 1.70 | 0.72 |
| 2:F:937:LYS:HG2 | 3:L:345:ASP:OD1 | 1.88 | 0.72 |
| 3:J:489:ALA:HB2 | 3:J:677:PRO:HG3 | 1.70 | 0.72 |
| 1:G:426:THR:HG21 | 1:G:432:ASN:N | 2.02 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:K:635:ALA:HB3 | 3:K:647:ILE:HD11 | 1.71 | 0.72 |
| 3:J:248:LEU:HD22 | 3:J:268:LEU:HD22 | 1.70 | 0.72 |
| 3:J:464:ASP:HB3 | 3:J:615:LEU:HB2 | 1.70 | 0.72 |
| 3:J:653:PRO:HD2 | 3:J:654:ARG:HH12 | 1.55 | 0.72 |
| 2:H:834:GLN:NE2 | 2:H:835:ASN:H | 1.86 | 0.72 |
| 1:C:6:ILE:HD13 | 1:C:22:LEU:HD23 | 1.72 | 0.71 |
| 1:G:6:ILE:HD13 | 1:G:22:LEU:HD23 | 1.72 | 0.71 |
| 3:L:461:LYS:HE2 | 3:L:461:LYS:HA | 1.73 | 0.71 |
| 3:J:539:LYS:HG2 | 3:J:544:ILE:HD12 | 1.73 | 0.71 |
| 3:J:576:GLU:HB3 | 3:J:580:ARG:HH22 | 1.55 | 0.71 |
| 3:K:539:LYS:HG2 | 3:K:544:ILE:HD12 | 1.73 | 0.71 |
| 1:C:13:ARG:HH22 | 1:C:476:GLY:HA3 | 1.54 | 0.71 |
| 3:J:635:ALA:HB3 | 3:J:647:ILE:HD11 | 1.71 | 0.71 |
| 3:K:461:LYS:HE2 | 3:K:461:LYS:HA | 1.73 | 0.71 |
| 3:I:461:LYS:HE2 | 3:I:461:LYS:HA | 1.73 | 0.71 |
| 3:I:653:PRO:HD2 | 3:I:654:ARG:HH12 | 1.55 | 0.71 |
| 3:J:461:LYS:HA | 3:J:461:LYS:HE2 | 1.73 | 0.71 |
| 3:K:576:GLU:HB3 | 3:K:580:ARG:HH22 | 1.55 | 0.71 |
| 1:C:439:LEU:HG | 1:E:439:LEU:HG | 1.71 | 0.71 |
| 3:I:635:ALA:HB3 | 3:I:647:ILE:HD11 | 1.71 | 0.71 |
| 3:K:248:LEU:HD22 | 3:K:268:LEU:HD22 | 1.70 | 0.71 |
| 3:L:635:ALA:HB3 | 3:L:647:ILE:HD11 | 1.71 | 0.70 |
| 1:E:6:ILE:HD13 | 1:E:22:LEU:HD23 | 1.72 | 0.70 |
| 1:C:98:VAL:HG11 | 2:D:1017:LEU:HD13 | 1.73 | 0.70 |
| 3:K:653:PRO:HD2 | 3:K:654:ARG:HH12 | 1.55 | 0.70 |
| 4:Q:71:GLN:HE21 | 4:Q:71:GLN:HA | 1.57 | 0.70 |
| 3:I:539:LYS:HG2 | 3:I:544:ILE:HD12 | 1.73 | 0.70 |
| 3:L:576:GLU:HB3 | 3:L:580:ARG:HH22 | 1.55 | 0.70 |
| 2:H:1446:ASN:HB2 | 4:N:4:LEU:HD13 | 1.74 | 0.70 |
| 4:P:71:GLN:HE21 | 4:P:71:GLN:HA | 1.57 | 0.70 |
| 3:I:576:GLU:HB3 | 3:I:580:ARG:HH22 | 1.55 | 0.70 |
| 2:B:742:ARG:HB3 | 2:B:775:ASP:HB3 | 1.74 | 0.70 |
| 3:L:539:LYS:HG2 | 3:L:544:ILE:HD12 | 1.73 | 0.69 |
| 1:A:6:ILE:HD13 | 1:A:22:LEU:HD23 | 1.72 | 0.69 |
| 2:D:1416:PHE:HZ | 2:D:1442:HIS:HB2 | 1.57 | 0.69 |
| 3:I:381:ARG:HH21 | 3:I:381:ARG:CG | 2.05 | 0.69 |
| 3:J:238:LEU:HD11 | 3:J:278:TYR:HB3 | 1.74 | 0.69 |
| 3:L:373:PRO:HB2 | 3:L:417:LEU:HD21 | 1.75 | 0.69 |
| 3:I:238:LEU:HD11 | 3:I:278:TYR:HB3 | 1.74 | 0.69 |
| 3:K:381:ARG:CG | 3:K:381:ARG:HH21 | 2.06 | 0.69 |
| 3:L:653:PRO:HD2 | 3:L:654:ARG:HH12 | 1.55 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:962:GLY:O | 2:H:964:PRO:HD3 | 1.92 | 0.69 |
| 1:E:426:THR:HG21 | 1:E:432:ASN:H | 1.57 | 0.69 |
| 2:F:1387:THR:HG22 | 2:F:1451:GLN:H | 1.58 | 0.69 |
| 3:L:238:LEU:HD11 | 3:L:278:TYR:HB3 | 1.74 | 0.69 |
| 2:H:1446:ASN:HB2 | 4:N:4:LEU:CD1 | 2.21 | 0.69 |
| 1:G:505:PRO:HG3 | 1:G:595:TRP:HE3 | 1.55 | 0.69 |
| 2:H:855:THR:HB | 2:H:1602:LYS:HZ3 | 1.56 | 0.69 |
| 4:N:71:GLN:HE21 | 4:N:71:GLN:HA | 1.56 | 0.69 |
| 3:J:381:ARG:HH21 | 3:J:381:ARG:CG | 2.05 | 0.69 |
| 2:H:1387:THR:HG22 | 2:H:1451:GLN:H | 1.58 | 0.69 |
| 2:D:962:GLY:O | 2:D:964:PRO:HD3 | 1.93 | 0.69 |
| 3:L:381:ARG:CG | 3:L:381:ARG:HH21 | 2.05 | 0.69 |
| 2:B:1416:PHE:HZ | 2:B:1442:HIS:HB2 | 1.57 | 0.68 |
| 3:J:705:ARG:HG3 | 3:J:705:ARG:O | 1.93 | 0.68 |
| 2:B:1488:LEU:HG | 2:B:1590:TRP:CZ2 | 2.27 | 0.68 |
| 2:B:841:ARG:NH1 | 2:B:841:ARG:HG2 | 2.08 | 0.68 |
| 2:F:841:ARG:NH1 | 2:F:841:ARG:HG2 | 2.08 | 0.68 |
| 2:D:1488:LEU:HG | 2:D:1590:TRP:CZ2 | 2.27 | 0.68 |
| 4:M:71:GLN:HA | 4:M:71:GLN:HE21 | 1.56 | 0.68 |
| 2:F:733:ILE:HG12 | 2:F:734:ILE:H | 1.58 | 0.68 |
| 3:I:373:PRO:HB2 | 3:I:417:LEU:HD21 | 1.75 | 0.68 |
| 3:J:373:PRO:HB2 | 3:J:417:LEU:HD21 | 1.75 | 0.68 |
| 3:K:373:PRO:HB2 | 3:K:417:LEU:HD21 | 1.75 | 0.68 |
| 3:J:435:ASN:ND2 | 3:J:460:ARG:HH21 | 1.90 | 0.68 |
| 1:G:100:LEU:HD21 | 1:G:638:LEU:HD23 | 1.76 | 0.68 |
| 1:G:567:HIS:ND1 | 2:H:760:PRO:HG3 | 2.09 | 0.68 |
| 1:C:606:THR:HG22 | 1:C:608:GLY:H | 1.59 | 0.68 |
| 2:D:1445:PHE:CZ | 4:P:7:SER:HA | 2.28 | 0.68 |
| 2:H:733:ILE:HG12 | 2:H:734:ILE:H | 1.58 | 0.68 |
| 3:J:432:ASP:HA | 4:Q:27:ASN:HD21 | 1.57 | 0.67 |
| 1:C:372:GLU:O | 1:C:375:VAL:HG12 | 1.95 | 0.67 |
| 3:K:446:GLU:HB3 | 3:K:449:SER:HB2 | 1.77 | 0.67 |
| 2:D:1518:GLY:HA3 | 2:D:1585:LEU:HD22 | 1.77 | 0.67 |
| 2:D:733:ILE:HG12 | 2:D:734:ILE:H | 1.58 | 0.67 |
| 3:K:705:ARG:HG3 | 3:K:705:ARG:O | 1.93 | 0.67 |
| 2:H:841:ARG:HG2 | 2:H:841:ARG:NH1 | 2.08 | 0.67 |
| 3:K:238:LEU:HD11 | 3:K:278:TYR:HB3 | 1.74 | 0.67 |
| 2:B:733:ILE:HG12 | 2:B:734:ILE:H | 1.58 | 0.67 |
| 3:I:705:ARG:HG3 | 3:I:705:ARG:O | 1.94 | 0.67 |
| 2:B:1518:GLY:HA3 | 2:B:1585:LEU:HD22 | 1.77 | 0.67 |
| 1:G:351:MET:SD | 1:G:440:ARG:HD2 | 2.35 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1268:GLN:CG | 2:H:1269:GLU:H | 2.00 | 0.67 |
| 2:H:1359:LYS:HD2 | 4:N:4:LEU:HD11 | 1.75 | 0.67 |
| 3:L:705:ARG:O | 3:L:705:ARG:HG3 | 1.94 | 0.67 |
| 2:D:876:TYR:HA | 2:D:1451:GLN:HE22 | 1.60 | 0.66 |
| 2:F:962:GLY:O | 2:F:964:PRO:HD3 | 1.95 | 0.66 |
| 2:H:1518:GLY:HA3 | 2:H:1585:LEU:HD22 | 1.77 | 0.66 |
| 2:D:1337:ASN:O | 2:D:1338:LYS:HB2 | 1.95 | 0.66 |
| 2:H:1499:GLN:HG2 | 2:H:1500:LYS:HG3 | 1.77 | 0.66 |
| 1:G:606:THR:HG22 | 1:G:608:GLY:H | 1.59 | 0.66 |
| 1:G:55:THR:HG22 | 1:G:57:ALA:H | 1.61 | 0.66 |
| 1:A:473:MET:HB2 | 1:A:508:ARG:HB2 | 1.78 | 0.66 |
| 1:A:606:THR:HG22 | 1:A:608:GLY:H | 1.59 | 0.66 |
| 2:B:877:VAL:HG22 | 2:B:1451:GLN:HE21 | 1.59 | 0.66 |
| 2:D:841:ARG:NH1 | 2:D:841:ARG:HG2 | 2.08 | 0.66 |
| 2:H:1498:ILE:HG12 | 2:H:1499:GLN:H | 1.60 | 0.66 |
| 1:E:606:THR:HG22 | 1:E:608:GLY:H | 1.59 | 0.66 |
| 2:B:1387:THR:HG22 | 2:B:1451:GLN:H | 1.60 | 0.66 |
| 3:J:446:GLU:HB3 | 3:J:449:SER:HB2 | 1.77 | 0.66 |
| 1:G:510:VAL:HG21 | 1:G:622:LEU:CD1 | 2.26 | 0.65 |
| 2:H:896:HIS:HB3 | 4:N:61:LYS:HD3 | 1.78 | 0.65 |
| 2:B:962:GLY:O | 2:B:964:PRO:HD3 | 1.96 | 0.65 |
| 1:E:473:MET:HB2 | 1:E:508:ARG:HB2 | 1.78 | 0.65 |
| 1:A:55:THR:HG22 | 1:A:57:ALA:H | 1.61 | 0.65 |
| 2:B:1417:SER:HB2 | 4:Q:14:LYS:NZ | 2.11 | 0.65 |
| 3:I:446:GLU:HB3 | 3:I:449:SER:HB2 | 1.79 | 0.65 |
| 3:I:478:ARG:HG3 | 3:I:479:PRO:HD2 | 1.79 | 0.65 |
| 2:F:1518:GLY:HA3 | 2:F:1585:LEU:HD22 | 1.77 | 0.65 |
| 1:C:473:MET:HB2 | 1:C:508:ARG:HB2 | 1.78 | 0.65 |
| 2:F:1126:LEU:HG | 2:F:1130:GLN:HE21 | 1.61 | 0.65 |
| 2:F:829:LEU:HD23 | 2:F:840:VAL:HG11 | 1.78 | 0.65 |
| 2:B:829:LEU:HD23 | 2:B:840:VAL:HG11 | 1.78 | 0.65 |
| 2:H:829:LEU:HD23 | 2:H:840:VAL:HG11 | 1.78 | 0.65 |
| 1:G:549:GLU:HG2 | 1:G:550:ASP:N | 2.12 | 0.65 |
| 2:B:1337:ASN:O | 2:B:1338:LYS:HB2 | 1.94 | 0.65 |
| 2:B:1126:LEU:HG | 2:B:1130:GLN:HE21 | 1.61 | 0.64 |
| 2:D:829:LEU:HD23 | 2:D:840:VAL:HG11 | 1.78 | 0.64 |
| 1:C:55:THR:HG22 | 1:C:57:ALA:H | 1.61 | 0.64 |
| 2:F:1265:PRO:O | 2:F:1266:ASP:HB2 | 1.96 | 0.64 |
| 3:I:446:GLU:O | 3:I:450:LEU:HG | 1.97 | 0.64 |
| 2:B:1265:PRO:O | 2:B:1266:ASP:HB2 | 1.97 | 0.64 |
| 2:D:1387:THR:HG22 | 2:D:1451:GLN:H | 1.60 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:55:THR:HG22 | 1:E:57:ALA:H | 1.61 | 0.64 |
| 2:D:1126:LEU:HG | 2:D:1130:GLN:HE21 | 1.61 | 0.64 |
| 1:G:473:MET:HB2 | 1:G:508:ARG:HB2 | 1.78 | 0.64 |
| 3:J:478:ARG:HG3 | 3:J:479:PRO:HD2 | 1.79 | 0.64 |
| 2:F:1268:GLN:O | 2:F:1269:GLU:HG2 | 1.97 | 0.64 |
| 3:K:478:ARG:HG3 | 3:K:479:PRO:HD2 | 1.79 | 0.64 |
| 3:L:446:GLU:HB3 | 3:L:449:SER:HB2 | 1.79 | 0.64 |
| 2:B:837:GLU:HG2 | 4:Q:64:SER:OG | 1.97 | 0.64 |
| 2:D:1265:PRO:O | 2:D:1266:ASP:HB2 | 1.98 | 0.64 |
| 2:F:1337:ASN:O | 2:F:1338:LYS:HB2 | 1.97 | 0.64 |
| 2:H:1338:LYS:HA | 2:H:1371:ARG:HB2 | 1.80 | 0.64 |
| 1:C:549:GLU:HG2 | 1:C:550:ASP:N | 2.12 | 0.63 |
| 2:D:1527:LEU:HD13 | 2:D:1541:MET:HG2 | 1.80 | 0.63 |
| 1:A:551:ARG:N | 1:A:551:ARG:HD2 | 2.13 | 0.63 |
| 2:D:1416:PHE:CZ | 2:D:1442:HIS:HB2 | 2.34 | 0.63 |
| 2:H:837:GLU:HG2 | 4:N:64:SER:OG | 1.98 | 0.63 |
| 3:K:460:ARG:HE | 4:P:28:VAL:HG21 | 1.63 | 0.63 |
| 3:K:513:LYS:HB3 | 3:K:522:ASP:HB3 | 1.81 | 0.63 |
| 1:A:147:ASN:HB2 | 1:A:148:PRO:HD2 | 1.81 | 0.63 |
| 2:H:1498:ILE:HG12 | 2:H:1499:GLN:N | 2.13 | 0.63 |
| 1:C:551:ARG:N | 1:C:551:ARG:HD2 | 2.13 | 0.63 |
| 2:F:1498:ILE:HG22 | 2:F:1499:GLN:N | 2.13 | 0.63 |
| 3:L:478:ARG:HG3 | 3:L:479:PRO:HD2 | 1.79 | 0.63 |
| 1:E:551:ARG:N | 1:E:551:ARG:HD2 | 2.13 | 0.63 |
| 1:E:567:HIS:ND1 | 2:F:760:PRO:HG3 | 2.13 | 0.63 |
| 1:G:551:ARG:HD2 | 1:G:551:ARG:N | 2.13 | 0.63 |
| 2:H:1337:ASN:O | 2:H:1338:LYS:HB2 | 1.97 | 0.63 |
| 2:H:876:TYR:HA | 2:H:1451:GLN:HE22 | 1.64 | 0.63 |
| 6:S:1:NAG:H61 | 6:S:2:NAG:C7 | 2.29 | 0.63 |
| 2:B:1527:LEU:HD13 | 2:B:1541:MET:HG2 | 1.80 | 0.63 |
| 1:C:147:ASN:HB2 | 1:C:148:PRO:HD2 | 1.80 | 0.63 |
| 1:C:634:GLN:HE22 | 2:D:1016:GLY:HA2 | 1.64 | 0.63 |
| 1:A:351:MET:SD | 1:A:440:ARG:HD2 | 2.39 | 0.63 |
| 2:B:1416:PHE:CZ | 2:B:1442:HIS:HB2 | 2.34 | 0.63 |
| 3:J:460:ARG:HE | 4:Q:28:VAL:HG21 | 1.64 | 0.62 |
| 1:E:147:ASN:HB2 | 1:E:148:PRO:HD2 | 1.81 | 0.62 |
| 1:G:512:TYR:CZ | 1:G:624:PHE:HE1 | 2.16 | 0.62 |
| 2:H:1527:LEU:HD13 | 2:H:1541:MET:HG2 | 1.80 | 0.62 |
| 3:K:432:ASP:HA | 4:P:27:ASN:HD21 | 1.63 | 0.62 |
| 3:L:513:LYS:HB3 | 3:L:522:ASP:HB3 | 1.81 | 0.62 |
| 2:B:1295:SER:O | 2:B:1297:LEU:HD12 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1295:SER:O | 2:D:1297:LEU:HD12 | 2.00 | 0.62 |
| 2:B:876:TYR:HA | 2:B:1451:GLN:HE22 | 1.63 | 0.62 |
| 3:I:513:LYS:HB3 | 3:I:522:ASP:HB3 | 1.81 | 0.62 |
| 3:K:433:MET:HE3 | 3:K:436:LEU:HD21 | 1.81 | 0.62 |
| 1:G:147:ASN:HB2 | 1:G:148:PRO:HD2 | 1.81 | 0.62 |
| 2:F:877:VAL:HG22 | 2:F:1451:GLN:HE21 | 1.65 | 0.62 |
| 2:H:1498:ILE:HG13 | 2:H:1605:TRP:CE3 | 2.34 | 0.62 |
| 2:B:1446:ASN:HB2 | 4:Q:4:LEU:HB2 | 1.81 | 0.62 |
| 1:A:549:GLU:HG2 | 1:A:550:ASP:N | 2.12 | 0.62 |
| 1:A:572:VAL:HG12 | 2:B:753:VAL:HG22 | 1.81 | 0.62 |
| 2:H:834:GLN:HE21 | 2:H:835:ASN:H | 1.47 | 0.62 |
| 2:H:855:THR:HB | 2:H:1602:LYS:NZ | 2.14 | 0.62 |
| 1:A:222:TYR:CE2 | 1:A:224:TYR:HB2 | 2.35 | 0.62 |
| 2:F:1527:LEU:HD13 | 2:F:1541:MET:HG2 | 1.80 | 0.62 |
| 3:J:513:LYS:HB3 | 3:J:522:ASP:HB3 | 1.81 | 0.62 |
| 3:I:423:ASN:HD22 | 3:I:423:ASN:N | 1.98 | 0.61 |
| 1:G:19:THR:HB | 1:G:478:LEU:HB2 | 1.81 | 0.61 |
| 2:B:834:GLN:HE21 | 2:B:835:ASN:H | 1.47 | 0.61 |
| 1:E:222:TYR:CE2 | 1:E:224:TYR:HB2 | 2.35 | 0.61 |
| 2:F:1295:SER:O | 2:F:1297:LEU:HD12 | 2.00 | 0.61 |
| 2:H:1611:GLU:HG3 | 2:H:1612:GLU:H | 1.66 | 0.61 |
| 3:I:650:VAL:HG23 | 3:I:651:VAL:HG23 | 1.83 | 0.61 |
| 1:C:13:ARG:NH2 | 1:C:476:GLY:HA3 | 2.15 | 0.61 |
| 2:H:1497:PHE:HB2 | 2:H:1498:ILE:HD13 | 1.82 | 0.61 |
| 3:I:267:CYS:HB2 | 3:I:433:MET:HE1 | 1.82 | 0.61 |
| 3:K:423:ASN:N | 3:K:423:ASN:HD22 | 1.98 | 0.61 |
| 3:L:461:LYS:HG2 | 4:N:28:VAL:HG12 | 1.81 | 0.61 |
| 2:B:1490:ARG:HB3 | 2:B:1590:TRP:CH2 | 2.36 | 0.61 |
| 1:E:372:GLU:O | 1:E:375:VAL:HG12 | 1.99 | 0.61 |
| 1:G:372:GLU:O | 1:G:375:VAL:HG12 | 2.01 | 0.61 |
| 1:G:222:TYR:CE2 | 1:G:224:TYR:HB2 | 2.35 | 0.61 |
| 3:K:478:ARG:HE | 3:K:481:LYS:HD2 | 1.65 | 0.61 |
| 3:I:461:LYS:HG2 | 4:M:28:VAL:HG12 | 1.82 | 0.61 |
| 2:B:1291:TRP:CG | 2:B:1292:GLU:N | 2.69 | 0.61 |
| 3:L:650:VAL:HG23 | 3:L:651:VAL:HG23 | 1.83 | 0.61 |
| 1:C:20:MET:HB3 | 1:C:64:VAL:HG23 | 1.83 | 0.61 |
| 2:D:1490:ARG:HB3 | 2:D:1590:TRP:CH2 | 2.36 | 0.61 |
| 2:H:1498:ILE:CG1 | 2:H:1499:GLN:H | 2.12 | 0.61 |
| 3:J:423:ASN:HD22 | 3:J:423:ASN:N | 1.98 | 0.61 |
| 1:C:222:TYR:CE2 | 1:C:224:TYR:HB2 | 2.35 | 0.61 |
| 2:H:923:ARG:HH22 | 2:H:940:ILE:HG12 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1338:LYS:HA | 2:F:1371:ARG:HB2 | 1.81 | 0.61 |
| 2:F:1527:LEU:HD21 | 2:F:1530:VAL:HG22 | 1.83 | 0.61 |
| 2:F:834:GLN:HE21 | 2:F:835:ASN:H | 1.47 | 0.61 |
| 3:K:650:VAL:HG23 | 3:K:651:VAL:HG23 | 1.83 | 0.61 |
| 2:B:1527:LEU:HD21 | 2:B:1530:VAL:HG22 | 1.83 | 0.60 |
| 2:F:1611:GLU:HG3 | 2:F:1612:GLU:H | 1.66 | 0.60 |
| 3:I:478:ARG:HE | 3:I:481:LYS:HD2 | 1.65 | 0.60 |
| 1:A:372:GLU:O | 1:A:375:VAL:HG12 | 2.01 | 0.60 |
| 2:D:1611:GLU:HG3 | 2:D:1612:GLU:H | 1.66 | 0.60 |
| 2:F:923:ARG:HH22 | 2:F:940:ILE:HG12 | 1.66 | 0.60 |
| 3:J:478:ARG:HE | 3:J:481:LYS:HD2 | 1.65 | 0.60 |
| 2:D:1291:TRP:CG | 2:D:1292:GLU:N | 2.69 | 0.60 |
| 1:G:20:MET:HB3 | 1:G:64:VAL:HG23 | 1.83 | 0.60 |
| 2:F:837:GLU:HG2 | 4:M:64:SER:OG | 2.00 | 0.60 |
| 1:C:426:THR:HG21 | 1:C:432:ASN:H | 1.65 | 0.60 |
| 2:H:1295:SER:O | 2:H:1297:LEU:HD12 | 2.00 | 0.60 |
| 3:L:449:SER:HA | 3:L:452:LEU:HD13 | 1.84 | 0.60 |
| 3:L:478:ARG:HE | 3:L:481:LYS:HD2 | 1.65 | 0.60 |
| 4:P:84:LYS:O | 4:P:85:TYR:HB2 | 2.02 | 0.60 |
| 2:B:973:VAL:HG11 | 2:B:978:LEU:HD12 | 1.83 | 0.60 |
| 1:C:572:VAL:HG12 | 2:D:753:VAL:HG22 | 1.82 | 0.60 |
| 2:D:772:PHE:HD1 | 4:M:37:ASN:ND2 | 1.99 | 0.60 |
| 2:D:973:VAL:HG11 | 2:D:978:LEU:HD12 | 1.83 | 0.60 |
| 1:A:20:MET:HB3 | 1:A:64:VAL:HG23 | 1.83 | 0.60 |
| 2:B:1532:LEU:HD11 | 2:B:1569:ARG:CD | 2.32 | 0.60 |
| 4:M:84:LYS:O | 4:M:85:TYR:HB2 | 2.02 | 0.60 |
| 2:B:1039:GLN:HB3 | 2:B:1040:PRO:HD2 | 1.83 | 0.60 |
| 1:C:10:ASN:HB2 | 1:C:621:GLY:C | 2.21 | 0.60 |
| 3:J:650:VAL:HG23 | 3:J:651:VAL:HG23 | 1.83 | 0.60 |
| 3:L:374:ILE:HD13 | 3:L:417:LEU:HD23 | 1.84 | 0.60 |
| 2:D:834:GLN:HE21 | 2:D:835:ASN:H | 1.47 | 0.60 |
| 1:E:20:MET:HB3 | 1:E:64:VAL:HG23 | 1.83 | 0.60 |
| 2:F:1291:TRP:CD1 | 2:F:1292:GLU:N | 2.70 | 0.60 |
| 2:F:1446:ASN:HB2 | 4:M:4:LEU:CD1 | 2.32 | 0.60 |
| 3:J:460:ARG:NE | 4:Q:28:VAL:HG21 | 2.16 | 0.60 |
| 2:D:1532:LEU:HD11 | 2:D:1569:ARG:CD | 2.32 | 0.59 |
| 1:E:220:PHE:CZ | 1:E:330:PRO:HB3 | 2.37 | 0.59 |
| 2:F:1039:GLN:HB3 | 2:F:1040:PRO:HD2 | 1.83 | 0.59 |
| 2:F:876:TYR:HA | 2:F:1451:GLN:HE22 | 1.67 | 0.59 |
| 2:D:1039:GLN:HB3 | 2:D:1040:PRO:HD2 | 1.83 | 0.59 |
| 2:D:877:VAL:HG22 | 2:D:1451:GLN:HE21 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:570:ILE:HD13 | 3:J:688:GLN:HB2 | 1.84 | 0.59 |
| 3:K:436:LEU:HB3 | 3:K:440:PHE:CE2 | 2.37 | 0.59 |
| 3:L:423:ASN:HD22 | 3:L:423:ASN:N | 1.98 | 0.59 |
| 2:B:1611:GLU:HG3 | 2:B:1612:GLU:H | 1.66 | 0.59 |
| 2:D:1527:LEU:HD21 | 2:D:1530:VAL:HG22 | 1.83 | 0.59 |
| 1:E:549:GLU:HG2 | 1:E:550:ASP:N | 2.12 | 0.59 |
| 1:G:13:ARG:NH2 | 1:G:476:GLY:HA3 | 2.18 | 0.59 |
| 2:H:833:ARG:CG | 2:H:833:ARG:HH11 | 2.15 | 0.59 |
| 3:I:563:TYR:CE2 | 3:I:569:PRO:HG3 | 2.38 | 0.59 |
| 3:I:570:ILE:HD13 | 3:I:688:GLN:HB2 | 1.84 | 0.59 |
| 1:G:555:PRO:HB3 | 2:H:775:ASP:HA | 1.83 | 0.59 |
| 2:D:1337:ASN:O | 2:D:1338:LYS:CB | 2.51 | 0.59 |
| 2:H:1527:LEU:HD21 | 2:H:1530:VAL:HG22 | 1.83 | 0.59 |
| 3:L:570:ILE:HD13 | 3:L:688:GLN:HB2 | 1.84 | 0.59 |
| 4:N:84:LYS:O | 4:N:85:TYR:HB2 | 2.02 | 0.59 |
| 3:K:563:TYR:CE2 | 3:K:569:PRO:HG3 | 2.38 | 0.59 |
| 1:C:558:GLN:HB3 | 2:D:770:ASN:HD21 | 1.68 | 0.59 |
| 1:G:350:LEU:HD21 | 1:G:400:ILE:HG21 | 1.83 | 0.59 |
| 3:J:436:LEU:HB3 | 3:J:440:PHE:CE2 | 2.37 | 0.59 |
| 3:J:563:TYR:CE2 | 3:J:569:PRO:HG3 | 2.38 | 0.59 |
| 3:L:508:LYS:HE2 | 3:L:508:LYS:HA | 1.85 | 0.59 |
| 4:N:22:LEU:HB3 | 4:N:74:TYR:HE2 | 1.68 | 0.59 |
| 4:Q:84:LYS:O | 4:Q:85:TYR:HB2 | 2.02 | 0.59 |
| 3:L:563:TYR:CE2 | 3:L:569:PRO:HG3 | 2.38 | 0.59 |
| 2:F:973:VAL:HG11 | 2:F:978:LEU:HD12 | 1.84 | 0.58 |
| 3:I:374:ILE:HD13 | 3:I:417:LEU:HD23 | 1.84 | 0.58 |
| 2:D:833:ARG:CG | 2:D:833:ARG:HH11 | 2.15 | 0.58 |
| 1:E:477:ARG:HH11 | 1:E:477:ARG:CG | 2.16 | 0.58 |
| 2:F:1215:LEU:HD23 | 2:F:1256:ALA:HB1 | 1.85 | 0.58 |
| 3:L:436:LEU:HB3 | 3:L:440:PHE:CE2 | 2.37 | 0.58 |
| 3:I:436:LEU:HB3 | 3:I:440:PHE:CE2 | 2.37 | 0.58 |
| 3:K:374:ILE:HD13 | 3:K:417:LEU:HD23 | 1.84 | 0.58 |
| 1:C:40:PHE:CE2 | 2:D:1017:LEU:HD22 | 2.38 | 0.58 |
| 2:F:1291:TRP:CG | 2:F:1292:GLU:N | 2.70 | 0.58 |
| 2:F:1532:LEU:HD11 | 2:F:1569:ARG:CD | 2.34 | 0.58 |
| 3:J:374:ILE:HD13 | 3:J:417:LEU:HD23 | 1.84 | 0.58 |
| 4:P:22:LEU:HB3 | 4:P:74:TYR:HE2 | 1.68 | 0.58 |
| 2:H:1535:ASP:O | 2:H:1536:PHE:HB3 | 2.04 | 0.58 |
| 4:M:22:LEU:HB3 | 4:M:74:TYR:HE2 | 1.68 | 0.58 |
| 3:I:508:LYS:HE2 | 3:I:508:LYS:HA | 1.85 | 0.58 |
| 3:J:508:LYS:HA | 3:J:508:LYS:HE2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:570:ILE:HD13 | 3:K:688:GLN:HB2 | 1.84 | 0.58 |
| 2:H:877:VAL:H | 2:H:1451:GLN:NE2 | 2.01 | 0.58 |
| 3:L:477:ILE:O | 3:L:511:SER:HB2 | 2.04 | 0.58 |
| 2:B:1215:LEU:HD23 | 2:B:1256:ALA:HB1 | 1.85 | 0.58 |
| 2:B:833:ARG:CG | 2:B:833:ARG:HH11 | 2.15 | 0.58 |
| 2:F:1359:LYS:HD2 | 4:M:4:LEU:CD1 | 2.32 | 0.58 |
| 2:H:1532:LEU:HD11 | 2:H:1569:ARG:CD | 2.34 | 0.58 |
| 3:J:477:ILE:O | 3:J:511:SER:HB2 | 2.04 | 0.58 |
| 2:D:1470:PHE:HB2 | 2:D:1478:GLY:HA3 | 1.86 | 0.57 |
| 1:G:527:ASP:N | 1:G:616:VAL:HG11 | 2.19 | 0.57 |
| 4:Q:6:THR:H | 4:Q:9:GLU:CB | 2.16 | 0.57 |
| 1:E:350:LEU:HD21 | 1:E:400:ILE:HG21 | 1.86 | 0.57 |
| 1:G:510:VAL:HG11 | 1:G:622:LEU:HD12 | 1.86 | 0.57 |
| 2:H:1291:TRP:CD1 | 2:H:1292:GLU:N | 2.70 | 0.57 |
| 2:H:1497:PHE:CZ | 2:H:1572:LEU:HD23 | 2.39 | 0.57 |
| 3:I:477:ILE:O | 3:I:511:SER:HB2 | 2.04 | 0.57 |
| 3:K:477:ILE:O | 3:K:511:SER:HB2 | 2.04 | 0.57 |
| 2:B:1445:PHE:CZ | 4:Q:7:SER:HA | 2.40 | 0.57 |
| 2:F:1133:LYS:O | 2:F:1137:GLU:HG3 | 2.04 | 0.57 |
| 2:H:1291:TRP:CG | 2:H:1292:GLU:N | 2.70 | 0.57 |
| 1:A:614:ALA:HB1 | 1:A:632:THR:HA | 1.86 | 0.57 |
| 2:D:1215:LEU:HD23 | 2:D:1256:ALA:HB1 | 1.85 | 0.57 |
| 2:D:809:ILE:HD11 | 2:D:892:ALA:HB3 | 1.87 | 0.57 |
| 1:G:13:ARG:HH22 | 1:G:476:GLY:HA3 | 1.69 | 0.57 |
| 4:Q:22:LEU:HB3 | 4:Q:74:TYR:HE2 | 1.68 | 0.57 |
| 2:B:1133:LYS:O | 2:B:1137:GLU:HG3 | 2.04 | 0.57 |
| 2:B:1337:ASN:O | 2:B:1338:LYS:CB | 2.51 | 0.57 |
| 2:F:1535:ASP:O | 2:F:1536:PHE:HB3 | 2.03 | 0.57 |
| 2:B:809:ILE:HD11 | 2:B:892:ALA:HB3 | 1.87 | 0.57 |
| 2:D:962:GLY:C | 2:D:964:PRO:HD3 | 2.24 | 0.57 |
| 2:F:1269:GLU:HG3 | 2:F:1315:LYS:CB | 2.35 | 0.57 |
| 2:F:1446:ASN:HB2 | 4:M:4:LEU:HD13 | 1.85 | 0.57 |
| 1:C:567:HIS:ND1 | 2:D:760:PRO:HG3 | 2.19 | 0.57 |
| 3:K:508:LYS:HA | 3:K:508:LYS:HE2 | 1.85 | 0.57 |
| 3:K:460:ARG:NE | 4:P:28:VAL:HG21 | 2.19 | 0.57 |
| 2:B:836:GLN:HG2 | 2:B:897:HIS:HE1 | 1.70 | 0.57 |
| 1:E:614:ALA:HB1 | 1:E:632:THR:HA | 1.86 | 0.57 |
| 2:B:1470:PHE:HB2 | 2:B:1478:GLY:HA3 | 1.86 | 0.57 |
| 2:D:1462:ASN:HD22 | 2:D:1463:LEU:N | 2.03 | 0.57 |
| 2:H:1582:MET:HA | 2:H:1605:TRP:O | 2.05 | 0.57 |
| 2:H:923:ARG:NH2 | 2:H:940:ILE:HG12 | 2.19 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1055:TRP:CZ2 | 2:F:1108:ILE:HA | 2.40 | 0.57 |
| 2:H:1462:ASN:HD22 | 2:H:1463:LEU:N | 2.03 | 0.57 |
| 2:H:819:ARG:HG2 | 2:H:819:ARG:NH1 | 2.19 | 0.57 |
| 2:B:1143:LEU:HB3 | 2:B:1144:PRO:HD3 | 1.86 | 0.56 |
| 2:B:965:VAL:O | 2:B:1267:HIS:HD2 | 1.88 | 0.56 |
| 1:C:268:ARG:HD3 | 2:D:1378:MET:SD | 2.44 | 0.56 |
| 2:D:1055:TRP:CZ2 | 2:D:1108:ILE:HA | 2.40 | 0.56 |
| 2:D:1143:LEU:HB3 | 2:D:1144:PRO:HD3 | 1.86 | 0.56 |
| 3:L:253:SER:HB2 | 3:L:326:SER:O | 2.05 | 0.56 |
| 2:F:1582:MET:HA | 2:F:1605:TRP:O | 2.05 | 0.56 |
| 2:F:833:ARG:HH11 | 2:F:833:ARG:CG | 2.15 | 0.56 |
| 2:F:809:ILE:HD11 | 2:F:892:ALA:HB3 | 1.87 | 0.56 |
| 1:G:614:ALA:HB1 | 1:G:632:THR:HA | 1.86 | 0.56 |
| 2:H:1494:GLU:HG2 | 2:H:1602:LYS:HD3 | 1.87 | 0.56 |
| 3:L:461:LYS:HD2 | 4:N:29:ASN:OD1 | 2.05 | 0.56 |
| 2:B:1462:ASN:HD22 | 2:B:1463:LEU:N | 2.03 | 0.56 |
| 2:B:923:ARG:HH22 | 2:B:940:ILE:HG12 | 1.70 | 0.56 |
| 2:D:925:LEU:HD11 | 2:D:1320:LEU:HD22 | 1.86 | 0.56 |
| 2:D:1535:ASP:O | 2:D:1536:PHE:HB3 | 2.05 | 0.56 |
| 2:H:1337:ASN:O | 2:H:1338:LYS:CB | 2.53 | 0.56 |
| 1:A:558:GLN:HB3 | 2:B:770:ASN:HD21 | 1.70 | 0.56 |
| 2:B:925:LEU:HD11 | 2:B:1320:LEU:HD22 | 1.87 | 0.56 |
| 2:B:1516:GLU:HB3 | 2:B:1517:PRO:HD2 | 1.88 | 0.56 |
| 1:C:614:ALA:HB1 | 1:C:632:THR:HA | 1.86 | 0.56 |
| 2:D:1133:LYS:O | 2:D:1137:GLU:HG3 | 2.05 | 0.56 |
| 2:F:1462:ASN:HD22 | 2:F:1463:LEU:N | 2.03 | 0.56 |
| 1:E:572:VAL:HG12 | 2:F:753:VAL:HG22 | 1.87 | 0.56 |
| 2:H:1566:ILE:O | 2:H:1569:ARG:HG3 | 2.06 | 0.56 |
| 3:K:364:ASP:O | 3:K:409:VAL:HG23 | 2.06 | 0.56 |
| 2:F:836:GLN:HG2 | 2:F:897:HIS:HE1 | 1.70 | 0.56 |
| 2:H:925:LEU:HD11 | 2:H:1320:LEU:HD22 | 1.88 | 0.56 |
| 3:I:353:ASN:HB2 | 3:I:394:ARG:NH1 | 2.20 | 0.56 |
| 3:K:253:SER:HB2 | 3:K:326:SER:O | 2.05 | 0.56 |
| 3:L:364:ASP:O | 3:L:409:VAL:HG23 | 2.06 | 0.56 |
| 2:B:1055:TRP:CZ2 | 2:B:1108:ILE:HA | 2.40 | 0.56 |
| 2:B:1180:LEU:HD23 | 2:B:1221:LEU:HD11 | 1.88 | 0.56 |
| 2:F:923:ARG:NH2 | 2:F:940:ILE:HG12 | 2.19 | 0.56 |
| 2:B:1535:ASP:O | 2:B:1536:PHE:HB3 | 2.05 | 0.56 |
| 1:C:441:THR:HG21 | 1:E:441:THR:HG21 | 1.88 | 0.56 |
| 1:E:116:ILE:HD11 | 1:E:203:LYS:HB3 | 1.88 | 0.56 |
| 1:G:477:ARG:HH11 | 1:G:477:ARG:CG | 2.16 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:836:GLN:HG2 | 2:H:897:HIS:HE1 | 1.70 | 0.56 |
| 3:I:253:SER:HB2 | 3:I:326:SER:O | 2.05 | 0.56 |
| 1:A:10:ASN:HB2 | 1:A:621:GLY:C | 2.25 | 0.56 |
| 2:D:1180:LEU:HD23 | 2:D:1221:LEU:HD11 | 1.88 | 0.56 |
| 3:J:253:SER:HB2 | 3:J:326:SER:O | 2.06 | 0.56 |
| 3:J:438:ASP:OD2 | 4:Q:28:VAL:HG13 | 2.05 | 0.56 |
| 2:D:1279:PRO:HG2 | 2:D:1306:GLU:HB3 | 1.88 | 0.56 |
| 2:D:923:ARG:HH22 | 2:D:940:ILE:HG12 | 1.70 | 0.56 |
| 2:F:1337:ASN:O | 2:F:1338:LYS:CB | 2.53 | 0.56 |
| 3:I:364:ASP:O | 3:I:409:VAL:HG23 | 2.06 | 0.56 |
| 3:L:381:ARG:CG | 3:L:381:ARG:NH2 | 2.68 | 0.56 |
| 2:D:1291:TRP:O | 2:D:1292:GLU:C | 2.45 | 0.56 |
| 2:F:1143:LEU:HB3 | 2:F:1144:PRO:HD3 | 1.86 | 0.56 |
| 2:H:964:PRO:HG3 | 2:H:1270:LEU:HD11 | 1.88 | 0.56 |
| 2:H:809:ILE:HD11 | 2:H:892:ALA:HB3 | 1.87 | 0.56 |
| 3:J:364:ASP:O | 3:J:409:VAL:HG23 | 2.06 | 0.56 |
| 3:L:353:ASN:HB2 | 3:L:394:ARG:NH1 | 2.20 | 0.56 |
| 3:L:513:LYS:HZ2 | 3:L:524:GLU:HG2 | 1.71 | 0.56 |
| 4:N:6:THR:H | 4:N:9:GLU:CB | 2.16 | 0.56 |
| 1:A:477:ARG:HH11 | 1:A:477:ARG:CG | 2.16 | 0.56 |
| 2:F:1012:TRP:HB3 | 2:F:1017:LEU:HD23 | 1.88 | 0.56 |
| 4:P:6:THR:H | 4:P:9:GLU:CB | 2.16 | 0.56 |
| 2:B:966:ALA:O | 2:B:967:GLN:CB | 2.54 | 0.55 |
| 2:F:1566:ILE:O | 2:F:1569:ARG:HG3 | 2.06 | 0.55 |
| 3:I:461:LYS:HG2 | 4:M:28:VAL:CG1 | 2.36 | 0.55 |
| 3:K:267:CYS:HB2 | 3:K:433:MET:HE1 | 1.87 | 0.55 |
| 1:A:350:LEU:HD21 | 1:A:400:ILE:HG21 | 1.88 | 0.55 |
| 2:D:1291:TRP:CD1 | 2:D:1292:GLU:N | 2.75 | 0.55 |
| 2:D:1516:GLU:HB3 | 2:D:1517:PRO:HD2 | 1.88 | 0.55 |
| 2:F:925:LEU:HD11 | 2:F:1320:LEU:HD22 | 1.88 | 0.55 |
| 2:F:804:MET:HG2 | 2:F:805:GLN:H | 1.72 | 0.55 |
| 2:B:1338:LYS:HA | 2:B:1371:ARG:HB2 | 1.88 | 0.55 |
| 2:B:1563:ILE:HB | 2:B:1599:ILE:HD13 | 1.88 | 0.55 |
| 1:A:569:ALA:HB2 | 2:B:788:SER:HB2 | 1.88 | 0.55 |
| 2:F:1516:GLU:HB3 | 2:F:1517:PRO:HD2 | 1.88 | 0.55 |
| 2:F:1640:PRO:O | 2:F:1641:ASN:HB2 | 2.07 | 0.55 |
| 1:G:143:VAL:C | 1:G:144:ASN:HD22 | 2.10 | 0.55 |
| 2:H:839:LYS:HE2 | 4:N:60:PHE:CD1 | 2.41 | 0.55 |
| 1:A:143:VAL:C | 1:A:144:ASN:HD22 | 2.09 | 0.55 |
| 2:B:804:MET:HG2 | 2:B:805:GLN:H | 1.71 | 0.55 |
| 1:C:465:ILE:HD11 | 1:C:515:LEU:HD22 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:477:ARG:CG | 1:C:477:ARG:HH11 | 2.16 | 0.55 |
| 1:G:116:ILE:HD11 | 1:G:203:LYS:HB3 | 1.88 | 0.55 |
| 2:H:1525:THR:HG22 | 2:H:1543:ILE:HA | 1.88 | 0.55 |
| 2:H:1563:ILE:HB | 2:H:1599:ILE:HD13 | 1.89 | 0.55 |
| 2:F:738:ASN:ND2 | 4:P:45:LYS:HE2 | 2.19 | 0.55 |
| 2:B:1566:ILE:O | 2:B:1569:ARG:HG3 | 2.07 | 0.55 |
| 1:C:350:LEU:HD21 | 1:C:400:ILE:HG21 | 1.88 | 0.55 |
| 2:D:836:GLN:HG2 | 2:D:897:HIS:HE1 | 1.70 | 0.55 |
| 1:E:143:VAL:C | 1:E:144:ASN:HD22 | 2.10 | 0.55 |
| 1:E:13:ARG:HH22 | 1:E:476:GLY:HA3 | 1.71 | 0.55 |
| 2:F:1498:ILE:HD12 | 2:F:1498:ILE:N | 2.21 | 0.55 |
| 2:H:1338:LYS:CA | 2:H:1371:ARG:HB2 | 2.36 | 0.55 |
| 3:K:353:ASN:HB2 | 3:K:394:ARG:NH1 | 2.21 | 0.55 |
| 2:F:740:VAL:O | 4:P:42:ARG:HD3 | 2.06 | 0.55 |
| 2:B:1291:TRP:CD1 | 2:B:1292:GLU:N | 2.75 | 0.55 |
| 1:C:252:GLY:HA2 | 1:C:262:LEU:HG | 1.89 | 0.55 |
| 2:D:1012:TRP:HB3 | 2:D:1017:LEU:HD23 | 1.88 | 0.55 |
| 2:F:1525:THR:HG22 | 2:F:1543:ILE:HA | 1.88 | 0.55 |
| 2:F:776:SER:HB2 | 2:F:780:TRP:CZ2 | 2.42 | 0.55 |
| 2:B:1012:TRP:HB3 | 2:B:1017:LEU:HD23 | 1.88 | 0.55 |
| 2:B:877:VAL:H | 2:B:1451:GLN:NE2 | 2.03 | 0.55 |
| 1:G:252:GLY:HA2 | 1:G:262:LEU:HG | 1.89 | 0.55 |
| 2:H:1498:ILE:CD1 | 2:H:1605:TRP:HA | 2.35 | 0.55 |
| 2:F:896:HIS:HB3 | 4:M:61:LYS:HD3 | 1.88 | 0.55 |
| 2:B:1417:SER:HB2 | 4:Q:14:LYS:HZ3 | 1.71 | 0.55 |
| 1:G:386:LYS:HD3 | 1:G:440:ARG:HG2 | 1.87 | 0.55 |
| 1:G:473:MET:CE | 1:G:603:ILE:HD11 | 2.37 | 0.55 |
| 1:G:465:ILE:HD11 | 1:G:515:LEU:HD22 | 1.89 | 0.55 |
| 2:H:1516:GLU:HB3 | 2:H:1517:PRO:HD2 | 1.88 | 0.55 |
| 1:A:116:ILE:HD11 | 1:A:203:LYS:HB3 | 1.88 | 0.55 |
| 2:D:1338:LYS:HA | 2:D:1371:ARG:HB2 | 1.89 | 0.55 |
| 2:F:1084:TRP:CD1 | 2:F:1088:GLU:HG3 | 2.42 | 0.55 |
| 2:F:1268:GLN:O | 2:F:1269:GLU:CG | 2.55 | 0.55 |
| 2:F:1291:TRP:O | 2:F:1292:GLU:C | 2.44 | 0.55 |
| 1:C:116:ILE:HD11 | 1:C:203:LYS:HB3 | 1.88 | 0.55 |
| 2:F:1338:LYS:CA | 2:F:1371:ARG:HB2 | 2.37 | 0.55 |
| 3:J:353:ASN:HB2 | 3:J:394:ARG:NH1 | 2.21 | 0.55 |
| 2:H:1641:ASN:HD21 | 3:J:366:LEU:HB3 | 1.72 | 0.55 |
| 2:D:776:SER:HB2 | 2:D:780:TRP:CZ2 | 2.42 | 0.54 |
| 1:E:10:ASN:HA | 1:E:623:THR:HG23 | 1.89 | 0.54 |
| 2:F:1180:LEU:HD23 | 2:F:1221:LEU:HD11 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1279:PRO:HG2 | 2:F:1306:GLU:HB3 | 1.88 | 0.54 |
| 1:G:508:ARG:NH1 | 1:G:604:GLY:HA3 | 2.22 | 0.54 |
| 2:D:1525:THR:HG22 | 2:D:1543:ILE:HA | 1.89 | 0.54 |
| 2:H:1279:PRO:HG2 | 2:H:1306:GLU:HB3 | 1.88 | 0.54 |
| 2:H:744:GLU:C | 2:H:746:PRO:HD3 | 2.28 | 0.54 |
| 3:L:461:LYS:HG2 | 4:N:28:VAL:CG1 | 2.37 | 0.54 |
| 2:B:776:SER:HB2 | 2:B:780:TRP:CZ2 | 2.42 | 0.54 |
| 1:C:143:VAL:C | 1:C:144:ASN:HD22 | 2.10 | 0.54 |
| 2:H:1291:TRP:O | 2:H:1292:GLU:C | 2.45 | 0.54 |
| 2:H:1445:PHE:CE2 | 4:N:7:SER:HA | 2.43 | 0.54 |
| 2:B:1291:TRP:O | 2:B:1292:GLU:C | 2.45 | 0.54 |
| 1:E:478:LEU:HD21 | 1:E:622:LEU:HD21 | 1.88 | 0.54 |
| 2:H:1289:ILE:HD13 | 2:H:1298:ARG:HE | 1.73 | 0.54 |
| 3:J:368:ASN:ND2 | 3:J:368:ASN:H | 2.06 | 0.54 |
| 1:A:465:ILE:HD11 | 1:A:515:LEU:HD22 | 1.89 | 0.54 |
| 1:E:252:GLY:HA2 | 1:E:262:LEU:HG | 1.89 | 0.54 |
| 3:I:535:ASN:O | 3:I:547:PHE:HB3 | 2.07 | 0.54 |
| 3:L:535:ASN:O | 3:L:547:PHE:HB3 | 2.07 | 0.54 |
| 2:D:804:MET:HG2 | 2:D:805:GLN:H | 1.71 | 0.54 |
| 2:H:804:MET:HG2 | 2:H:805:GLN:H | 1.72 | 0.54 |
| 3:K:535:ASN:O | 3:K:547:PHE:HB3 | 2.07 | 0.54 |
| 2:B:1084:TRP:CD1 | 2:B:1088:GLU:HG3 | 2.42 | 0.54 |
| 2:D:1566:ILE:O | 2:D:1569:ARG:HG3 | 2.07 | 0.54 |
| 2:D:966:ALA:O | 2:D:967:GLN:CB | 2.54 | 0.54 |
| 1:E:396:LYS:HG3 | 1:E:397:PRO:HD2 | 1.90 | 0.54 |
| 1:E:555:PRO:HB3 | 2:F:775:ASP:HA | 1.90 | 0.54 |
| 2:H:1268:GLN:CG | 2:H:1269:GLU:N | 2.70 | 0.54 |
| 1:A:269:ILE:HD13 | 1:A:278:VAL:HB | 1.90 | 0.54 |
| 2:B:1525:THR:HG22 | 2:B:1543:ILE:HA | 1.89 | 0.54 |
| 2:D:1563:ILE:HB | 2:D:1599:ILE:HD13 | 1.88 | 0.54 |
| 2:F:1289:ILE:HD13 | 2:F:1298:ARG:HE | 1.73 | 0.54 |
| 1:G:534:LYS:HD2 | 1:G:535:ASP:H | 1.72 | 0.54 |
| 3:J:631:CYS:SG | 3:J:714:ARG:HD2 | 2.48 | 0.54 |
| 3:K:631:CYS:SG | 3:K:714:ARG:HD2 | 2.48 | 0.54 |
| 3:L:478:ARG:NE | 3:L:481:LYS:HD2 | 2.23 | 0.54 |
| 2:D:837:GLU:HG2 | 4:P:64:SER:OG | 2.07 | 0.54 |
| 2:F:1563:ILE:HB | 2:F:1599:ILE:HD13 | 1.89 | 0.54 |
| 1:G:396:LYS:HG3 | 1:G:397:PRO:HD2 | 1.90 | 0.54 |
| 3:K:478:ARG:NE | 3:K:481:LYS:HD2 | 2.23 | 0.54 |
| 2:B:1582:MET:HA | 2:B:1605:TRP:O | 2.08 | 0.53 |
| 2:B:819:ARG:HG2 | 2:B:819:ARG:NH1 | 2.19 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:D:1084:TRP:CD1 | 2:D:1088:GLU:HG3 | 2.41 | 0.53 |
| 3:K:381:ARG:CG | 3:K:381:ARG:NH2 | 2.68 | 0.53 |
| 3:L:436:LEU:HB3 | 3:L:440:PHE:HE2 | 1.73 | 0.53 |
| 1:A:13:ARG:HH22 | 1:A:476:GLY:HA3 | 1.73 | 0.53 |
| 2:B:1279:PRO:HG2 | 2:B:1306:GLU:HB3 | 1.88 | 0.53 |
| 2:B:923:ARG:NH2 | 2:B:940:ILE:HG12 | 2.23 | 0.53 |
| 1:C:436:LEU:HD11 | 1:C:511:ALA:HB3 | 1.90 | 0.53 |
| 1:C:505:PRO:HG3 | 1:C:595:TRP:CE3 | 2.42 | 0.53 |
| 2:D:997:THR:N | 2:D:998:PRO:HD2 | 2.24 | 0.53 |
| 1:E:568:GLY:HA2 | 2:F:757:LYS:HE2 | 1.89 | 0.53 |
| 2:F:804:MET:HG2 | 2:F:805:GLN:N | 2.23 | 0.53 |
| 1:G:451:VAL:HB | 1:G:495:LEU:HB3 | 1.91 | 0.53 |
| 1:A:472:ILE:HD13 | 1:A:509:LEU:HD23 | 1.90 | 0.53 |
| 2:D:804:MET:HG2 | 2:D:805:GLN:N | 2.23 | 0.53 |
| 3:J:535:ASN:O | 3:J:547:PHE:HB3 | 2.07 | 0.53 |
| 2:F:744:GLU:C | 2:F:746:PRO:HD3 | 2.29 | 0.53 |
| 3:K:435:ASN:ND2 | 3:K:460:ARG:HH21 | 2.06 | 0.53 |
| 3:L:631:CYS:SG | 3:L:714:ARG:HD2 | 2.48 | 0.53 |
| 1:A:252:GLY:HA2 | 1:A:262:LEU:HG | 1.89 | 0.53 |
| 1:A:436:LEU:HD11 | 1:A:511:ALA:HB3 | 1.90 | 0.53 |
| 1:E:465:ILE:HD11 | 1:E:515:LEU:HD22 | 1.89 | 0.53 |
| 2:F:940:ILE:HD12 | 2:F:1308:PHE:CE1 | 2.44 | 0.53 |
| 2:D:1289:ILE:HD13 | 2:D:1298:ARG:HE | 1.74 | 0.53 |
| 2:D:1582:MET:HA | 2:D:1605:TRP:O | 2.08 | 0.53 |
| 1:E:219:LYS:NZ | 1:E:356:ASN:HD22 | 2.07 | 0.53 |
| 1:G:269:ILE:HD13 | 1:G:278:VAL:HB | 1.90 | 0.53 |
| 3:J:478:ARG:NE | 3:J:481:LYS:HD2 | 2.23 | 0.53 |
| 1:A:451:VAL:HB | 1:A:495:LEU:HB3 | 1.91 | 0.53 |
| 2:B:997:THR:N | 2:B:998:PRO:HD2 | 2.24 | 0.53 |
| 1:C:269:ILE:HD13 | 1:C:278:VAL:HB | 1.90 | 0.53 |
| 2:D:923:ARG:NH2 | 2:D:940:ILE:HG12 | 2.23 | 0.53 |
| 2:D:967:GLN:O | 2:D:968:MET:HB2 | 2.08 | 0.53 |
| 2:H:940:ILE:HD12 | 2:H:1308:PHE:CE1 | 2.43 | 0.53 |
| 2:B:804:MET:HG2 | 2:B:805:GLN:N | 2.23 | 0.53 |
| 1:E:477:ARG:HG2 | 1:E:477:ARG:NH1 | 2.21 | 0.53 |
| 2:H:1521:TYR:HB2 | 2:H:1523:TYR:CE2 | 2.44 | 0.53 |
| 3:I:478:ARG:NE | 3:I:481:LYS:HD2 | 2.23 | 0.53 |
| 3:K:456:VAL:HG13 | 3:K:467:LYS:HA | 1.91 | 0.53 |
| 1:A:506:SER:CB | 1:A:530:TRP:HE1 | 2.21 | 0.53 |
| 2:F:937:LYS:HD2 | 2:F:937:LYS:O | 2.09 | 0.53 |
| 2:H:776:SER:HB2 | 2:H:780:TRP:CZ2 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:456:VAL:HG13 | 3:I:467:LYS:HA | 1.91 | 0.53 |
| 3:J:456:VAL:HG13 | 3:J:467:LYS:HA | 1.91 | 0.53 |
| 3:L:438:ASP:OD2 | 4:N:28:VAL:HG13 | 2.09 | 0.53 |
| 4:M:6:THR:H | 4:M:9:GLU:CB | 2.16 | 0.53 |
| 2:D:877:VAL:H | 2:D:1451:GLN:NE2 | 2.07 | 0.53 |
| 2:D:1470:PHE:CB | 2:D:1478:GLY:HA3 | 2.39 | 0.53 |
| 2:D:865:THR:OG1 | 4:P:11:GLN:HG2 | 2.08 | 0.53 |
| 1:E:505:PRO:HG3 | 1:E:595:TRP:CE3 | 2.44 | 0.53 |
| 2:F:1387:THR:CG2 | 2:F:1451:GLN:H | 2.21 | 0.53 |
| 2:F:822:GLN:OE1 | 2:F:1479:LYS:HA | 2.09 | 0.53 |
| 2:F:973:VAL:HG12 | 2:F:975:ALA:H | 1.73 | 0.53 |
| 2:F:997:THR:N | 2:F:998:PRO:HD2 | 2.24 | 0.53 |
| 3:I:631:CYS:SG | 3:I:714:ARG:HD2 | 2.48 | 0.53 |
| 3:J:436:LEU:HB3 | 3:J:440:PHE:HE2 | 1.73 | 0.53 |
| 3:K:436:LEU:HB3 | 3:K:440:PHE:HE2 | 1.73 | 0.53 |
| 2:B:1289:ILE:HD13 | 2:B:1298:ARG:HE | 1.73 | 0.52 |
| 1:C:439:LEU:HD12 | 1:C:439:LEU:H | 1.74 | 0.52 |
| 1:E:590:THR:HG22 | 1:E:592:SER:H | 1.75 | 0.52 |
| 1:G:569:ALA:HB2 | 2:H:788:SER:HB2 | 1.90 | 0.52 |
| 2:H:740:VAL:O | 4:Q:42:ARG:HD3 | 2.09 | 0.52 |
| 2:B:962:GLY:C | 2:B:964:PRO:HD3 | 2.29 | 0.52 |
| 2:D:1196:ASN:HD22 | 2:D:1196:ASN:N | 2.07 | 0.52 |
| 2:F:978:LEU:HG | 2:F:1240:TYR:HB3 | 1.91 | 0.52 |
| 1:G:342:PHE:CE1 | 1:G:391:THR:HG21 | 2.45 | 0.52 |
| 1:G:472:ILE:HD13 | 1:G:509:LEU:HD23 | 1.90 | 0.52 |
| 3:K:654:ARG:HA | 3:K:722:GLN:HG3 | 1.91 | 0.52 |
| 3:L:368:ASN:ND2 | 3:L:368:ASN:H | 2.08 | 0.52 |
| 3:K:438:ASP:OD2 | 4:P:28:VAL:HG13 | 2.09 | 0.52 |
| 2:B:1387:THR:CG2 | 2:B:1451:GLN:H | 2.22 | 0.52 |
| 2:B:1470:PHE:CB | 2:B:1478:GLY:HA3 | 2.39 | 0.52 |
| 1:C:396:LYS:HG3 | 1:C:397:PRO:HD2 | 1.90 | 0.52 |
| 1:C:19:THR:HB | 1:C:478:LEU:HB2 | 1.91 | 0.52 |
| 2:D:1387:THR:CG2 | 2:D:1451:GLN:H | 2.22 | 0.52 |
| 1:C:569:ALA:HB2 | 2:D:788:SER:HB2 | 1.89 | 0.52 |
| 1:E:439:LEU:H | 1:E:439:LEU:HD12 | 1.74 | 0.52 |
| 1:G:527:ASP:CA | 1:G:616:VAL:HG11 | 2.40 | 0.52 |
| 2:H:804:MET:HG2 | 2:H:805:GLN:N | 2.23 | 0.52 |
| 3:K:461:LYS:HD2 | 4:P:29:ASN:OD1 | 2.10 | 0.52 |
| 3:K:598:LEU:HA | 3:K:603:ILE:HD13 | 1.91 | 0.52 |
| 2:B:1446:ASN:CB | 4:Q:4:LEU:HB2 | 2.40 | 0.52 |
| 2:B:978:LEU:HG | 2:B:1240:TYR:HB3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:973:VAL:HG12 | 2:B:975:ALA:H | 1.73 | 0.52 |
| 2:D:1360:ASN:O | 2:D:1361:THR:C | 2.48 | 0.52 |
| 1:E:451:VAL:HB | 1:E:495:LEU:HB3 | 1.91 | 0.52 |
| 3:J:654:ARG:HA | 3:J:722:GLN:HG3 | 1.91 | 0.52 |
| 2:B:1344:THR:HG21 | 2:B:1346:LYS:HE2 | 1.92 | 0.52 |
| 2:D:973:VAL:HG12 | 2:D:975:ALA:H | 1.73 | 0.52 |
| 3:I:461:LYS:HD2 | 4:M:29:ASN:OD1 | 2.09 | 0.52 |
| 2:F:932:ARG:HH11 | 3:L:339:SER:HB2 | 1.73 | 0.52 |
| 1:A:344:PRO:HD2 | 1:A:433:TYR:CE1 | 2.44 | 0.52 |
| 1:A:434:LEU:HB2 | 1:A:513:TYR:HE2 | 1.75 | 0.52 |
| 1:C:451:VAL:HB | 1:C:495:LEU:HB3 | 1.91 | 0.52 |
| 2:D:1521:TYR:HB2 | 2:D:1523:TYR:CE2 | 2.44 | 0.52 |
| 1:E:434:LEU:HB2 | 1:E:513:TYR:HE2 | 1.75 | 0.52 |
| 1:G:339:PRO:HB3 | 1:G:608:GLY:O | 2.09 | 0.52 |
| 1:G:436:LEU:HD11 | 1:G:511:ALA:HB3 | 1.90 | 0.52 |
| 2:H:1578:LYS:HD3 | 2:H:1608:HIS:HE1 | 1.74 | 0.52 |
| 3:J:598:LEU:HA | 3:J:603:ILE:HD13 | 1.91 | 0.52 |
| 3:K:531:HIS:CD2 | 3:K:533:ASN:H | 2.27 | 0.52 |
| 8:X:2:NAG:O3 | 8:X:2:NAG:H82 | 2.10 | 0.52 |
| 1:C:434:LEU:HB2 | 1:C:513:TYR:HE2 | 1.75 | 0.52 |
| 1:E:472:ILE:HD13 | 1:E:509:LEU:HD23 | 1.90 | 0.52 |
| 2:F:1196:ASN:N | 2:F:1196:ASN:HD22 | 2.07 | 0.52 |
| 2:F:1521:TYR:HB2 | 2:F:1523:TYR:CE2 | 2.44 | 0.52 |
| 2:H:1470:PHE:HB2 | 2:H:1478:GLY:HA3 | 1.92 | 0.52 |
| 3:I:313:GLN:O | 3:I:317:ILE:HG13 | 2.10 | 0.52 |
| 3:I:513:LYS:HZ2 | 3:I:524:GLU:HG2 | 1.75 | 0.52 |
| 3:I:531:HIS:CD2 | 3:I:533:ASN:H | 2.27 | 0.52 |
| 3:L:256:ILE:HD12 | 3:L:405:VAL:HG23 | 1.92 | 0.52 |
| 1:A:214:VAL:HG23 | 1:A:321:ARG:HB2 | 1.92 | 0.52 |
| 1:C:472:ILE:HD13 | 1:C:509:LEU:HD23 | 1.90 | 0.52 |
| 3:I:292:TYR:HD1 | 3:I:325:LYS:HD3 | 1.74 | 0.52 |
| 3:I:368:ASN:H | 3:I:368:ASN:ND2 | 2.08 | 0.52 |
| 3:I:654:ARG:HA | 3:I:722:GLN:HG3 | 1.91 | 0.52 |
| 3:J:531:HIS:CD2 | 3:J:533:ASN:H | 2.27 | 0.52 |
| 3:L:292:TYR:HD1 | 3:L:325:LYS:HD3 | 1.74 | 0.52 |
| 2:B:1521:TYR:HB2 | 2:B:1523:TYR:CE2 | 2.44 | 0.52 |
| 2:D:978:LEU:HG | 2:D:1240:TYR:HB3 | 1.91 | 0.52 |
| 2:F:1470:PHE:HB2 | 2:F:1478:GLY:HA3 | 1.92 | 0.52 |
| 1:G:214:VAL:HG23 | 1:G:321:ARG:HB2 | 1.92 | 0.52 |
| 1:G:506:SER:CB | 1:G:530:TRP:HE1 | 2.21 | 0.52 |
| 2:H:1387:THR:CG2 | 2:H:1451:GLN:H | 2.21 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:239:ASP:HB3 | 3:J:448:GLN:HB2 | 1.92 | 0.52 |
| 2:H:1641:ASN:O | 3:J:368:ASN:ND2 | 2.43 | 0.52 |
| 3:J:381:ARG:CG | 3:J:381:ARG:NH2 | 2.68 | 0.52 |
| 3:J:256:ILE:HD12 | 3:J:405:VAL:HG23 | 1.92 | 0.52 |
| 3:L:598:LEU:HA | 3:L:603:ILE:HD13 | 1.91 | 0.52 |
| 2:H:1359:LYS:HD2 | 4:N:4:LEU:CD1 | 2.40 | 0.52 |
| 1:A:396:LYS:HG3 | 1:A:397:PRO:HD2 | 1.90 | 0.52 |
| 1:A:404:THR:HG23 | 1:A:414:GLN:HB3 | 1.92 | 0.52 |
| 1:E:269:ILE:HD13 | 1:E:278:VAL:HB | 1.90 | 0.52 |
| 1:E:436:LEU:HD11 | 1:E:511:ALA:HB3 | 1.90 | 0.52 |
| 1:G:424:TYR:O | 1:G:433:TYR:CE1 | 2.59 | 0.52 |
| 3:I:436:LEU:HB3 | 3:I:440:PHE:HE2 | 1.73 | 0.52 |
| 3:L:654:ARG:HA | 3:L:722:GLN:HG3 | 1.91 | 0.52 |
| 4:P:30:GLU:HA | 4:P:44:ILE:HD13 | 1.92 | 0.52 |
| 2:B:1196:ASN:N | 2:B:1196:ASN:HD22 | 2.07 | 0.51 |
| 2:F:1228:PRO:HB2 | 2:F:1229:PRO:HD3 | 1.92 | 0.51 |
| 3:L:239:ASP:HB3 | 3:L:448:GLN:HB2 | 1.92 | 0.51 |
| 1:A:439:LEU:HD12 | 1:A:439:LEU:H | 1.74 | 0.51 |
| 2:B:1360:ASN:O | 2:B:1361:THR:C | 2.48 | 0.51 |
| 2:H:860:HIS:CE1 | 2:H:862:GLN:HE22 | 2.29 | 0.51 |
| 3:K:313:GLN:O | 3:K:317:ILE:HG13 | 2.10 | 0.51 |
| 3:K:368:ASN:H | 3:K:368:ASN:ND2 | 2.07 | 0.51 |
| 3:L:531:HIS:CD2 | 3:L:533:ASN:H | 2.27 | 0.51 |
| 4:N:30:GLU:HA | 4:N:44:ILE:HD13 | 1.92 | 0.51 |
| 1:C:126:ARG:HG2 | 1:C:168:PRO:HA | 1.93 | 0.51 |
| 1:E:214:VAL:HG23 | 1:E:321:ARG:HB2 | 1.92 | 0.51 |
| 1:A:590:THR:HG22 | 1:A:592:SER:H | 1.75 | 0.51 |
| 2:D:972:ALA:HB1 | 2:D:1005:TYR:OH | 2.10 | 0.51 |
| 2:D:1228:PRO:HB2 | 2:D:1229:PRO:HD3 | 1.92 | 0.51 |
| 2:D:1344:THR:HG21 | 2:D:1346:LYS:HE2 | 1.92 | 0.51 |
| 1:E:410:SER:O | 1:E:414:GLN:HG2 | 2.11 | 0.51 |
| 2:F:754:GLU:HG3 | 2:F:769:MET:SD | 2.51 | 0.51 |
| 3:I:598:LEU:HA | 3:I:603:ILE:HD13 | 1.91 | 0.51 |
| 3:J:292:TYR:HD1 | 3:J:325:LYS:HD3 | 1.74 | 0.51 |
| 3:L:313:GLN:O | 3:L:317:ILE:HG13 | 2.10 | 0.51 |
| 1:C:568:GLY:HA2 | 2:D:757:LYS:HE2 | 1.93 | 0.51 |
| 2:D:1381:LEU:HD23 | 2:D:1457:VAL:HG12 | 1.92 | 0.51 |
| 2:F:972:ALA:HB1 | 2:F:1005:TYR:OH | 2.09 | 0.51 |
| 2:F:1578:LYS:HD3 | 2:F:1608:HIS:HE1 | 1.74 | 0.51 |
| 3:K:256:ILE:HD12 | 3:K:405:VAL:HG23 | 1.92 | 0.51 |
| 4:M:70:LEU:HG | 4:M:74:TYR:CE2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:972:ALA:HB1 | 2:B:1005:TYR:OH | 2.10 | 0.51 |
| 1:C:478:LEU:HD21 | 1:C:622:LEU:HD21 | 1.91 | 0.51 |
| 2:D:754:GLU:HG3 | 2:D:769:MET:SD | 2.51 | 0.51 |
| 3:J:461:LYS:HD2 | 4:Q:29:ASN:OD1 | 2.10 | 0.51 |
| 3:K:292:TYR:HD1 | 3:K:325:LYS:HD3 | 1.74 | 0.51 |
| 1:A:640:CYS:HB3 | 1:A:641:PRO:HD2 | 1.93 | 0.51 |
| 2:B:1126:LEU:HD23 | 2:B:1173:ALA:HB1 | 1.93 | 0.51 |
| 2:B:1381:LEU:HD23 | 2:B:1457:VAL:HG12 | 1.92 | 0.51 |
| 2:B:754:GLU:HG3 | 2:B:769:MET:SD | 2.51 | 0.51 |
| 2:D:1233:TRP:O | 2:D:1237:GLN:HG2 | 2.11 | 0.51 |
| 1:E:19:THR:HB | 1:E:478:LEU:HB2 | 1.93 | 0.51 |
| 1:E:506:SER:CB | 1:E:530:TRP:HE1 | 2.21 | 0.51 |
| 1:G:439:LEU:HD12 | 1:G:439:LEU:H | 1.74 | 0.51 |
| 1:G:36:THR:HG23 | 1:G:48:SER:HA | 1.93 | 0.51 |
| 1:G:590:THR:HG22 | 1:G:592:SER:H | 1.74 | 0.51 |
| 2:H:937:LYS:HD2 | 2:H:937:LYS:O | 2.10 | 0.51 |
| 3:L:235:LYS:O | 3:L:236:ILE:HB | 2.11 | 0.51 |
| 3:L:456:VAL:HG13 | 3:L:467:LYS:HA | 1.91 | 0.51 |
| 1:A:36:THR:HG23 | 1:A:48:SER:HA | 1.93 | 0.51 |
| 1:A:410:SER:O | 1:A:414:GLN:HG2 | 2.11 | 0.51 |
| 2:B:1228:PRO:HB2 | 2:B:1229:PRO:HD3 | 1.91 | 0.51 |
| 2:B:860:HIS:CE1 | 2:B:862:GLN:HE22 | 2.29 | 0.51 |
| 1:C:214:VAL:HG23 | 1:C:321:ARG:HB2 | 1.93 | 0.51 |
| 2:D:1126:LEU:HD23 | 2:D:1173:ALA:HB1 | 1.93 | 0.51 |
| 2:D:1480:LEU:HB3 | 2:D:1493:GLU:OE2 | 2.10 | 0.51 |
| 1:G:404:THR:HG23 | 1:G:414:GLN:HB3 | 1.92 | 0.51 |
| 1:G:640:CYS:HB3 | 1:G:641:PRO:HD2 | 1.93 | 0.51 |
| 1:C:590:THR:HG22 | 1:C:592:SER:H | 1.75 | 0.51 |
| 2:D:819:ARG:HG2 | 2:D:819:ARG:NH1 | 2.19 | 0.51 |
| 1:G:126:ARG:HG2 | 1:G:168:PRO:HA | 1.93 | 0.51 |
| 4:Q:30:GLU:HA | 4:Q:44:ILE:HD13 | 1.92 | 0.51 |
| 2:B:839:LYS:HE2 | 4:Q:60:PHE:CD1 | 2.46 | 0.51 |
| 4:Q:70:LEU:HG | 4:Q:74:TYR:CE2 | 2.46 | 0.51 |
| 2:B:1578:LYS:HD3 | 2:B:1608:HIS:HE1 | 1.75 | 0.51 |
| 1:C:640:CYS:HB3 | 1:C:641:PRO:HD2 | 1.93 | 0.51 |
| 2:D:772:PHE:CD1 | 4:M:37:ASN:ND2 | 2.78 | 0.51 |
| 2:F:1126:LEU:HD23 | 2:F:1173:ALA:HB1 | 1.93 | 0.51 |
| 2:F:1233:TRP:O | 2:F:1237:GLN:HG2 | 2.11 | 0.51 |
| 2:F:860:HIS:CE1 | 2:F:862:GLN:HE22 | 2.29 | 0.51 |
| 2:F:966:ALA:O | 2:F:967:GLN:CB | 2.57 | 0.51 |
| 1:G:434:LEU:HB2 | 1:G:513:TYR:HE2 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:754:GLU:HG3 | 2:H:769:MET:SD | 2.51 | 0.51 |
| 3:I:334:LEU:HB3 | 3:I:376:VAL:HG11 | 1.93 | 0.51 |
| 3:I:381:ARG:CG | 3:I:381:ARG:NH2 | 2.68 | 0.51 |
| 3:L:339:SER:HA | 3:L:342:SER:HB3 | 1.93 | 0.51 |
| 3:L:724:LEU:HB3 | 3:L:725:PRO:HD3 | 1.92 | 0.51 |
| 2:H:738:ASN:ND2 | 4:Q:45:LYS:HE2 | 2.22 | 0.51 |
| 1:E:36:THR:HG23 | 1:E:48:SER:HA | 1.93 | 0.50 |
| 3:I:256:ILE:HD12 | 3:I:405:VAL:HG23 | 1.92 | 0.50 |
| 3:J:563:TYR:CZ | 3:J:569:PRO:HG3 | 2.47 | 0.50 |
| 3:K:724:LEU:HB3 | 3:K:725:PRO:HD3 | 1.92 | 0.50 |
| 4:P:70:LEU:HG | 4:P:74:TYR:CE2 | 2.46 | 0.50 |
| 1:C:36:THR:HG23 | 1:C:48:SER:HA | 1.93 | 0.50 |
| 2:D:1593:LYS:HG2 | 2:D:1596:LEU:HD11 | 1.94 | 0.50 |
| 1:E:404:THR:HG23 | 1:E:414:GLN:HB3 | 1.92 | 0.50 |
| 1:E:640:CYS:HB3 | 1:E:641:PRO:HD2 | 1.93 | 0.50 |
| 2:F:882:LYS:HG3 | 2:F:886:GLN:NE2 | 2.27 | 0.50 |
| 2:H:1381:LEU:HD23 | 2:H:1457:VAL:HG12 | 1.93 | 0.50 |
| 3:I:724:LEU:HB3 | 3:I:725:PRO:HD3 | 1.92 | 0.50 |
| 3:L:334:LEU:HB3 | 3:L:376:VAL:HG11 | 1.93 | 0.50 |
| 2:B:1233:TRP:O | 2:B:1237:GLN:HG2 | 2.11 | 0.50 |
| 2:B:772:PHE:HD1 | 4:N:37:ASN:ND2 | 2.10 | 0.50 |
| 1:C:410:SER:O | 1:C:414:GLN:HG2 | 2.11 | 0.50 |
| 2:F:1344:THR:HG21 | 2:F:1346:LYS:HE2 | 1.93 | 0.50 |
| 3:J:313:GLN:O | 3:J:317:ILE:HG13 | 2.10 | 0.50 |
| 3:K:239:ASP:HB3 | 3:K:448:GLN:HB2 | 1.92 | 0.50 |
| 3:L:439:VAL:HG22 | 4:N:31:LEU:HD21 | 1.91 | 0.50 |
| 1:G:554:VAL:HG13 | 1:G:555:PRO:HD2 | 1.94 | 0.50 |
| 3:I:239:ASP:HB3 | 3:I:448:GLN:HB2 | 1.92 | 0.50 |
| 3:J:334:LEU:HB3 | 3:J:376:VAL:HG11 | 1.93 | 0.50 |
| 3:L:278:TYR:HA | 3:L:455:MET:HE1 | 1.92 | 0.50 |
| 3:L:465:TYR:CD1 | 3:L:517:GLY:HA2 | 2.46 | 0.50 |
| 3:L:641:TYR:HE2 | 3:L:650:VAL:HB | 1.77 | 0.50 |
| 2:B:964:PRO:HG3 | 2:B:1270:LEU:HD11 | 1.92 | 0.50 |
| 2:B:940:ILE:HD12 | 2:B:1308:PHE:CE1 | 2.47 | 0.50 |
| 2:B:1569:ARG:CG | 2:B:1569:ARG:HH11 | 2.25 | 0.50 |
| 1:C:404:THR:HG23 | 1:C:414:GLN:HB3 | 1.92 | 0.50 |
| 2:D:1578:LYS:HD3 | 2:D:1608:HIS:HE1 | 1.75 | 0.50 |
| 2:D:860:HIS:CE1 | 2:D:862:GLN:HE22 | 2.29 | 0.50 |
| 2:F:819:ARG:HH11 | 2:F:819:ARG:CG | 2.22 | 0.50 |
| 1:G:369:VAL:HG12 | 1:G:370:GLN:H | 1.77 | 0.50 |
| 1:G:410:SER:O | 1:G:414:GLN:HG2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:882:LYS:HG3 | 2:H:886:GLN:NE2 | 2.27 | 0.50 |
| 3:I:563:TYR:CZ | 3:I:569:PRO:HG3 | 2.46 | 0.50 |
| 3:I:641:TYR:HE2 | 3:I:650:VAL:HB | 1.77 | 0.50 |
| 3:J:235:LYS:O | 3:J:236:ILE:HB | 2.11 | 0.50 |
| 3:J:724:LEU:HB3 | 3:J:725:PRO:HD3 | 1.92 | 0.50 |
| 2:B:1593:LYS:HG2 | 2:B:1596:LEU:HD11 | 1.94 | 0.50 |
| 2:B:882:LYS:HG3 | 2:B:886:GLN:NE2 | 2.27 | 0.50 |
| 3:J:339:SER:HA | 3:J:342:SER:HB3 | 1.93 | 0.50 |
| 3:J:465:TYR:CD1 | 3:J:517:GLY:HA2 | 2.46 | 0.50 |
| 3:K:641:TYR:HE2 | 3:K:650:VAL:HB | 1.77 | 0.50 |
| 3:L:513:LYS:NZ | 3:L:524:GLU:HG2 | 2.27 | 0.50 |
| 4:M:30:GLU:HA | 4:M:44:ILE:HD13 | 1.92 | 0.50 |
| 1:A:126:ARG:HG2 | 1:A:168:PRO:HA | 1.93 | 0.50 |
| 1:E:126:ARG:HG2 | 1:E:168:PRO:HA | 1.93 | 0.50 |
| 2:F:964:PRO:HG3 | 2:F:1270:LEU:HD11 | 1.93 | 0.50 |
| 1:E:268:ARG:HD3 | 2:F:1378:MET:SD | 2.51 | 0.50 |
| 2:H:1617:ASP:O | 2:H:1621:GLN:HG3 | 2.12 | 0.50 |
| 3:K:339:SER:HA | 3:K:342:SER:HB3 | 1.93 | 0.50 |
| 1:A:554:VAL:HG13 | 1:A:555:PRO:HD2 | 1.94 | 0.50 |
| 2:D:907:LEU:H | 2:D:907:LEU:HD23 | 1.77 | 0.50 |
| 2:F:1617:ASP:O | 2:F:1621:GLN:HG3 | 2.12 | 0.50 |
| 2:F:855:THR:HB | 2:F:1602:LYS:HZ3 | 1.76 | 0.50 |
| 2:H:907:LEU:HD23 | 2:H:907:LEU:H | 1.77 | 0.50 |
| 2:H:962:GLY:C | 2:H:964:PRO:HD3 | 2.31 | 0.50 |
| 3:I:339:SER:HA | 3:I:342:SER:HB3 | 1.93 | 0.50 |
| 3:J:478:ARG:CG | 3:J:479:PRO:HD2 | 2.42 | 0.50 |
| 2:H:839:LYS:HE2 | 4:N:60:PHE:CE1 | 2.47 | 0.50 |
| 1:C:222:TYR:HB3 | 1:C:225:ASN:HB2 | 1.94 | 0.50 |
| 1:C:10:ASN:HA | 1:C:623:THR:HG23 | 1.93 | 0.50 |
| 1:E:222:TYR:HB3 | 1:E:225:ASN:HB2 | 1.94 | 0.50 |
| 2:F:1268:GLN:O | 2:F:1269:GLU:CB | 2.59 | 0.50 |
| 3:K:334:LEU:HB3 | 3:K:376:VAL:HG11 | 1.93 | 0.50 |
| 3:K:563:TYR:CZ | 3:K:569:PRO:HG3 | 2.47 | 0.50 |
| 3:L:431:LYS:HG3 | 4:N:27:ASN:ND2 | 2.27 | 0.50 |
| 1:A:103:LEU:HB3 | 1:A:193:GLN:HE21 | 1.77 | 0.49 |
| 1:A:568:GLY:HA2 | 2:B:757:LYS:HE2 | 1.94 | 0.49 |
| 2:B:1617:ASP:O | 2:B:1621:GLN:HG3 | 2.12 | 0.49 |
| 2:H:1488:LEU:HG | 2:H:1590:TRP:CH2 | 2.35 | 0.49 |
| 3:J:267:CYS:HB2 | 3:J:433:MET:HE1 | 1.94 | 0.49 |
| 3:J:641:TYR:HE2 | 3:J:650:VAL:HB | 1.77 | 0.49 |
| 1:A:426:THR:HG21 | 1:A:432:ASN:H | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:733:ILE:HG12 | 2:D:734:ILE:N | 2.26 | 0.49 |
| 2:F:1593:LYS:HG2 | 2:F:1596:LEU:HD11 | 1.94 | 0.49 |
| 3:I:465:TYR:CD1 | 3:I:517:GLY:HA2 | 2.46 | 0.49 |
| 3:K:465:TYR:CD1 | 3:K:517:GLY:HA2 | 2.46 | 0.49 |
| 1:C:351:MET:SD | 1:C:440:ARG:HD2 | 2.53 | 0.49 |
| 2:D:940:ILE:HD12 | 2:D:1308:PHE:CE1 | 2.47 | 0.49 |
| 2:D:1617:ASP:O | 2:D:1621:GLN:HG3 | 2.12 | 0.49 |
| 2:D:841:ARG:HH11 | 2:D:841:ARG:CG | 2.23 | 0.49 |
| 2:D:882:LYS:HG3 | 2:D:886:GLN:NE2 | 2.27 | 0.49 |
| 1:G:572:VAL:CG2 | 2:H:785:VAL:HB | 2.42 | 0.49 |
| 3:I:438:ASP:OD2 | 4:M:28:VAL:HG13 | 2.12 | 0.49 |
| 3:J:435:ASN:HD21 | 3:J:460:ARG:HH21 | 1.57 | 0.49 |
| 2:B:1505:VAL:HG23 | 2:B:1505:VAL:O | 2.12 | 0.49 |
| 2:D:1505:VAL:HG23 | 2:D:1505:VAL:O | 2.12 | 0.49 |
| 1:E:554:VAL:HG13 | 1:E:555:PRO:HD2 | 1.94 | 0.49 |
| 2:F:1495:ASN:O | 2:F:1602:LYS:HA | 2.13 | 0.49 |
| 3:I:328:THR:HB | 3:I:367:HIS:HA | 1.94 | 0.49 |
| 3:K:235:LYS:O | 3:K:236:ILE:HB | 2.11 | 0.49 |
| 3:L:478:ARG:CG | 3:L:479:PRO:HD2 | 2.42 | 0.49 |
| 4:N:70:LEU:HG | 4:N:74:TYR:CE2 | 2.46 | 0.49 |
| 2:B:1239:TYR:OH | 2:B:1246:SER:HB2 | 2.13 | 0.49 |
| 2:F:1569:ARG:HH11 | 2:F:1569:ARG:CG | 2.26 | 0.49 |
| 2:F:841:ARG:CG | 2:F:841:ARG:HH11 | 2.23 | 0.49 |
| 1:G:439:LEU:HD12 | 1:G:439:LEU:N | 2.28 | 0.49 |
| 2:H:1593:LYS:HG2 | 2:H:1596:LEU:HD11 | 1.94 | 0.49 |
| 2:H:733:ILE:HG12 | 2:H:734:ILE:N | 2.26 | 0.49 |
| 3:J:513:LYS:NZ | 3:J:524:GLU:HG2 | 2.27 | 0.49 |
| 3:L:328:THR:HB | 3:L:367:HIS:HA | 1.94 | 0.49 |
| 2:H:1344:THR:HG21 | 2:H:1346:LYS:HE2 | 1.93 | 0.49 |
| 2:H:1635:VAL:HG23 | 2:H:1636:VAL:H | 1.78 | 0.49 |
| 2:D:1485:ARG:HD3 | 2:D:1536:PHE:HZ | 1.78 | 0.49 |
| 1:E:108:LEU:HB2 | 1:E:196:PHE:CD1 | 2.48 | 0.49 |
| 2:F:1381:LEU:HD23 | 2:F:1457:VAL:HG12 | 1.93 | 0.49 |
| 3:I:573:PRO:HB3 | 3:I:721:PHE:CZ | 2.48 | 0.49 |
| 3:K:328:THR:HB | 3:K:367:HIS:HA | 1.95 | 0.49 |
| 3:L:563:TYR:CZ | 3:L:569:PRO:HG3 | 2.47 | 0.49 |
| 1:A:108:LEU:HB2 | 1:A:196:PHE:CD1 | 2.48 | 0.49 |
| 1:C:554:VAL:HG13 | 1:C:555:PRO:HD2 | 1.94 | 0.49 |
| 2:D:1569:ARG:HH11 | 2:D:1569:ARG:CG | 2.24 | 0.49 |
| 2:F:907:LEU:HD23 | 2:F:907:LEU:H | 1.77 | 0.49 |
| 1:G:369:VAL:HG12 | 1:G:370:GLN:N | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:L:268:LEU:O | 3:L:272:ILE:HG13 | 2.13 | 0.49 |
| 1:A:222:TYR:HB3 | 1:A:225:ASN:HB2 | 1.94 | 0.49 |
| 1:A:505:PRO:HG3 | 1:A:595:TRP:CE3 | 2.48 | 0.49 |
| 1:A:567:HIS:ND1 | 2:B:760:PRO:HG3 | 2.27 | 0.49 |
| 2:B:813:LEU:HD23 | 2:B:907:LEU:HB3 | 1.95 | 0.49 |
| 3:I:235:LYS:O | 3:I:236:ILE:HB | 2.11 | 0.49 |
| 2:B:738:ASN:HD22 | 4:N:45:LYS:HE2 | 1.78 | 0.49 |
| 1:A:477:ARG:NH1 | 1:A:477:ARG:CG | 2.76 | 0.48 |
| 2:B:907:LEU:HD23 | 2:B:907:LEU:H | 1.77 | 0.48 |
| 2:D:1239:TYR:OH | 2:D:1246:SER:HB2 | 2.13 | 0.48 |
| 2:D:813:LEU:HD23 | 2:D:907:LEU:HB3 | 1.95 | 0.48 |
| 2:D:833:ARG:CG | 2:D:833:ARG:NH1 | 2.76 | 0.48 |
| 1:G:454:LEU:HA | 1:G:491:ASP:O | 2.13 | 0.48 |
| 1:G:477:ARG:CG | 1:G:477:ARG:NH1 | 2.76 | 0.48 |
| 2:H:813:LEU:HD23 | 2:H:907:LEU:HB3 | 1.95 | 0.48 |
| 3:J:268:LEU:O | 3:J:272:ILE:HG13 | 2.13 | 0.48 |
| 3:J:573:PRO:HB3 | 3:J:721:PHE:CZ | 2.48 | 0.48 |
| 3:L:372:ASP:O | 3:L:375:THR:HG22 | 2.13 | 0.48 |
| 3:L:573:PRO:HB3 | 3:L:721:PHE:CZ | 2.48 | 0.48 |
| 2:D:1417:SER:HB2 | 4:P:14:LYS:NZ | 2.27 | 0.48 |
| 1:C:477:ARG:CG | 1:C:477:ARG:NH1 | 2.76 | 0.48 |
| 2:H:1446:ASN:HB2 | 4:N:4:LEU:HB2 | 1.94 | 0.48 |
| 2:H:1492:ALA:O | 2:H:1494:GLU:N | 2.46 | 0.48 |
| 3:I:620:VAL:HG12 | 3:I:667:PRO:HD2 | 1.95 | 0.48 |
| 3:K:372:ASP:O | 3:K:375:THR:HG22 | 2.13 | 0.48 |
| 3:K:513:LYS:NZ | 3:K:524:GLU:HG2 | 2.27 | 0.48 |
| 3:L:620:VAL:HG12 | 3:L:667:PRO:HD2 | 1.95 | 0.48 |
| 2:F:1635:VAL:HG23 | 2:F:1636:VAL:H | 1.78 | 0.48 |
| 2:H:1338:LYS:H | 2:H:1371:ARG:HD2 | 1.78 | 0.48 |
| 2:H:1499:GLN:HG2 | 2:H:1500:LYS:N | 2.27 | 0.48 |
| 3:I:372:ASP:O | 3:I:375:THR:HG22 | 2.13 | 0.48 |
| 3:I:513:LYS:NZ | 3:I:524:GLU:HG2 | 2.27 | 0.48 |
| 3:J:328:THR:HB | 3:J:367:HIS:HA | 1.95 | 0.48 |
| 3:J:372:ASP:O | 3:J:375:THR:HG22 | 2.13 | 0.48 |
| 3:K:268:LEU:O | 3:K:272:ILE:HG13 | 2.13 | 0.48 |
| 3:K:478:ARG:CG | 3:K:479:PRO:HD2 | 2.42 | 0.48 |
| 1:A:439:LEU:HD12 | 1:A:439:LEU:N | 2.28 | 0.48 |
| 1:C:108:LEU:HB2 | 1:C:196:PHE:CD1 | 2.48 | 0.48 |
| 3:I:268:LEU:O | 3:I:272:ILE:HG13 | 2.13 | 0.48 |
| 3:I:270:ASN:HD22 | 3:I:270:ASN:N | 2.12 | 0.48 |
| 3:J:493:GLU:HG3 | 3:J:563:TYR:OH | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:620:VAL:HG12 | 3:J:667:PRO:HD2 | 1.95 | 0.48 |
| 5:U:1:NAG:H61 | 5:U:2:NAG:H83 | 1.94 | 0.48 |
| 2:D:744:GLU:C | 2:D:746:PRO:HD3 | 2.34 | 0.48 |
| 2:F:1239:TYR:OH | 2:F:1246:SER:HB2 | 2.13 | 0.48 |
| 1:G:108:LEU:HB2 | 1:G:196:PHE:CD1 | 2.48 | 0.48 |
| 2:H:1569:ARG:CG | 2:H:1569:ARG:HH11 | 2.26 | 0.48 |
| 3:I:478:ARG:CG | 3:I:479:PRO:HD2 | 2.42 | 0.48 |
| 2:F:1445:PHE:CE2 | 4:M:7:SER:HA | 2.48 | 0.48 |
| 2:B:1485:ARG:HD3 | 2:B:1536:PHE:HZ | 1.78 | 0.48 |
| 3:J:270:ASN:N | 3:J:270:ASN:HD22 | 2.11 | 0.48 |
| 3:K:267:CYS:HB2 | 3:K:433:MET:CE | 2.44 | 0.48 |
| 3:K:362:MET:HG2 | 3:K:403:PHE:HB2 | 1.95 | 0.48 |
| 4:N:11:GLN:NE2 | 4:N:11:GLN:H | 2.11 | 0.48 |
| 3:L:493:GLU:HG3 | 3:L:563:TYR:OH | 2.14 | 0.48 |
| 2:D:738:ASN:HD22 | 4:M:45:LYS:HE2 | 1.77 | 0.48 |
| 4:P:11:GLN:H | 4:P:11:GLN:NE2 | 2.11 | 0.48 |
| 4:Q:11:GLN:NE2 | 4:Q:11:GLN:H | 2.11 | 0.48 |
| 1:C:506:SER:CB | 1:C:530:TRP:HE1 | 2.21 | 0.48 |
| 1:E:369:VAL:HG12 | 1:E:370:GLN:H | 1.78 | 0.48 |
| 1:G:222:TYR:HB3 | 1:G:225:ASN:HB2 | 1.94 | 0.48 |
| 3:I:439:VAL:HG22 | 4:M:31:LEU:HD21 | 1.95 | 0.48 |
| 3:I:465:TYR:CE1 | 3:I:517:GLY:HA2 | 2.49 | 0.48 |
| 3:I:493:GLU:HG3 | 3:I:563:TYR:OH | 2.14 | 0.48 |
| 3:K:378:ASP:HA | 3:K:381:ARG:HB2 | 1.96 | 0.48 |
| 3:K:573:PRO:HB3 | 3:K:721:PHE:CZ | 2.48 | 0.48 |
| 2:D:1291:TRP:O | 2:D:1294:ALA:N | 2.47 | 0.48 |
| 2:D:1361:THR:HA | 2:D:1441:VAL:O | 2.14 | 0.48 |
| 1:G:624:PHE:HB3 | 1:G:632:THR:HG23 | 1.96 | 0.48 |
| 3:J:465:TYR:CE1 | 3:J:517:GLY:HA2 | 2.49 | 0.48 |
| 3:K:465:TYR:CE1 | 3:K:517:GLY:HA2 | 2.49 | 0.48 |
| 3:L:328:THR:O | 3:L:367:HIS:HB2 | 2.14 | 0.48 |
| 3:L:544:ILE:HD13 | 3:L:650:VAL:HG12 | 1.96 | 0.48 |
| 4:M:11:GLN:NE2 | 4:M:11:GLN:H | 2.11 | 0.48 |
| 1:A:624:PHE:HB3 | 1:A:632:THR:HG23 | 1.96 | 0.48 |
| 1:C:439:LEU:HD12 | 1:C:439:LEU:N | 2.28 | 0.48 |
| 1:E:606:THR:HB | 1:E:619:ASP:HB3 | 1.96 | 0.48 |
| 2:F:819:ARG:HG2 | 2:F:819:ARG:NH1 | 2.19 | 0.48 |
| 1:G:528:SER:N | 1:G:616:VAL:HG13 | 2.29 | 0.48 |
| 2:H:932:ARG:O | 2:H:934:GLY:N | 2.47 | 0.48 |
| 3:K:493:GLU:HG3 | 3:K:563:TYR:OH | 2.14 | 0.48 |
| 2:B:865:THR:OG1 | 4:Q:11:GLN:HG2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:470:TYR:HA | 1:A:510:VAL:O | 2.14 | 0.47 |
| 2:B:1361:THR:HA | 2:B:1441:VAL:O | 2.14 | 0.47 |
| 2:D:964:PRO:HB3 | 2:D:1270:LEU:HD11 | 1.95 | 0.47 |
| 1:E:439:LEU:N | 1:E:439:LEU:HD12 | 2.28 | 0.47 |
| 2:F:733:ILE:HG12 | 2:F:734:ILE:N | 2.26 | 0.47 |
| 1:G:35:VAL:HG21 | 1:G:64:VAL:HG21 | 1.96 | 0.47 |
| 3:J:267:CYS:HB2 | 3:J:433:MET:CE | 2.44 | 0.47 |
| 3:J:539:LYS:HD2 | 3:J:539:LYS:N | 2.30 | 0.47 |
| 3:K:328:THR:O | 3:K:367:HIS:HB2 | 2.14 | 0.47 |
| 3:L:361:LEU:O | 3:L:402:VAL:HA | 2.14 | 0.47 |
| 3:L:465:TYR:CE1 | 3:L:517:GLY:HA2 | 2.49 | 0.47 |
| 1:A:382:ASP:OD2 | 1:A:440:ARG:NH2 | 2.47 | 0.47 |
| 1:C:35:VAL:HG21 | 1:C:64:VAL:HG21 | 1.96 | 0.47 |
| 2:F:1338:LYS:H | 2:F:1371:ARG:HD2 | 1.79 | 0.47 |
| 2:F:877:VAL:H | 2:F:1451:GLN:NE2 | 2.12 | 0.47 |
| 1:G:470:TYR:HA | 1:G:510:VAL:O | 2.14 | 0.47 |
| 1:G:510:VAL:HG21 | 1:G:622:LEU:HD12 | 1.96 | 0.47 |
| 3:I:278:TYR:HA | 3:I:455:MET:HE1 | 1.97 | 0.47 |
| 5:O:1:NAG:H4 | 5:O:2:NAG:H2 | 1.61 | 0.47 |
| 1:A:6:ILE:HD12 | 1:A:21:VAL:O | 2.15 | 0.47 |
| 2:D:1521:TYR:HB2 | 2:D:1523:TYR:CZ | 2.50 | 0.47 |
| 1:G:345:GLY:HA2 | 1:G:391:THR:O | 2.14 | 0.47 |
| 3:I:544:ILE:HD13 | 3:I:650:VAL:HG12 | 1.96 | 0.47 |
| 3:K:620:VAL:HG12 | 3:K:667:PRO:HD2 | 1.95 | 0.47 |
| 2:B:1291:TRP:O | 2:B:1294:ALA:N | 2.47 | 0.47 |
| 1:C:555:PRO:HB3 | 2:D:775:ASP:HA | 1.96 | 0.47 |
| 2:D:965:VAL:O | 2:D:1267:HIS:HD2 | 1.97 | 0.47 |
| 2:F:813:LEU:HD23 | 2:F:907:LEU:HB3 | 1.95 | 0.47 |
| 3:J:378:ASP:HA | 3:J:381:ARG:HB2 | 1.96 | 0.47 |
| 3:J:362:MET:HG2 | 3:J:403:PHE:HB2 | 1.95 | 0.47 |
| 3:L:334:LEU:HD12 | 3:L:373:PRO:HB3 | 1.97 | 0.47 |
| 4:N:10:TYR:HE2 | 4:N:14:LYS:HE3 | 1.80 | 0.47 |
| 2:B:1521:TYR:HB2 | 2:B:1523:TYR:CZ | 2.50 | 0.47 |
| 1:C:624:PHE:HB3 | 1:C:632:THR:HG23 | 1.96 | 0.47 |
| 1:E:369:VAL:HG12 | 1:E:370:GLN:N | 2.29 | 0.47 |
| 1:E:13:ARG:NH2 | 1:E:476:GLY:HA3 | 2.28 | 0.47 |
| 1:E:624:PHE:HB3 | 1:E:632:THR:HG23 | 1.96 | 0.47 |
| 2:H:1270:LEU:O | 2:H:1290:HIS:HA | 2.15 | 0.47 |
| 3:I:378:ASP:HA | 3:I:381:ARG:HB2 | 1.96 | 0.47 |
| 3:I:538:GLY:C | 3:I:539:LYS:HD2 | 2.35 | 0.47 |
| 3:K:334:LEU:HD12 | 3:K:373:PRO:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:M:10:TYR:HE2 | 4:M:14:LYS:HE3 | 1.79 | 0.47 |
| 1:C:166:VAL:O | 1:C:168:PRO:HD3 | 2.15 | 0.47 |
| 1:E:35:VAL:HG21 | 1:E:64:VAL:HG21 | 1.96 | 0.47 |
| 2:F:932:ARG:O | 2:F:934:GLY:N | 2.47 | 0.47 |
| 1:G:606:THR:HB | 1:G:619:ASP:HB3 | 1.96 | 0.47 |
| 3:I:334:LEU:HD12 | 3:I:373:PRO:HB3 | 1.97 | 0.47 |
| 3:I:349:PRO:O | 3:I:352:TRP:HD1 | 1.98 | 0.47 |
| 3:I:361:LEU:O | 3:I:402:VAL:HA | 2.14 | 0.47 |
| 3:I:362:MET:HG2 | 3:I:403:PHE:HB2 | 1.95 | 0.47 |
| 3:J:349:PRO:O | 3:J:352:TRP:HD1 | 1.98 | 0.47 |
| 3:J:538:GLY:C | 3:J:539:LYS:HD2 | 2.35 | 0.47 |
| 1:C:10:ASN:HB2 | 1:C:621:GLY:HA2 | 1.95 | 0.47 |
| 2:F:1269:GLU:HG3 | 2:F:1269:GLU:O | 2.15 | 0.47 |
| 3:J:236:ILE:HG21 | 3:J:443:MET:O | 2.15 | 0.47 |
| 3:J:513:LYS:HZ2 | 3:J:524:GLU:HG2 | 1.78 | 0.47 |
| 3:K:544:ILE:HD13 | 3:K:650:VAL:HG12 | 1.96 | 0.47 |
| 3:L:362:MET:HG2 | 3:L:403:PHE:HB2 | 1.95 | 0.47 |
| 3:L:539:LYS:N | 3:L:539:LYS:HD2 | 2.30 | 0.47 |
| 1:A:35:VAL:HG21 | 1:A:64:VAL:HG21 | 1.96 | 0.47 |
| 1:C:470:TYR:HA | 1:C:510:VAL:O | 2.14 | 0.47 |
| 2:F:1270:LEU:O | 2:F:1290:HIS:HA | 2.15 | 0.47 |
| 2:H:1521:TYR:HB2 | 2:H:1523:TYR:CZ | 2.49 | 0.47 |
| 2:H:1359:LYS:HD2 | 4:N:4:LEU:CG | 2.45 | 0.47 |
| 1:A:606:THR:HB | 1:A:619:ASP:HB3 | 1.96 | 0.47 |
| 2:B:967:GLN:O | 2:B:968:MET:HB2 | 2.13 | 0.47 |
| 3:I:236:ILE:O | 3:I:236:ILE:HG23 | 2.15 | 0.47 |
| 3:J:328:THR:O | 3:J:367:HIS:HB2 | 2.15 | 0.47 |
| 3:J:544:ILE:HD13 | 3:J:650:VAL:HG12 | 1.96 | 0.47 |
| 3:K:363:THR:HG23 | 3:K:365:GLY:H | 1.80 | 0.47 |
| 3:K:538:GLY:C | 3:K:539:LYS:HD2 | 2.35 | 0.47 |
| 2:H:1446:ASN:CB | 4:N:4:LEU:HB2 | 2.44 | 0.47 |
| 1:A:541:LEU:HD22 | 2:B:786:SER:HB3 | 1.97 | 0.47 |
| 1:C:510:VAL:HG12 | 1:C:528:SER:HB3 | 1.97 | 0.47 |
| 1:E:219:LYS:HZ2 | 1:E:356:ASN:HD22 | 1.63 | 0.47 |
| 1:E:6:ILE:HG22 | 1:E:625:THR:O | 2.14 | 0.47 |
| 2:F:1521:TYR:HB2 | 2:F:1523:TYR:CZ | 2.49 | 0.47 |
| 1:G:522:ARG:HG2 | 1:G:628:SER:CB | 2.44 | 0.47 |
| 2:H:1291:TRP:O | 2:H:1294:ALA:N | 2.48 | 0.47 |
| 2:H:1498:ILE:HG13 | 2:H:1605:TRP:CZ3 | 2.50 | 0.47 |
| 3:K:236:ILE:HG21 | 3:K:443:MET:O | 2.15 | 0.47 |
| 1:C:325:PRO:HG2 | 1:C:357:PRO:HB2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:470:TYR:HA | 1:E:510:VAL:O | 2.14 | 0.47 |
| 3:K:270:ASN:N | 3:K:270:ASN:HD22 | 2.12 | 0.47 |
| 3:K:539:LYS:N | 3:K:539:LYS:HD2 | 2.30 | 0.47 |
| 3:L:236:ILE:HG23 | 3:L:236:ILE:O | 2.15 | 0.47 |
| 2:B:733:ILE:HD13 | 2:B:841:ARG:HD3 | 1.98 | 0.46 |
| 1:C:378:LEU:HD13 | 1:E:446:GLY:O | 2.16 | 0.46 |
| 1:C:541:LEU:HD22 | 2:D:786:SER:HB3 | 1.96 | 0.46 |
| 2:D:1524:LYS:HB3 | 2:D:1545:GLN:HG2 | 1.97 | 0.46 |
| 1:E:34:THR:HG22 | 1:E:51:LYS:HE3 | 1.97 | 0.46 |
| 2:F:1269:GLU:CG | 2:F:1315:LYS:HB3 | 2.40 | 0.46 |
| 2:F:1524:LYS:HB3 | 2:F:1545:GLN:HG2 | 1.97 | 0.46 |
| 2:B:1640:PRO:HA | 3:L:326:SER:OG | 2.14 | 0.46 |
| 3:L:236:ILE:HG21 | 3:L:443:MET:O | 2.15 | 0.46 |
| 1:A:166:VAL:O | 1:A:168:PRO:HD3 | 2.15 | 0.46 |
| 1:A:213:ILE:HG22 | 1:A:215:GLU:HG3 | 1.97 | 0.46 |
| 2:B:1524:LYS:HB3 | 2:B:1545:GLN:HG2 | 1.97 | 0.46 |
| 1:C:369:VAL:HG12 | 1:C:370:GLN:N | 2.31 | 0.46 |
| 1:C:6:ILE:HD12 | 1:C:21:VAL:O | 2.14 | 0.46 |
| 2:D:1172:TYR:CE1 | 2:D:1216:LEU:HB3 | 2.51 | 0.46 |
| 2:D:990:GLU:O | 2:D:994:ILE:HG13 | 2.16 | 0.46 |
| 2:F:1265:PRO:O | 2:F:1266:ASP:CB | 2.64 | 0.46 |
| 2:F:733:ILE:HD13 | 2:F:841:ARG:HD3 | 1.97 | 0.46 |
| 3:I:328:THR:O | 3:I:367:HIS:HB2 | 2.14 | 0.46 |
| 3:L:270:ASN:HD22 | 3:L:270:ASN:N | 2.11 | 0.46 |
| 2:B:1172:TYR:CE1 | 2:B:1216:LEU:HB3 | 2.51 | 0.46 |
| 1:E:207:LEU:HA | 1:E:208:PRO:HD2 | 1.82 | 0.46 |
| 1:E:6:ILE:HD12 | 1:E:21:VAL:O | 2.14 | 0.46 |
| 2:F:1291:TRP:O | 2:F:1294:ALA:N | 2.48 | 0.46 |
| 2:F:990:GLU:O | 2:F:994:ILE:HG13 | 2.16 | 0.46 |
| 1:G:477:ARG:NH1 | 1:G:477:ARG:HG2 | 2.21 | 0.46 |
| 1:G:34:THR:HG22 | 1:G:51:LYS:HE3 | 1.97 | 0.46 |
| 3:I:700:CYS:O | 3:I:701:LYS:C | 2.53 | 0.46 |
| 3:J:361:LEU:O | 3:J:402:VAL:HA | 2.14 | 0.46 |
| 3:L:538:GLY:C | 3:L:539:LYS:HD2 | 2.35 | 0.46 |
| 3:L:679:ILE:HG21 | 3:L:686:PHE:HB3 | 1.97 | 0.46 |
| 3:L:700:CYS:O | 3:L:701:LYS:C | 2.53 | 0.46 |
| 2:H:1444:TYR:HB2 | 4:N:10:TYR:CE1 | 2.50 | 0.46 |
| 1:A:34:THR:HG22 | 1:A:51:LYS:HE3 | 1.97 | 0.46 |
| 2:B:733:ILE:HG12 | 2:B:734:ILE:N | 2.26 | 0.46 |
| 2:B:990:GLU:O | 2:B:994:ILE:HG13 | 2.16 | 0.46 |
| 1:E:166:VAL:O | 1:E:168:PRO:HD3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:80:ARG:HD2 | 2:F:1010:GLU:HG3 | 1.97 | 0.46 |
| 3:K:361:LEU:O | 3:K:402:VAL:HA | 2.14 | 0.46 |
| 3:K:700:CYS:O | 3:K:701:LYS:C | 2.53 | 0.46 |
| 3:L:378:ASP:HA | 3:L:381:ARG:HB2 | 1.96 | 0.46 |
| 4:Q:10:TYR:HE2 | 4:Q:14:LYS:HE3 | 1.79 | 0.46 |
| 4:Q:73:ILE:O | 4:Q:77:ILE:HG13 | 2.16 | 0.46 |
| 1:G:154:LYS:HD2 | 1:G:171:TRP:CD1 | 2.51 | 0.46 |
| 2:H:833:ARG:CG | 2:H:833:ARG:NH1 | 2.75 | 0.46 |
| 3:I:363:THR:HG23 | 3:I:365:GLY:H | 1.80 | 0.46 |
| 3:I:236:ILE:HG21 | 3:I:443:MET:O | 2.15 | 0.46 |
| 3:I:539:LYS:HD2 | 3:I:539:LYS:N | 2.30 | 0.46 |
| 3:J:236:ILE:O | 3:J:236:ILE:HG23 | 2.15 | 0.46 |
| 3:J:700:CYS:O | 3:J:701:LYS:C | 2.53 | 0.46 |
| 3:K:349:PRO:O | 3:K:352:TRP:HD1 | 1.98 | 0.46 |
| 3:L:349:PRO:O | 3:L:352:TRP:HD1 | 1.98 | 0.46 |
| 2:F:740:VAL:CB | 4:P:42:ARG:HB2 | 2.43 | 0.46 |
| 1:A:154:LYS:HD2 | 1:A:171:TRP:CD1 | 2.51 | 0.46 |
| 1:C:213:ILE:HG22 | 1:C:215:GLU:HG3 | 1.97 | 0.46 |
| 1:C:639:GLN:NE2 | 1:C:639:GLN:H | 2.14 | 0.46 |
| 2:F:1172:TYR:CE1 | 2:F:1216:LEU:HB3 | 2.51 | 0.46 |
| 1:G:6:ILE:HD12 | 1:G:21:VAL:O | 2.15 | 0.46 |
| 3:I:531:HIS:HD2 | 3:I:533:ASN:H | 1.64 | 0.46 |
| 3:K:236:ILE:HG23 | 3:K:236:ILE:O | 2.15 | 0.46 |
| 4:M:73:ILE:O | 4:M:77:ILE:HG13 | 2.16 | 0.46 |
| 8:X:3:MAN:H62 | 8:X:4:MAN:H2 | 1.43 | 0.46 |
| 1:C:606:THR:HB | 1:C:619:ASP:HB3 | 1.96 | 0.46 |
| 1:E:342:PHE:CE1 | 1:E:391:THR:HG21 | 2.50 | 0.46 |
| 2:F:1494:GLU:HB2 | 2:F:1602:LYS:HB3 | 1.97 | 0.46 |
| 1:G:247:ALA:HB2 | 1:G:308:VAL:HG22 | 1.97 | 0.46 |
| 2:H:837:GLU:HB3 | 2:H:868:PRO:HD3 | 1.97 | 0.46 |
| 3:J:531:HIS:HD2 | 3:J:533:ASN:H | 1.64 | 0.46 |
| 3:K:292:TYR:CD1 | 3:K:325:LYS:HD3 | 2.51 | 0.46 |
| 3:L:363:THR:HG23 | 3:L:365:GLY:H | 1.80 | 0.46 |
| 1:A:47:LEU:HD13 | 1:A:66:PHE:HB2 | 1.97 | 0.46 |
| 2:B:1393:THR:O | 2:B:1397:LYS:HD3 | 2.16 | 0.46 |
| 2:B:744:GLU:C | 2:B:746:PRO:HD3 | 2.35 | 0.46 |
| 1:C:154:LYS:HD2 | 1:C:171:TRP:CD1 | 2.51 | 0.46 |
| 1:C:47:LEU:HD13 | 1:C:66:PHE:HB2 | 1.97 | 0.46 |
| 2:D:1393:THR:O | 2:D:1397:LYS:HD3 | 2.16 | 0.46 |
| 1:G:354:VAL:HG11 | 1:G:365:VAL:HG11 | 1.98 | 0.46 |
| 3:J:363:THR:HG23 | 3:J:365:GLY:H | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:261:PHE:HB3 | 3:K:319:TYR:HD1 | 1.81 | 0.46 |
| 3:K:679:ILE:HG21 | 3:K:686:PHE:HB3 | 1.97 | 0.46 |
| 3:L:345:ASP:HB3 | 3:L:346:ASP:H | 1.49 | 0.46 |
| 3:L:531:HIS:HD2 | 3:L:533:ASN:H | 1.64 | 0.46 |
| 4:N:73:ILE:O | 4:N:77:ILE:HG13 | 2.15 | 0.46 |
| 1:A:639:GLN:NE2 | 1:A:639:GLN:H | 2.14 | 0.46 |
| 1:C:6:ILE:HG22 | 1:C:625:THR:O | 2.16 | 0.46 |
| 1:E:10:ASN:HB2 | 1:E:621:GLY:C | 2.36 | 0.46 |
| 2:F:1290:HIS:O | 2:F:1291:TRP:O | 2.34 | 0.46 |
| 2:F:811:LEU:HG | 2:F:813:LEU:HD13 | 1.98 | 0.46 |
| 3:I:700:CYS:HA | 3:I:704:LYS:O | 2.16 | 0.46 |
| 3:J:334:LEU:HD12 | 3:J:373:PRO:HB3 | 1.97 | 0.46 |
| 3:L:261:PHE:HB3 | 3:L:319:TYR:HD1 | 1.81 | 0.46 |
| 4:P:73:ILE:O | 4:P:77:ILE:HG13 | 2.16 | 0.46 |
| 7:V:4:BMA:H62 | 7:V:6:BMA:H2 | 1.36 | 0.46 |
| 1:E:147:ASN:HB2 | 1:E:148:PRO:CD | 2.46 | 0.46 |
| 1:E:354:VAL:HG11 | 1:E:365:VAL:HG11 | 1.98 | 0.46 |
| 1:G:144:ASN:HD22 | 1:G:144:ASN:N | 2.14 | 0.46 |
| 1:G:166:VAL:O | 1:G:168:PRO:HD3 | 2.15 | 0.46 |
| 1:G:47:LEU:HD13 | 1:G:66:PHE:HB2 | 1.97 | 0.46 |
| 3:I:267:CYS:HB2 | 3:I:433:MET:CE | 2.44 | 0.46 |
| 4:M:66:ALA:HA | 4:M:69:GLN:HB2 | 1.98 | 0.46 |
| 2:B:819:ARG:CG | 2:B:819:ARG:HH11 | 2.22 | 0.45 |
| 1:C:34:THR:HG22 | 1:C:51:LYS:HE3 | 1.97 | 0.45 |
| 1:G:213:ILE:HG22 | 1:G:215:GLU:HG3 | 1.97 | 0.45 |
| 3:J:679:ILE:HG21 | 3:J:686:PHE:HB3 | 1.97 | 0.45 |
| 3:K:646:ASP:OD2 | 3:K:648:SER:HB3 | 2.17 | 0.45 |
| 4:N:66:ALA:HA | 4:N:69:GLN:HB2 | 1.98 | 0.45 |
| 4:P:10:TYR:HE2 | 4:P:14:LYS:HE3 | 1.79 | 0.45 |
| 1:A:369:VAL:HG12 | 1:A:370:GLN:N | 2.31 | 0.45 |
| 1:A:426:THR:HG22 | 1:A:427:VAL:N | 2.31 | 0.45 |
| 3:I:646:ASP:OD2 | 3:I:648:SER:HB3 | 2.16 | 0.45 |
| 3:L:653:PRO:CD | 3:L:654:ARG:HH12 | 2.27 | 0.45 |
| 1:A:144:ASN:HD22 | 1:A:144:ASN:N | 2.14 | 0.45 |
| 1:A:427:VAL:HB | 1:A:523:GLU:HG3 | 1.99 | 0.45 |
| 1:A:538:VAL:HB | 2:B:791:LYS:O | 2.16 | 0.45 |
| 1:E:351:MET:SD | 1:E:440:ARG:HD2 | 2.57 | 0.45 |
| 1:E:47:LEU:HD13 | 1:E:66:PHE:HB2 | 1.97 | 0.45 |
| 1:G:639:GLN:H | 1:G:639:GLN:NE2 | 2.14 | 0.45 |
| 2:H:1524:LYS:HB3 | 2:H:1545:GLN:HG2 | 1.97 | 0.45 |
| 3:I:261:PHE:HB3 | 3:I:319:TYR:HD1 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:700:CYS:HA | 3:J:704:LYS:O | 2.16 | 0.45 |
| 3:L:292:TYR:CD1 | 3:L:325:LYS:HD3 | 2.51 | 0.45 |
| 2:B:819:ARG:O | 2:B:820:ASN:HB2 | 2.17 | 0.45 |
| 2:B:837:GLU:HB3 | 2:B:868:PRO:HD3 | 1.97 | 0.45 |
| 1:E:154:LYS:HD2 | 1:E:171:TRP:CD1 | 2.51 | 0.45 |
| 2:F:837:GLU:HB3 | 2:F:868:PRO:HD3 | 1.97 | 0.45 |
| 1:G:473:MET:HE2 | 1:G:603:ILE:HD11 | 1.98 | 0.45 |
| 2:H:733:ILE:HD13 | 2:H:841:ARG:HD3 | 1.98 | 0.45 |
| 3:K:239:ASP:HA | 3:K:240:PRO:HD3 | 1.86 | 0.45 |
| 3:K:702:ASN:O | 3:K:703:GLN:HG3 | 2.17 | 0.45 |
| 3:L:702:ASN:O | 3:L:703:GLN:HG3 | 2.17 | 0.45 |
| 2:B:1264:ALA:HA | 2:B:1265:PRO:HD3 | 1.73 | 0.45 |
| 2:D:1223:ASP:O | 2:D:1227:VAL:HG23 | 2.17 | 0.45 |
| 2:D:1280:SER:O | 2:D:1281:ARG:C | 2.55 | 0.45 |
| 2:D:1288:ARG:HD3 | 2:D:1290:HIS:NE2 | 2.32 | 0.45 |
| 2:D:1364:LEU:HD23 | 2:D:1439:PHE:CZ | 2.52 | 0.45 |
| 1:E:569:ALA:HB2 | 2:F:788:SER:HB2 | 1.99 | 0.45 |
| 1:G:100:LEU:HD21 | 1:G:638:LEU:CD2 | 2.44 | 0.45 |
| 1:G:567:HIS:CG | 2:H:760:PRO:HG3 | 2.52 | 0.45 |
| 3:I:679:ILE:HG21 | 3:I:686:PHE:HB3 | 1.97 | 0.45 |
| 3:J:646:ASP:OD2 | 3:J:648:SER:HB3 | 2.17 | 0.45 |
| 3:J:705:ARG:O | 3:J:706:GLN:CB | 2.60 | 0.45 |
| 5:T:1:NAG:H61 | 5:T:2:NAG:C7 | 2.46 | 0.45 |
| 2:B:1123:ALA:O | 2:B:1127:ILE:HG13 | 2.17 | 0.45 |
| 2:B:1288:ARG:HD3 | 2:B:1290:HIS:NE2 | 2.32 | 0.45 |
| 1:C:342:PHE:CE1 | 1:C:391:THR:HG21 | 2.52 | 0.45 |
| 1:C:427:VAL:HB | 1:C:523:GLU:HG3 | 1.99 | 0.45 |
| 2:D:1192:ALA:HB2 | 2:D:1198:TRP:CZ2 | 2.52 | 0.45 |
| 1:E:510:VAL:HG12 | 1:E:528:SER:HB3 | 1.97 | 0.45 |
| 1:G:424:TYR:OH | 1:G:613:TYR:HB3 | 2.16 | 0.45 |
| 2:H:1492:ALA:O | 2:H:1493:GLU:C | 2.55 | 0.45 |
| 2:H:1495:ASN:O | 2:H:1496:CYS:C | 2.54 | 0.45 |
| 3:I:292:TYR:CD1 | 3:I:325:LYS:HD3 | 2.51 | 0.45 |
| 3:J:261:PHE:HB3 | 3:J:319:TYR:HD1 | 1.81 | 0.45 |
| 3:L:646:ASP:OD2 | 3:L:648:SER:HB3 | 2.16 | 0.45 |
| 2:B:1192:ALA:HB2 | 2:B:1198:TRP:CZ2 | 2.52 | 0.45 |
| 2:B:1203:LYS:HD2 | 2:B:1206:TYR:CE2 | 2.52 | 0.45 |
| 2:F:1470:PHE:CB | 2:F:1478:GLY:HA3 | 2.47 | 0.45 |
| 2:H:819:ARG:O | 2:H:820:ASN:HB2 | 2.17 | 0.45 |
| 3:I:653:PRO:CD | 3:I:654:ARG:HH12 | 2.27 | 0.45 |
| 3:K:653:PRO:CD | 3:K:654:ARG:HH12 | 2.27 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:428:PHE:CE1 | 4:P:31:LEU:HD11 | 2.52 | 0.45 |
| 4:P:66:ALA:HA | 4:P:69:GLN:HB2 | 1.98 | 0.45 |
| 1:A:354:VAL:HG11 | 1:A:365:VAL:HG11 | 1.98 | 0.45 |
| 1:A:510:VAL:HG12 | 1:A:528:SER:HB3 | 1.98 | 0.45 |
| 2:B:1280:SER:O | 2:B:1281:ARG:C | 2.55 | 0.45 |
| 2:B:729:LEU:O | 2:B:729:LEU:HD22 | 2.17 | 0.45 |
| 2:B:851:CYS:HB2 | 2:B:1491:CYS:HB2 | 1.90 | 0.45 |
| 2:D:1123:ALA:O | 2:D:1127:ILE:HG13 | 2.17 | 0.45 |
| 2:D:811:LEU:HG | 2:D:813:LEU:HD13 | 1.98 | 0.45 |
| 2:D:837:GLU:HB3 | 2:D:868:PRO:HD3 | 1.97 | 0.45 |
| 2:F:1182:GLY:HA3 | 2:F:1183:PRO:HD2 | 1.82 | 0.45 |
| 1:G:516:ILE:N | 1:G:516:ILE:HD12 | 2.32 | 0.45 |
| 2:H:1497:PHE:C | 2:H:1498:ILE:HD13 | 2.37 | 0.45 |
| 3:J:292:TYR:CD1 | 3:J:325:LYS:HD3 | 2.51 | 0.45 |
| 2:D:937:LYS:HD2 | 2:D:937:LYS:O | 2.17 | 0.45 |
| 1:E:213:ILE:HG22 | 1:E:215:GLU:HG3 | 1.97 | 0.45 |
| 1:E:639:GLN:H | 1:E:639:GLN:NE2 | 2.14 | 0.45 |
| 2:F:1203:LYS:HD2 | 2:F:1206:TYR:CE2 | 2.52 | 0.45 |
| 2:F:1280:SER:O | 2:F:1281:ARG:C | 2.55 | 0.45 |
| 2:F:1288:ARG:HD3 | 2:F:1290:HIS:NE2 | 2.32 | 0.45 |
| 2:F:1364:LEU:HD23 | 2:F:1439:PHE:CZ | 2.52 | 0.45 |
| 2:F:962:GLY:C | 2:F:964:PRO:HD3 | 2.37 | 0.45 |
| 2:H:811:LEU:HG | 2:H:813:LEU:HD13 | 1.98 | 0.45 |
| 14:G:1651:MAN:C1 | 6:W:3:BMA:H3 | 2.46 | 0.45 |
| 1:A:369:VAL:HG12 | 1:A:370:GLN:H | 1.82 | 0.45 |
| 2:D:1126:LEU:HD21 | 2:D:1177:MET:HE3 | 1.99 | 0.45 |
| 2:D:1444:TYR:HB2 | 4:P:10:TYR:CE1 | 2.52 | 0.45 |
| 2:D:733:ILE:HD13 | 2:D:841:ARG:HD3 | 1.98 | 0.45 |
| 2:F:1506:THR:OG1 | 2:F:1509:GLU:HG2 | 2.17 | 0.45 |
| 2:H:1498:ILE:HD13 | 2:H:1498:ILE:N | 2.32 | 0.45 |
| 2:H:734:ILE:N | 2:H:734:ILE:HD12 | 2.32 | 0.45 |
| 3:J:702:ASN:O | 3:J:703:GLN:HG3 | 2.17 | 0.45 |
| 3:K:554:LEU:H | 3:K:726:TRP:HH2 | 1.65 | 0.45 |
| 3:L:272:ILE:HG12 | 3:L:284:TYR:CE1 | 2.52 | 0.45 |
| 3:L:432:ASP:HA | 4:N:27:ASN:HD21 | 1.82 | 0.45 |
| 2:B:1126:LEU:HD21 | 2:B:1177:MET:HE3 | 1.99 | 0.44 |
| 2:B:1223:ASP:O | 2:B:1227:VAL:HG23 | 2.17 | 0.44 |
| 1:C:344:PRO:HD2 | 1:C:433:TYR:CE1 | 2.51 | 0.44 |
| 1:C:354:VAL:HG11 | 1:C:365:VAL:HG11 | 1.98 | 0.44 |
| 1:E:477:ARG:NH1 | 1:E:477:ARG:CG | 2.76 | 0.44 |
| 2:F:1192:ALA:HB2 | 2:F:1198:TRP:CZ2 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1290:HIS:O | 2:H:1291:TRP:O | 2.34 | 0.44 |
| 3:K:238:LEU:HD22 | 3:K:280:VAL:HG21 | 1.99 | 0.44 |
| 3:K:531:HIS:HD2 | 3:K:533:ASN:H | 1.64 | 0.44 |
| 3:L:700:CYS:HA | 3:L:704:LYS:O | 2.16 | 0.44 |
| 3:L:705:ARG:O | 3:L:706:GLN:CB | 2.60 | 0.44 |
| 1:A:147:ASN:HB2 | 1:A:148:PRO:CD | 2.46 | 0.44 |
| 1:A:516:ILE:HD12 | 1:A:516:ILE:N | 2.32 | 0.44 |
| 1:C:369:VAL:HG12 | 1:C:370:GLN:H | 1.82 | 0.44 |
| 2:F:1126:LEU:O | 2:F:1130:GLN:HG3 | 2.17 | 0.44 |
| 2:F:1223:ASP:O | 2:F:1227:VAL:HG23 | 2.17 | 0.44 |
| 1:G:526:ALA:HB2 | 1:G:617:PHE:CE2 | 2.52 | 0.44 |
| 2:H:1497:PHE:O | 2:H:1498:ILE:C | 2.56 | 0.44 |
| 3:J:272:ILE:HG12 | 3:J:284:TYR:CE1 | 2.52 | 0.44 |
| 3:J:554:LEU:H | 3:J:726:TRP:HH2 | 1.65 | 0.44 |
| 3:K:491:VAL:HB | 3:K:572:LEU:HD11 | 1.99 | 0.44 |
| 3:L:554:LEU:H | 3:L:726:TRP:HH2 | 1.65 | 0.44 |
| 1:A:100:LEU:HD21 | 1:A:638:LEU:HD23 | 2.00 | 0.44 |
| 2:B:1126:LEU:O | 2:B:1130:GLN:HG3 | 2.17 | 0.44 |
| 2:B:1283:SER:O | 2:B:1284:LYS:HG2 | 2.18 | 0.44 |
| 2:B:734:ILE:N | 2:B:734:ILE:HD12 | 2.33 | 0.44 |
| 2:D:1203:LYS:HD2 | 2:D:1206:TYR:CE2 | 2.52 | 0.44 |
| 2:D:819:ARG:O | 2:D:820:ASN:HB2 | 2.17 | 0.44 |
| 2:F:1360:ASN:O | 2:F:1361:THR:O | 2.36 | 0.44 |
| 2:H:1470:PHE:CB | 2:H:1478:GLY:HA3 | 2.47 | 0.44 |
| 3:I:433:MET:HE3 | 3:I:433:MET:HB3 | 1.83 | 0.44 |
| 3:K:489:ALA:HB2 | 3:K:677:PRO:CG | 2.45 | 0.44 |
| 6:W:2:NAG:H3 | 6:W:4:BMA:O3 | 2.17 | 0.44 |
| 1:A:459:ARG:HH21 | 1:G:459:ARG:HE | 1.66 | 0.44 |
| 2:B:847:ASN:HA | 2:B:848:PRO:HD2 | 1.83 | 0.44 |
| 1:C:250:ILE:HG22 | 1:C:305:SER:HB3 | 2.00 | 0.44 |
| 1:E:144:ASN:N | 1:E:144:ASN:HD22 | 2.14 | 0.44 |
| 1:E:247:ALA:HB2 | 1:E:308:VAL:HG22 | 1.98 | 0.44 |
| 1:E:427:VAL:HB | 1:E:523:GLU:HG3 | 1.99 | 0.44 |
| 2:F:734:ILE:HD12 | 2:F:734:ILE:N | 2.33 | 0.44 |
| 2:F:943:ALA:O | 2:F:1305:ASN:ND2 | 2.49 | 0.44 |
| 2:H:1288:ARG:HD3 | 2:H:1290:HIS:NE2 | 2.32 | 0.44 |
| 2:H:1360:ASN:O | 2:H:1361:THR:O | 2.36 | 0.44 |
| 2:H:1364:LEU:HD23 | 2:H:1439:PHE:CZ | 2.52 | 0.44 |
| 2:H:943:ALA:O | 2:H:1305:ASN:ND2 | 2.49 | 0.44 |
| 1:A:342:PHE:CE1 | 1:A:391:THR:HG21 | 2.53 | 0.44 |
| 1:A:555:PRO:HB3 | 2:B:775:ASP:HA | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1364:LEU:HD23 | 2:B:1439:PHE:CZ | 2.52 | 0.44 |
| 2:B:1639:CYS:HB2 | 3:L:368:ASN:OD1 | 2.18 | 0.44 |
| 2:H:1280:SER:O | 2:H:1281:ARG:C | 2.55 | 0.44 |
| 2:H:847:ASN:HA | 2:H:848:PRO:HD2 | 1.83 | 0.44 |
| 3:I:272:ILE:HG12 | 3:I:284:TYR:CE1 | 2.52 | 0.44 |
| 3:I:554:LEU:H | 3:I:726:TRP:HH2 | 1.65 | 0.44 |
| 3:K:238:LEU:HD11 | 3:K:278:TYR:CB | 2.46 | 0.44 |
| 3:L:491:VAL:HB | 3:L:572:LEU:HD11 | 1.99 | 0.44 |
| 2:B:811:LEU:HG | 2:B:813:LEU:HD13 | 1.98 | 0.44 |
| 2:D:1265:PRO:O | 2:D:1266:ASP:CB | 2.65 | 0.44 |
| 2:D:1292:GLU:HG2 | 2:D:1293:SER:H | 1.83 | 0.44 |
| 2:F:847:ASN:HA | 2:F:848:PRO:HD2 | 1.83 | 0.44 |
| 2:D:1639:CYS:HB2 | 3:I:368:ASN:OD1 | 2.18 | 0.44 |
| 3:I:375:THR:O | 3:I:379:GLU:HG3 | 2.18 | 0.44 |
| 3:K:446:GLU:OE2 | 3:K:457:TRP:NE1 | 2.50 | 0.44 |
| 3:L:375:THR:O | 3:L:379:GLU:HG3 | 2.18 | 0.44 |
| 4:Q:66:ALA:HA | 4:Q:69:GLN:HB2 | 1.98 | 0.44 |
| 1:A:459:ARG:HE | 1:G:459:ARG:NH2 | 2.16 | 0.44 |
| 2:B:840:VAL:HG22 | 2:B:894:VAL:HG12 | 2.00 | 0.44 |
| 2:B:937:LYS:O | 2:B:937:LYS:HD2 | 2.17 | 0.44 |
| 1:C:22:LEU:HD13 | 1:C:33:VAL:HG11 | 2.00 | 0.44 |
| 2:D:1446:ASN:HB2 | 4:P:4:LEU:HB2 | 1.99 | 0.44 |
| 1:E:516:ILE:N | 1:E:516:ILE:HD12 | 2.32 | 0.44 |
| 1:E:558:GLN:HB3 | 2:F:770:ASN:HD21 | 1.82 | 0.44 |
| 1:E:567:HIS:CG | 2:F:760:PRO:HG3 | 2.53 | 0.44 |
| 2:F:1370:TYR:CD1 | 2:F:1376:ALA:HB2 | 2.52 | 0.44 |
| 1:G:147:ASN:HB2 | 1:G:148:PRO:CD | 2.46 | 0.44 |
| 3:J:375:THR:O | 3:J:379:GLU:HG3 | 2.18 | 0.44 |
| 1:A:329:SER:HA | 1:A:330:PRO:HD3 | 1.78 | 0.44 |
| 2:B:1462:ASN:C | 2:B:1462:ASN:HD22 | 2.21 | 0.44 |
| 2:D:1283:SER:O | 2:D:1284:LYS:HG2 | 2.18 | 0.44 |
| 2:F:1126:LEU:HD21 | 2:F:1177:MET:HE3 | 1.99 | 0.44 |
| 2:F:1264:ALA:HA | 2:F:1265:PRO:HD3 | 1.74 | 0.44 |
| 2:F:1375:ASP:OD1 | 2:F:1431:HIS:HD2 | 2.01 | 0.44 |
| 2:H:1283:SER:O | 2:H:1284:LYS:HG2 | 2.18 | 0.44 |
| 2:H:1375:ASP:OD1 | 2:H:1431:HIS:HD2 | 2.01 | 0.44 |
| 3:I:543:GLY:O | 3:I:545:PRO:HD3 | 2.18 | 0.44 |
| 3:J:366:LEU:HB2 | 17:J:2002:HOH:O | 2.18 | 0.44 |
| 3:J:433:MET:HE1 | 3:J:436:LEU:HD21 | 1.99 | 0.44 |
| 3:K:245:ASN:OD1 | 3:K:283:ARG:HB2 | 2.18 | 0.44 |
| 1:A:407:GLN:C | 1:A:409:LEU:H | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:10:ASN:HB2 | 1:C:621:GLY:CA | 2.48 | 0.44 |
| 2:D:1338:LYS:H | 2:D:1371:ARG:HD2 | 1.83 | 0.44 |
| 2:D:1375:ASP:OD1 | 2:D:1431:HIS:HD2 | 2.01 | 0.44 |
| 2:D:1462:ASN:HD21 | 2:D:1464:GLU:HB2 | 1.83 | 0.44 |
| 2:D:734:ILE:N | 2:D:734:ILE:HD12 | 2.33 | 0.44 |
| 2:F:1123:ALA:O | 2:F:1127:ILE:HG13 | 2.17 | 0.44 |
| 1:G:407:GLN:C | 1:G:409:LEU:H | 2.21 | 0.44 |
| 1:G:510:VAL:HG12 | 1:G:528:SER:HB3 | 1.99 | 0.44 |
| 2:H:1292:GLU:HG2 | 2:H:1293:SER:H | 1.83 | 0.44 |
| 3:I:702:ASN:O | 3:I:703:GLN:HG3 | 2.17 | 0.44 |
| 3:J:238:LEU:HD22 | 3:J:280:VAL:HG21 | 1.99 | 0.44 |
| 3:J:491:VAL:HB | 3:J:572:LEU:HD11 | 1.99 | 0.44 |
| 3:J:654:ARG:HG3 | 3:J:722:GLN:CB | 2.48 | 0.44 |
| 3:K:272:ILE:HG12 | 3:K:284:TYR:CE1 | 2.52 | 0.44 |
| 3:K:375:THR:O | 3:K:379:GLU:HG3 | 2.18 | 0.44 |
| 1:A:207:LEU:HA | 1:A:208:PRO:HD2 | 1.81 | 0.43 |
| 2:B:1056:LEU:O | 2:B:1060:VAL:HG23 | 2.18 | 0.43 |
| 1:C:144:ASN:N | 1:C:144:ASN:HD22 | 2.14 | 0.43 |
| 2:D:1126:LEU:O | 2:D:1130:GLN:HG3 | 2.17 | 0.43 |
| 1:E:407:GLN:C | 1:E:409:LEU:H | 2.21 | 0.43 |
| 2:F:1497:PHE:CZ | 2:F:1572:LEU:HD23 | 2.52 | 0.43 |
| 2:F:819:ARG:O | 2:F:820:ASN:HB2 | 2.17 | 0.43 |
| 3:I:491:VAL:HB | 3:I:572:LEU:HD11 | 1.99 | 0.43 |
| 3:K:654:ARG:HG3 | 3:K:722:GLN:CB | 2.48 | 0.43 |
| 3:K:700:CYS:HA | 3:K:704:LYS:O | 2.16 | 0.43 |
| 1:A:247:ALA:HB2 | 1:A:308:VAL:HG22 | 1.99 | 0.43 |
| 1:A:19:THR:HB | 1:A:478:LEU:HB2 | 1.99 | 0.43 |
| 2:B:1038:ARG:NH1 | 2:B:1077:VAL:HG22 | 2.33 | 0.43 |
| 1:E:343:LYS:HB2 | 1:E:346:MET:HB2 | 2.00 | 0.43 |
| 2:F:1283:SER:O | 2:F:1284:LYS:HG2 | 2.18 | 0.43 |
| 2:F:1359:LYS:HB2 | 4:M:4:LEU:HD21 | 2.00 | 0.43 |
| 2:F:1462:ASN:HD21 | 2:F:1464:GLU:HB2 | 1.84 | 0.43 |
| 2:H:1370:TYR:CD1 | 2:H:1376:ALA:HB2 | 2.52 | 0.43 |
| 2:H:840:VAL:HG22 | 2:H:894:VAL:HG12 | 2.00 | 0.43 |
| 9:Y:1:NAG:H61 | 9:Y:2:NAG:C7 | 2.48 | 0.43 |
| 2:D:1056:LEU:O | 2:D:1060:VAL:HG23 | 2.19 | 0.43 |
| 2:D:887:GLU:OE2 | 2:D:904:ARG:HD2 | 2.19 | 0.43 |
| 2:F:1038:ARG:NH1 | 2:F:1077:VAL:HG22 | 2.33 | 0.43 |
| 1:G:343:LYS:N | 1:G:343:LYS:HD2 | 2.33 | 0.43 |
| 2:H:887:GLU:OE2 | 2:H:904:ARG:HD2 | 2.18 | 0.43 |
| 3:J:543:GLY:O | 3:J:545:PRO:HD3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:653:PRO:CD | 3:J:654:ARG:HH12 | 2.27 | 0.43 |
| 3:K:513:LYS:HZ2 | 3:K:524:GLU:HG2 | 1.82 | 0.43 |
| 3:L:654:ARG:HG3 | 3:L:722:GLN:CB | 2.48 | 0.43 |
| 1:A:126:ARG:HG3 | 2:B:751:TRP:CZ2 | 2.54 | 0.43 |
| 1:E:208:PRO:CD | 1:E:583:LEU:HD11 | 2.48 | 0.43 |
| 2:F:1639:CYS:HA | 2:F:1640:PRO:HD3 | 1.69 | 0.43 |
| 2:F:833:ARG:NH1 | 2:F:833:ARG:CG | 2.75 | 0.43 |
| 1:G:473:MET:HE1 | 1:G:603:ILE:HD11 | 1.99 | 0.43 |
| 1:G:427:VAL:HB | 1:G:523:GLU:HG3 | 1.99 | 0.43 |
| 1:G:341:TYR:CE1 | 1:G:611:LYS:HB3 | 2.53 | 0.43 |
| 3:I:245:ASN:OD1 | 3:I:283:ARG:HB2 | 2.18 | 0.43 |
| 6:W:2:NAG:H61 | 6:W:3:BMA:H2 | 1.99 | 0.43 |
| 1:A:22:LEU:HD13 | 1:A:33:VAL:HG11 | 2.00 | 0.43 |
| 2:B:1338:LYS:H | 2:B:1371:ARG:HD2 | 1.83 | 0.43 |
| 2:B:1482:LYS:HA | 2:B:1492:ALA:HB3 | 2.00 | 0.43 |
| 1:C:407:GLN:C | 1:C:409:LEU:H | 2.21 | 0.43 |
| 1:C:516:ILE:HD12 | 1:C:516:ILE:N | 2.32 | 0.43 |
| 1:E:250:ILE:HG12 | 1:E:251:PHE:H | 1.84 | 0.43 |
| 1:E:22:LEU:HD13 | 1:E:33:VAL:HG11 | 2.00 | 0.43 |
| 1:E:343:LYS:HD2 | 1:E:343:LYS:N | 2.33 | 0.43 |
| 2:F:1462:ASN:HD22 | 2:F:1462:ASN:C | 2.21 | 0.43 |
| 3:L:238:LEU:HD22 | 3:L:280:VAL:HG21 | 1.99 | 0.43 |
| 2:B:1290:HIS:O | 2:B:1291:TRP:O | 2.37 | 0.43 |
| 2:B:1336:CYS:O | 2:B:1337:ASN:O | 2.37 | 0.43 |
| 2:B:1375:ASP:OD1 | 2:B:1431:HIS:HD2 | 2.01 | 0.43 |
| 2:D:1336:CYS:O | 2:D:1337:ASN:O | 2.36 | 0.43 |
| 2:D:840:VAL:HG22 | 2:D:894:VAL:HG12 | 2.00 | 0.43 |
| 1:G:2:PRO:HA | 1:G:25:HIS:O | 2.19 | 0.43 |
| 2:H:1506:THR:OG1 | 2:H:1509:GLU:HG2 | 2.17 | 0.43 |
| 3:I:654:ARG:HG3 | 3:I:722:GLN:CB | 2.48 | 0.43 |
| 3:J:245:ASN:OD1 | 3:J:283:ARG:HB2 | 2.18 | 0.43 |
| 2:B:944:ASP:O | 2:B:945:LEU:C | 2.57 | 0.43 |
| 1:C:343:LYS:HD2 | 1:C:343:LYS:N | 2.33 | 0.43 |
| 2:D:944:ASP:O | 2:D:945:LEU:C | 2.57 | 0.43 |
| 1:E:282:ARG:CZ | 1:E:286:LEU:HD11 | 2.49 | 0.43 |
| 2:F:1078:LEU:HD23 | 2:F:1135:ILE:HG21 | 2.01 | 0.43 |
| 2:F:840:VAL:HG22 | 2:F:894:VAL:HG12 | 2.00 | 0.43 |
| 1:G:572:VAL:HG23 | 2:H:785:VAL:HB | 2.01 | 0.43 |
| 3:I:238:LEU:HD22 | 3:I:280:VAL:HG21 | 1.99 | 0.43 |
| 3:K:543:GLY:O | 3:K:545:PRO:HD3 | 2.18 | 0.43 |
| 3:K:655:PHE:HD2 | 3:K:716:PHE:HB3 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:543:GLY:O | 3:L:545:PRO:HD3 | 2.18 | 0.43 |
| 1:A:343:LYS:HD2 | 1:A:343:LYS:N | 2.33 | 0.43 |
| 1:C:2:PRO:HA | 1:C:25:HIS:O | 2.19 | 0.43 |
| 1:E:251:PHE:CG | 1:E:280:LEU:HD22 | 2.54 | 0.43 |
| 1:E:2:PRO:HA | 1:E:25:HIS:O | 2.19 | 0.43 |
| 1:G:526:ALA:O | 1:G:616:VAL:HG21 | 2.19 | 0.43 |
| 3:I:655:PHE:HD2 | 3:I:716:PHE:HB3 | 1.84 | 0.43 |
| 1:C:282:ARG:CZ | 1:C:286:LEU:HD11 | 2.49 | 0.43 |
| 1:C:503:PHE:HD1 | 1:C:507:PHE:CG | 2.37 | 0.43 |
| 1:G:250:ILE:HG12 | 1:G:251:PHE:H | 1.84 | 0.43 |
| 1:G:343:LYS:HB2 | 1:G:346:MET:HB2 | 2.00 | 0.43 |
| 2:H:1528:VAL:HG21 | 2:H:1559:GLN:HE21 | 1.84 | 0.43 |
| 3:I:431:LYS:HG3 | 4:M:27:ASN:ND2 | 2.34 | 0.43 |
| 3:I:446:GLU:H | 3:I:446:GLU:HG3 | 1.66 | 0.43 |
| 2:B:1386:MET:O | 2:B:1387:THR:C | 2.57 | 0.43 |
| 2:B:1462:ASN:HD21 | 2:B:1464:GLU:HB2 | 1.83 | 0.43 |
| 2:B:1523:TYR:HB3 | 2:B:1543:ILE:HG23 | 2.01 | 0.43 |
| 2:B:824:GLU:OE2 | 2:B:875:PRO:HB3 | 2.19 | 0.43 |
| 2:B:887:GLU:OE2 | 2:B:904:ARG:HD2 | 2.18 | 0.43 |
| 1:C:506:SER:HB2 | 1:C:530:TRP:NE1 | 2.27 | 0.43 |
| 2:D:1038:ARG:NH1 | 2:D:1077:VAL:HG22 | 2.33 | 0.43 |
| 2:D:1523:TYR:HB3 | 2:D:1543:ILE:HG23 | 2.01 | 0.43 |
| 2:F:1056:LEU:O | 2:F:1060:VAL:HG23 | 2.19 | 0.43 |
| 2:F:1227:VAL:HB | 2:F:1228:PRO:HD3 | 2.01 | 0.43 |
| 2:H:1376:ALA:HB3 | 2:H:1429:VAL:CG2 | 2.49 | 0.43 |
| 3:L:238:LEU:HD11 | 3:L:278:TYR:CB | 2.46 | 0.43 |
| 2:B:896:HIS:HB3 | 4:Q:61:LYS:HD3 | 2.00 | 0.43 |
| 1:A:251:PHE:CG | 1:A:280:LEU:HD22 | 2.54 | 0.42 |
| 1:A:577:ASP:CG | 2:B:778:THR:HG21 | 2.40 | 0.42 |
| 2:B:1334:LEU:HD13 | 2:B:1334:LEU:HA | 1.80 | 0.42 |
| 1:C:251:PHE:CG | 1:C:280:LEU:HD22 | 2.54 | 0.42 |
| 1:C:538:VAL:HB | 2:D:791:LYS:O | 2.18 | 0.42 |
| 1:G:282:ARG:CZ | 1:G:286:LEU:HD11 | 2.49 | 0.42 |
| 2:H:1462:ASN:HD21 | 2:H:1464:GLU:HB2 | 1.84 | 0.42 |
| 2:H:851:CYS:HB2 | 2:H:1491:CYS:HB2 | 1.81 | 0.42 |
| 3:J:607:PHE:CE1 | 3:J:669:THR:HG22 | 2.54 | 0.42 |
| 3:K:503:PHE:HB2 | 3:K:530:PHE:CZ | 2.54 | 0.42 |
| 3:K:607:PHE:CE1 | 3:K:669:THR:HG22 | 2.54 | 0.42 |
| 2:B:1215:LEU:O | 2:B:1219:LEU:HG | 2.19 | 0.42 |
| 1:C:247:ALA:HB2 | 1:C:308:VAL:HG22 | 2.02 | 0.42 |
| 2:D:819:ARG:NH1 | 2:D:819:ARG:CG | 2.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1292:GLU:HG2 | 2:F:1293:SER:H | 1.83 | 0.42 |
| 2:F:745:PHE:N | 2:F:746:PRO:HD3 | 2.32 | 0.42 |
| 2:H:824:GLU:OE2 | 2:H:875:PRO:HB3 | 2.19 | 0.42 |
| 3:I:238:LEU:HD11 | 3:I:278:TYR:CB | 2.46 | 0.42 |
| 3:J:446:GLU:HG3 | 3:J:446:GLU:H | 1.66 | 0.42 |
| 3:L:245:ASN:OD1 | 3:L:283:ARG:HB2 | 2.18 | 0.42 |
| 2:B:772:PHE:CD1 | 4:N:37:ASN:ND2 | 2.87 | 0.42 |
| 1:A:439:LEU:CD1 | 1:A:439:LEU:H | 2.32 | 0.42 |
| 2:B:1265:PRO:O | 2:B:1266:ASP:CB | 2.64 | 0.42 |
| 2:B:1292:GLU:HG2 | 2:B:1293:SER:H | 1.83 | 0.42 |
| 2:B:932:ARG:O | 2:B:933:GLU:C | 2.57 | 0.42 |
| 1:C:343:LYS:HB2 | 1:C:346:MET:HB2 | 2.00 | 0.42 |
| 2:D:1482:LYS:HA | 2:D:1492:ALA:HB3 | 2.01 | 0.42 |
| 2:D:824:GLU:OE2 | 2:D:875:PRO:HB3 | 2.19 | 0.42 |
| 1:E:111:GLN:O | 1:E:125:TYR:HA | 2.20 | 0.42 |
| 1:G:22:LEU:HD13 | 1:G:33:VAL:HG11 | 2.00 | 0.42 |
| 2:H:1500:LYS:NZ | 2:H:1504:LYS:HB2 | 2.34 | 0.42 |
| 3:I:449:SER:HA | 3:I:452:LEU:HD13 | 2.01 | 0.42 |
| 3:J:437:GLU:CD | 3:J:458:GLU:HB2 | 2.40 | 0.42 |
| 3:J:655:PHE:HD2 | 3:J:716:PHE:HB3 | 1.84 | 0.42 |
| 3:L:655:PHE:HD2 | 3:L:716:PHE:HB3 | 1.84 | 0.42 |
| 6:W:2:NAG:N2 | 6:W:4:BMA:O3 | 2.52 | 0.42 |
| 1:A:503:PHE:HD1 | 1:A:507:PHE:CG | 2.37 | 0.42 |
| 1:A:549:GLU:O | 1:A:550:ASP:HB2 | 2.20 | 0.42 |
| 2:B:1446:ASN:HB2 | 4:Q:4:LEU:CD1 | 2.49 | 0.42 |
| 2:D:932:ARG:O | 2:D:933:GLU:C | 2.57 | 0.42 |
| 1:G:127:ILE:N | 1:G:127:ILE:HD12 | 2.35 | 0.42 |
| 3:I:607:PHE:CE1 | 3:I:669:THR:HG22 | 2.55 | 0.42 |
| 3:L:607:PHE:CE1 | 3:L:669:THR:HG22 | 2.54 | 0.42 |
| 1:A:10:ASN:HB2 | 1:A:621:GLY:HA2 | 2.01 | 0.42 |
| 1:A:127:ILE:HD12 | 1:A:127:ILE:N | 2.35 | 0.42 |
| 1:A:282:ARG:CZ | 1:A:286:LEU:HD11 | 2.49 | 0.42 |
| 1:C:111:GLN:O | 1:C:125:TYR:HA | 2.20 | 0.42 |
| 2:D:1078:LEU:HD23 | 2:D:1135:ILE:HG21 | 2.01 | 0.42 |
| 2:D:1082:VAL:HG13 | 2:D:1129:LEU:HD22 | 2.01 | 0.42 |
| 2:F:1528:VAL:HG21 | 2:F:1559:GLN:HE21 | 1.84 | 0.42 |
| 2:F:969:THR:O | 2:F:970:GLU:C | 2.57 | 0.42 |
| 2:H:745:PHE:N | 2:H:746:PRO:HD3 | 2.35 | 0.42 |
| 3:I:432:ASP:HA | 4:M:27:ASN:HD21 | 1.84 | 0.42 |
| 3:I:709:VAL:HA | 3:I:710:PRO:HD3 | 1.92 | 0.42 |
| 3:K:354:ARG:HB2 | 16:K:1749:NAG:C8 | 2.42 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Y:2:NAG:H82 | 9:Y:2:NAG:H2 | 1.91 | 0.42 |
| 1:A:40:PHE:HA | 1:A:41:PRO:HA | 1.84 | 0.42 |
| 2:B:1506:THR:OG1 | 2:B:1509:GLU:HG2 | 2.20 | 0.42 |
| 2:D:1215:LEU:O | 2:D:1219:LEU:HG | 2.19 | 0.42 |
| 2:D:1290:HIS:O | 2:D:1291:TRP:O | 2.37 | 0.42 |
| 2:D:1506:THR:OG1 | 2:D:1509:GLU:HG2 | 2.20 | 0.42 |
| 1:E:454:LEU:HA | 1:E:491:ASP:O | 2.19 | 0.42 |
| 1:G:251:PHE:CG | 1:G:280:LEU:HD22 | 2.54 | 0.42 |
| 3:I:289:TYR:HA | 3:I:293:PRO:HA | 2.01 | 0.42 |
| 3:K:353:ASN:OD1 | 16:K:1749:NAG:C7 | 2.67 | 0.42 |
| 3:L:489:ALA:HB2 | 3:L:677:PRO:CG | 2.45 | 0.42 |
| 2:B:1227:VAL:HB | 2:B:1228:PRO:HD3 | 2.01 | 0.42 |
| 1:C:147:ASN:HB2 | 1:C:148:PRO:CD | 2.46 | 0.42 |
| 1:C:218:GLU:C | 1:C:220:PHE:H | 2.23 | 0.42 |
| 1:E:127:ILE:HD12 | 1:E:127:ILE:N | 2.35 | 0.42 |
| 1:G:439:LEU:H | 1:G:439:LEU:CD1 | 2.32 | 0.42 |
| 2:H:1516:GLU:HB3 | 2:H:1517:PRO:CD | 2.50 | 0.42 |
| 2:H:1485:ARG:HH21 | 2:H:1590:TRP:HE1 | 1.67 | 0.42 |
| 3:J:531:HIS:CD2 | 3:J:533:ASN:HB2 | 2.55 | 0.42 |
| 1:A:218:GLU:C | 1:A:220:PHE:H | 2.23 | 0.42 |
| 2:B:1078:LEU:HD23 | 2:B:1135:ILE:HG21 | 2.01 | 0.42 |
| 1:C:127:ILE:N | 1:C:127:ILE:HD12 | 2.35 | 0.42 |
| 2:D:943:ALA:O | 2:D:1305:ASN:ND2 | 2.53 | 0.42 |
| 1:E:219:LYS:NZ | 1:E:356:ASN:ND2 | 2.68 | 0.42 |
| 1:E:6:ILE:HD11 | 1:E:20:MET:CG | 2.50 | 0.42 |
| 2:F:1215:LEU:O | 2:F:1219:LEU:HG | 2.19 | 0.42 |
| 2:F:1216:LEU:HD21 | 2:F:1256:ALA:HA | 2.02 | 0.42 |
| 2:F:887:GLU:OE2 | 2:F:904:ARG:HD2 | 2.19 | 0.42 |
| 2:F:944:ASP:O | 2:F:945:LEU:C | 2.57 | 0.42 |
| 1:G:512:TYR:CE1 | 1:G:624:PHE:HE1 | 2.37 | 0.42 |
| 2:H:1386:MET:O | 2:H:1387:THR:C | 2.58 | 0.42 |
| 2:H:944:ASP:O | 2:H:945:LEU:C | 2.57 | 0.42 |
| 3:I:531:HIS:CD2 | 3:I:533:ASN:HB2 | 2.55 | 0.42 |
| 3:L:289:TYR:HA | 3:L:293:PRO:HA | 2.02 | 0.42 |
| 3:L:503:PHE:HB2 | 3:L:530:PHE:CZ | 2.54 | 0.42 |
| 3:L:531:HIS:CD2 | 3:L:533:ASN:HB2 | 2.55 | 0.42 |
| 1:A:250:ILE:HG22 | 1:A:305:SER:HB3 | 2.01 | 0.42 |
| 2:B:1376:ALA:HB3 | 2:B:1429:VAL:CG2 | 2.49 | 0.42 |
| 1:C:330:PRO:HG2 | 1:C:409:LEU:HD21 | 2.01 | 0.42 |
| 2:D:1386:MET:O | 2:D:1387:THR:C | 2.58 | 0.42 |
| 1:G:111:GLN:O | 1:G:125:TYR:HA | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1334:LEU:HD13 | 2:H:1334:LEU:HA | 1.80 | 0.42 |
| 1:G:574:VAL:HG13 | 2:H:783:LEU:HB3 | 2.01 | 0.42 |
| 3:I:676:GLY:HA2 | 3:I:677:PRO:HD3 | 1.83 | 0.42 |
| 3:I:705:ARG:O | 3:I:706:GLN:CB | 2.60 | 0.42 |
| 3:J:443:MET:HB3 | 3:J:443:MET:HE2 | 1.86 | 0.42 |
| 3:K:244:MET:HG2 | 3:K:245:ASN:N | 2.35 | 0.42 |
| 4:Q:84:LYS:O | 4:Q:84:LYS:HG3 | 2.20 | 0.42 |
| 1:C:250:ILE:HG12 | 1:C:251:PHE:H | 1.84 | 0.42 |
| 2:D:1009:THR:HB | 2:D:1011:GLN:HE21 | 1.85 | 0.42 |
| 2:D:1462:ASN:HD22 | 2:D:1462:ASN:C | 2.21 | 0.42 |
| 2:D:1518:GLY:CA | 2:D:1585:LEU:HD22 | 2.48 | 0.42 |
| 2:F:1009:THR:HB | 2:F:1011:GLN:HE21 | 1.85 | 0.42 |
| 2:F:1269:GLU:O | 2:F:1271:ASN:N | 2.52 | 0.42 |
| 2:F:1522:VAL:HG22 | 2:F:1583:TRP:HB3 | 2.02 | 0.42 |
| 1:G:19:THR:HG22 | 1:G:20:MET:N | 2.35 | 0.42 |
| 1:G:503:PHE:HD1 | 1:G:507:PHE:CG | 2.37 | 0.42 |
| 3:I:503:PHE:HB2 | 3:I:530:PHE:CZ | 2.54 | 0.42 |
| 3:J:503:PHE:HB2 | 3:J:530:PHE:CZ | 2.54 | 0.42 |
| 3:L:298:LYS:HB2 | 3:L:301:GLU:HG3 | 2.02 | 0.42 |
| 3:L:443:MET:HE2 | 3:L:443:MET:HB3 | 1.87 | 0.42 |
| 2:B:1082:VAL:HG13 | 2:B:1129:LEU:HD22 | 2.02 | 0.41 |
| 1:C:6:ILE:HD11 | 1:C:20:MET:CG | 2.50 | 0.41 |
| 1:C:439:LEU:CD1 | 1:C:439:LEU:H | 2.32 | 0.41 |
| 2:D:1227:VAL:HB | 2:D:1228:PRO:HD3 | 2.01 | 0.41 |
| 2:F:1336:CYS:O | 2:F:1337:ASN:C | 2.59 | 0.41 |
| 2:F:1390:ALA:HA | 2:F:1391:PRO:HD3 | 1.91 | 0.41 |
| 1:G:526:ALA:CB | 1:G:617:PHE:CE2 | 3.03 | 0.41 |
| 1:G:6:ILE:HD11 | 1:G:20:MET:CG | 2.50 | 0.41 |
| 2:H:1338:LYS:N | 2:H:1371:ARG:HB2 | 2.34 | 0.41 |
| 2:H:841:ARG:CG | 2:H:841:ARG:HH11 | 2.23 | 0.41 |
| 2:H:854:ALA:HB2 | 2:H:860:HIS:HB3 | 2.02 | 0.41 |
| 2:H:877:VAL:H | 2:H:1451:GLN:HE21 | 1.68 | 0.41 |
| 4:M:23:LEU:HD21 | 4:M:51:ALA:HB3 | 2.02 | 0.41 |
| 4:N:56:LYS:HG3 | 4:N:57:SER:N | 2.34 | 0.41 |
| 1:A:330:PRO:HG2 | 1:A:409:LEU:HD21 | 2.00 | 0.41 |
| 1:A:80:ARG:HD2 | 2:B:1010:GLU:HG3 | 2.01 | 0.41 |
| 2:B:1165:TYR:HD1 | 2:B:1210:ALA:HB2 | 1.85 | 0.41 |
| 2:B:932:ARG:O | 2:B:934:GLY:N | 2.53 | 0.41 |
| 2:B:943:ALA:O | 2:B:1305:ASN:ND2 | 2.53 | 0.41 |
| 2:D:1528:VAL:HG21 | 2:D:1559:GLN:HE21 | 1.84 | 0.41 |
| 2:D:932:ARG:O | 2:D:934:GLY:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:350:LEU:CD2 | 1:G:400:ILE:HG21 | 2.50 | 0.41 |
| 3:J:489:ALA:HB2 | 3:J:677:PRO:CG | 2.45 | 0.41 |
| 3:K:540:LYS:HB2 | 3:K:540:LYS:NZ | 2.36 | 0.41 |
| 3:L:239:ASP:HA | 3:L:240:PRO:HD3 | 1.86 | 0.41 |
| 4:M:56:LYS:HG3 | 4:M:57:SER:N | 2.34 | 0.41 |
| 4:Q:23:LEU:HD21 | 4:Q:51:ALA:HB3 | 2.02 | 0.41 |
| 1:A:111:GLN:O | 1:A:125:TYR:HA | 2.20 | 0.41 |
| 1:A:249:VAL:HG13 | 1:A:267:LYS:HB2 | 2.02 | 0.41 |
| 2:B:1009:THR:HB | 2:B:1011:GLN:HE21 | 1.85 | 0.41 |
| 2:B:1541:MET:HE3 | 2:B:1541:MET:HB2 | 1.96 | 0.41 |
| 2:B:1528:VAL:HG21 | 2:B:1559:GLN:HE21 | 1.84 | 0.41 |
| 1:C:19:THR:HG22 | 1:C:20:MET:N | 2.35 | 0.41 |
| 2:D:1370:TYR:CG | 2:D:1376:ALA:HB2 | 2.55 | 0.41 |
| 2:D:1376:ALA:HB3 | 2:D:1429:VAL:CG2 | 2.49 | 0.41 |
| 1:E:126:ARG:CZ | 1:E:572:VAL:HB | 2.50 | 0.41 |
| 1:E:365:VAL:HA | 1:E:366:PRO:HD2 | 1.80 | 0.41 |
| 1:E:386:LYS:HD3 | 1:E:440:ARG:HG2 | 2.02 | 0.41 |
| 2:F:1165:TYR:HD1 | 2:F:1210:ALA:HB2 | 1.85 | 0.41 |
| 2:F:1472:HIS:HA | 2:F:1473:PRO:HD3 | 1.94 | 0.41 |
| 2:F:915:ARG:O | 2:F:916:MET:HG3 | 2.21 | 0.41 |
| 1:G:341:TYR:CD2 | 1:G:610:GLY:HA2 | 2.56 | 0.41 |
| 2:H:1611:GLU:HG3 | 2:H:1612:GLU:N | 2.34 | 0.41 |
| 3:I:666:ASP:HA | 3:I:667:PRO:HD3 | 1.95 | 0.41 |
| 3:J:244:MET:HG2 | 3:J:245:ASN:N | 2.35 | 0.41 |
| 3:J:298:LYS:HB2 | 3:J:301:GLU:HG3 | 2.02 | 0.41 |
| 3:J:433:MET:HE3 | 3:J:433:MET:HB3 | 1.82 | 0.41 |
| 3:K:443:MET:HE2 | 3:K:443:MET:HB3 | 1.87 | 0.41 |
| 3:K:531:HIS:CD2 | 3:K:533:ASN:HB2 | 2.55 | 0.41 |
| 3:L:540:LYS:NZ | 3:L:540:LYS:HB2 | 2.36 | 0.41 |
| 3:L:503:PHE:CZ | 3:L:555:ILE:HD11 | 2.55 | 0.41 |
| 3:L:494:TYR:O | 3:L:556:LYS:HA | 2.21 | 0.41 |
| 4:N:84:LYS:O | 4:N:84:LYS:HG3 | 2.20 | 0.41 |
| 4:Q:56:LYS:HG3 | 4:Q:57:SER:N | 2.34 | 0.41 |
| 7:V:3:BMA:H5 | 7:V:4:BMA:H2 | 2.01 | 0.41 |
| 1:G:481:ALA:O | 6:W:1:NAG:H82 | 2.20 | 0.41 |
| 1:A:343:LYS:HB2 | 1:A:346:MET:HB2 | 2.00 | 0.41 |
| 1:A:454:LEU:HA | 1:A:491:ASP:O | 2.21 | 0.41 |
| 2:B:1055:TRP:CD1 | 2:B:1111:LEU:HD22 | 2.56 | 0.41 |
| 1:C:100:LEU:HD12 | 1:C:101:VAL:H | 1.86 | 0.41 |
| 2:F:1055:TRP:CD1 | 2:F:1111:LEU:HD22 | 2.56 | 0.41 |
| 2:F:1518:GLY:CA | 2:F:1585:LEU:HD22 | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:932:ARG:HH11 | 3:L:339:SER:CB | 2.34 | 0.41 |
| 1:G:218:GLU:C | 1:G:220:PHE:H | 2.23 | 0.41 |
| 2:H:1514:ALA:O | 2:H:1519:VAL:HG11 | 2.20 | 0.41 |
| 3:I:503:PHE:CZ | 3:I:555:ILE:HD11 | 2.55 | 0.41 |
| 3:J:494:TYR:O | 3:J:556:LYS:HA | 2.21 | 0.41 |
| 3:L:278:TYR:CE2 | 3:L:455:MET:SD | 3.13 | 0.41 |
| 4:N:41:LYS:O | 4:N:45:LYS:HG3 | 2.21 | 0.41 |
| 4:P:84:LYS:HG3 | 4:P:84:LYS:O | 2.20 | 0.41 |
| 2:H:740:VAL:CB | 4:Q:42:ARG:HB2 | 2.45 | 0.41 |
| 1:A:250:ILE:HG12 | 1:A:251:PHE:H | 1.84 | 0.41 |
| 1:A:2:PRO:HA | 1:A:25:HIS:O | 2.19 | 0.41 |
| 1:A:13:ARG:NH2 | 1:A:476:GLY:HA3 | 2.35 | 0.41 |
| 2:B:1451:GLN:HA | 2:B:1452:PRO:HD3 | 1.94 | 0.41 |
| 2:D:1055:TRP:CD1 | 2:D:1111:LEU:HD22 | 2.56 | 0.41 |
| 2:D:1516:GLU:HB3 | 2:D:1517:PRO:CD | 2.50 | 0.41 |
| 2:F:1082:VAL:HG13 | 2:F:1129:LEU:HD22 | 2.02 | 0.41 |
| 2:F:759:PRO:HA | 2:F:760:PRO:HD3 | 1.84 | 0.41 |
| 2:F:932:ARG:O | 2:F:933:GLU:C | 2.58 | 0.41 |
| 2:H:1462:ASN:HD22 | 2:H:1462:ASN:C | 2.21 | 0.41 |
| 3:I:244:MET:HG2 | 3:I:245:ASN:N | 2.35 | 0.41 |
| 3:J:289:TYR:HA | 3:J:293:PRO:HA | 2.02 | 0.41 |
| 3:J:676:GLY:HA2 | 3:J:677:PRO:HD3 | 1.83 | 0.41 |
| 3:K:446:GLU:H | 3:K:446:GLU:HG3 | 1.66 | 0.41 |
| 3:K:503:PHE:CZ | 3:K:555:ILE:HD11 | 2.55 | 0.41 |
| 2:H:1359:LYS:CB | 4:N:4:LEU:HD21 | 2.50 | 0.41 |
| 3:J:461:LYS:HG2 | 4:Q:28:VAL:HG12 | 2.03 | 0.41 |
| 2:B:813:LEU:HD23 | 2:B:907:LEU:HD22 | 2.02 | 0.41 |
| 1:C:549:GLU:O | 1:C:550:ASP:HB2 | 2.20 | 0.41 |
| 2:D:1357:ASP:C | 2:D:1359:LYS:H | 2.24 | 0.41 |
| 2:F:1334:LEU:HA | 2:F:1334:LEU:HD13 | 1.80 | 0.41 |
| 2:F:824:GLU:OE2 | 2:F:875:PRO:HB3 | 2.19 | 0.41 |
| 1:G:549:GLU:O | 1:G:550:ASP:HB2 | 2.20 | 0.41 |
| 2:H:1500:LYS:HE3 | 2:H:1504:LYS:O | 2.21 | 0.41 |
| 3:J:368:ASN:ND2 | 3:J:368:ASN:N | 2.69 | 0.41 |
| 3:J:540:LYS:NZ | 3:J:540:LYS:HB2 | 2.35 | 0.41 |
| 4:M:84:LYS:O | 4:M:84:LYS:HG3 | 2.20 | 0.41 |
| 4:P:56:LYS:HG3 | 4:P:57:SER:N | 2.34 | 0.41 |
| 1:A:10:ASN:HA | 1:A:623:THR:HG23 | 2.03 | 0.41 |
| 2:B:1522:VAL:HG22 | 2:B:1583:TRP:HB3 | 2.02 | 0.41 |
| 2:B:854:ALA:HB2 | 2:B:860:HIS:HB3 | 2.02 | 0.41 |
| 2:D:851:CYS:HB2 | 2:D:1491:CYS:HB2 | 1.78 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1522:VAL:HG22 | 2:D:1583:TRP:HB3 | 2.02 | 0.41 |
| 2:D:1611:GLU:HG3 | 2:D:1612:GLU:N | 2.34 | 0.41 |
| 1:E:503:PHE:HD1 | 1:E:507:PHE:CG | 2.37 | 0.41 |
| 2:F:1386:MET:O | 2:F:1387:THR:C | 2.58 | 0.41 |
| 2:F:1514:ALA:O | 2:F:1519:VAL:HG11 | 2.20 | 0.41 |
| 1:A:459:ARG:NH2 | 1:G:459:ARG:HE | 2.19 | 0.41 |
| 1:G:7:ILE:HG21 | 1:G:471:LEU:HD22 | 2.02 | 0.41 |
| 2:H:1518:GLY:CA | 2:H:1585:LEU:HD22 | 2.48 | 0.41 |
| 3:I:494:TYR:O | 3:I:556:LYS:HA | 2.21 | 0.41 |
| 3:K:298:LYS:HB2 | 3:K:301:GLU:HG3 | 2.02 | 0.41 |
| 1:E:481:ALA:N | 5:U:1:NAG:H81 | 2.35 | 0.41 |
| 1:A:363:TYR:CD2 | 1:A:381:GLY:HA2 | 2.56 | 0.41 |
| 1:A:6:ILE:HD11 | 1:A:20:MET:CG | 2.50 | 0.41 |
| 2:B:1216:LEU:HD21 | 2:B:1256:ALA:HA | 2.02 | 0.41 |
| 2:B:1444:TYR:HB2 | 4:Q:10:TYR:CE1 | 2.55 | 0.41 |
| 2:B:1522:VAL:HG12 | 2:B:1547:ILE:HD12 | 2.03 | 0.41 |
| 2:B:841:ARG:HH11 | 2:B:841:ARG:CG | 2.23 | 0.41 |
| 1:C:207:LEU:HA | 1:C:208:PRO:HD2 | 1.82 | 0.41 |
| 1:E:549:GLU:O | 1:E:550:ASP:HB2 | 2.20 | 0.41 |
| 2:F:1338:LYS:N | 2:F:1371:ARG:HB2 | 2.36 | 0.41 |
| 1:G:23:GLU:OE1 | 1:G:469:THR:HG21 | 2.21 | 0.41 |
| 1:G:249:VAL:HG13 | 1:G:267:LYS:HB2 | 2.02 | 0.41 |
| 2:H:1639:CYS:HA | 2:H:1640:PRO:HD3 | 1.76 | 0.41 |
| 2:H:813:LEU:HA | 2:H:814:PRO:HD3 | 1.97 | 0.41 |
| 3:L:428:PHE:CE1 | 3:L:439:VAL:HG13 | 2.56 | 0.41 |
| 1:A:250:ILE:HG12 | 1:A:251:PHE:N | 2.36 | 0.41 |
| 2:B:1192:ALA:HB2 | 2:B:1198:TRP:CE2 | 2.56 | 0.41 |
| 2:B:1370:TYR:CG | 2:B:1376:ALA:HB2 | 2.55 | 0.41 |
| 2:B:1611:GLU:HB3 | 2:B:1614:GLU:HG3 | 2.03 | 0.41 |
| 1:C:10:ASN:HB2 | 1:C:622:LEU:N | 2.36 | 0.41 |
| 1:C:454:LEU:HA | 1:C:491:ASP:O | 2.21 | 0.41 |
| 2:D:1611:GLU:HB3 | 2:D:1614:GLU:HG3 | 2.03 | 0.41 |
| 1:E:19:THR:HG22 | 1:E:20:MET:N | 2.35 | 0.41 |
| 1:E:250:ILE:HG22 | 1:E:305:SER:HB3 | 2.03 | 0.41 |
| 1:E:640:CYS:HB3 | 1:E:641:PRO:CD | 2.51 | 0.41 |
| 2:H:1522:VAL:HG22 | 2:H:1583:TRP:HB3 | 2.02 | 0.41 |
| 3:I:239:ASP:HA | 3:I:240:PRO:HD3 | 1.86 | 0.41 |
| 3:J:503:PHE:CZ | 3:J:555:ILE:HD11 | 2.55 | 0.41 |
| 3:K:289:TYR:HA | 3:K:293:PRO:HA | 2.02 | 0.41 |
| 4:P:23:LEU:HD21 | 4:P:51:ALA:HB3 | 2.02 | 0.41 |
| 3:J:428:PHE:CE1 | 4:Q:31:LEU:HD11 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:506:SER:HB2 | 1:A:530:TRP:NE1 | 2.27 | 0.41 |
| 1:A:552:GLN:HA | 1:A:553:PRO:HD3 | 1.81 | 0.41 |
| 1:A:24:ALA:HB3 | 1:A:60:HIS:HB3 | 2.03 | 0.41 |
| 2:D:1165:TYR:HD1 | 2:D:1210:ALA:HB2 | 1.85 | 0.41 |
| 1:E:218:GLU:C | 1:E:220:PHE:H | 2.23 | 0.41 |
| 1:E:250:ILE:HG12 | 1:E:251:PHE:N | 2.36 | 0.41 |
| 1:E:324:ILE:HA | 1:E:325:PRO:HD3 | 1.89 | 0.41 |
| 2:F:1376:ALA:HB3 | 2:F:1429:VAL:CG2 | 2.49 | 0.41 |
| 2:F:745:PHE:HA | 2:F:776:SER:OG | 2.21 | 0.41 |
| 1:G:207:LEU:HA | 1:G:208:PRO:HD2 | 1.82 | 0.41 |
| 2:H:1523:TYR:HB3 | 2:H:1543:ILE:HG23 | 2.02 | 0.41 |
| 2:H:1541:MET:HB2 | 2:H:1541:MET:HE3 | 1.96 | 0.41 |
| 3:J:238:LEU:HD11 | 3:J:278:TYR:CB | 2.46 | 0.41 |
| 3:J:423:ASN:ND2 | 3:J:423:ASN:N | 2.68 | 0.41 |
| 3:J:638:ALA:HA | 3:J:639:PRO:HD3 | 1.98 | 0.41 |
| 3:K:676:GLY:HA2 | 3:K:677:PRO:HD3 | 1.83 | 0.41 |
| 4:M:69:GLN:HB3 | 4:M:69:GLN:HE21 | 1.68 | 0.41 |
| 1:A:100:LEU:HD12 | 1:A:101:VAL:H | 1.86 | 0.41 |
| 1:A:19:THR:HG22 | 1:A:20:MET:N | 2.35 | 0.41 |
| 2:B:1229:PRO:HA | 2:B:1232:ARG:NH1 | 2.36 | 0.41 |
| 2:B:729:LEU:C | 2:B:729:LEU:HD13 | 2.41 | 0.41 |
| 1:C:477:ARG:HG2 | 1:C:477:ARG:NH1 | 2.21 | 0.41 |
| 2:D:1216:LEU:HD21 | 2:D:1256:ALA:HA | 2.02 | 0.41 |
| 2:D:745:PHE:N | 2:D:746:PRO:HD3 | 2.35 | 0.41 |
| 1:E:439:LEU:CD1 | 1:E:439:LEU:H | 2.32 | 0.41 |
| 1:E:438:VAL:HG13 | 1:E:449:LEU:HD11 | 2.03 | 0.41 |
| 2:F:1522:VAL:HG12 | 2:F:1547:ILE:HD12 | 2.03 | 0.41 |
| 2:F:813:LEU:HD23 | 2:F:907:LEU:HD22 | 2.02 | 0.41 |
| 1:G:391:THR:HG22 | 1:G:392:HIS:N | 2.36 | 0.41 |
| 2:H:1635:VAL:HG23 | 2:H:1636:VAL:N | 2.36 | 0.41 |
| 3:I:503:PHE:HB2 | 3:I:530:PHE:HZ | 1.86 | 0.41 |
| 3:J:428:PHE:CE1 | 3:J:439:VAL:HG13 | 2.56 | 0.41 |
| 3:K:244:MET:HG2 | 3:K:245:ASN:H | 1.86 | 0.41 |
| 1:A:400:ILE:N | 1:A:400:ILE:HD12 | 2.36 | 0.40 |
| 2:B:917:ASN:OD1 | 5:R:1:NAG:O5 | 2.38 | 0.40 |
| 1:C:365:VAL:HA | 1:C:366:PRO:HD2 | 1.81 | 0.40 |
| 2:D:1192:ALA:HB2 | 2:D:1198:TRP:CE2 | 2.56 | 0.40 |
| 1:E:249:VAL:HG13 | 1:E:267:LYS:HB2 | 2.03 | 0.40 |
| 2:F:1229:PRO:HA | 2:F:1232:ARG:NH1 | 2.36 | 0.40 |
| 2:F:1516:GLU:HB3 | 2:F:1517:PRO:CD | 2.50 | 0.40 |
| 1:E:541:LEU:HD22 | 2:F:786:SER:HB3 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:819:ARG:CG | 2:F:819:ARG:NH1 | 2.80 | 0.40 |
| 2:F:854:ALA:HB2 | 2:F:860:HIS:HB3 | 2.02 | 0.40 |
| 1:G:400:ILE:N | 1:G:400:ILE:HD12 | 2.36 | 0.40 |
| 2:H:1522:VAL:HG12 | 2:H:1547:ILE:HD12 | 2.03 | 0.40 |
| 2:H:915:ARG:O | 2:H:916:MET:HG3 | 2.21 | 0.40 |
| 2:H:965:VAL:HG23 | 2:H:1268:GLN:OE1 | 2.22 | 0.40 |
| 3:K:439:VAL:HA | 4:P:31:LEU:HD21 | 2.02 | 0.40 |
| 3:K:428:PHE:CE1 | 3:K:439:VAL:HG13 | 2.56 | 0.40 |
| 4:M:41:LYS:O | 4:M:45:LYS:HG3 | 2.21 | 0.40 |
| 4:P:41:LYS:O | 4:P:45:LYS:HG3 | 2.21 | 0.40 |
| 1:A:344:PRO:HG3 | 1:A:423:PRO:HB3 | 2.02 | 0.40 |
| 1:E:391:THR:HG22 | 1:E:392:HIS:N | 2.36 | 0.40 |
| 1:E:552:GLN:HA | 1:E:553:PRO:HD3 | 1.81 | 0.40 |
| 1:E:24:ALA:HB3 | 1:E:60:HIS:HB3 | 2.03 | 0.40 |
| 2:F:1000:VAL:HG22 | 2:F:1027:ILE:HG23 | 2.04 | 0.40 |
| 2:F:1192:ALA:HB2 | 2:F:1198:TRP:CE2 | 2.56 | 0.40 |
| 2:F:1370:TYR:CE2 | 2:F:1372:GLY:HA3 | 2.56 | 0.40 |
| 2:F:1611:GLU:HB3 | 2:F:1614:GLU:HG3 | 2.03 | 0.40 |
| 2:H:1370:TYR:CG | 2:H:1376:ALA:HB2 | 2.56 | 0.40 |
| 2:H:1503:ASP:O | 2:H:1504:LYS:HG3 | 2.21 | 0.40 |
| 1:G:558:GLN:HB3 | 2:H:770:ASN:HD21 | 1.86 | 0.40 |
| 2:H:813:LEU:HD23 | 2:H:907:LEU:HD22 | 2.02 | 0.40 |
| 2:H:877:VAL:HG22 | 2:H:1451:GLN:NE2 | 2.28 | 0.40 |
| 1:C:109:PHE:CZ | 1:C:594:ILE:HG23 | 2.56 | 0.40 |
| 2:D:813:LEU:HD23 | 2:D:907:LEU:HD22 | 2.02 | 0.40 |
| 1:E:480:LYS:HG2 | 1:E:481:ALA:N | 2.36 | 0.40 |
| 2:F:1523:TYR:HB3 | 2:F:1543:ILE:HG23 | 2.02 | 0.40 |
| 1:G:126:ARG:HG3 | 2:H:751:TRP:CZ2 | 2.56 | 0.40 |
| 1:G:480:LYS:HG2 | 1:G:481:ALA:N | 2.37 | 0.40 |
| 1:G:505:PRO:O | 1:G:533:VAL:HB | 2.21 | 0.40 |
| 1:G:506:SER:HB2 | 1:G:530:TRP:NE1 | 2.27 | 0.40 |
| 2:H:1527:LEU:HD22 | 2:H:1574:LEU:HB3 | 2.04 | 0.40 |
| 2:H:809:ILE:HD11 | 2:H:892:ALA:CB | 2.52 | 0.40 |
| 3:I:345:ASP:HB3 | 3:I:346:ASP:H | 1.49 | 0.40 |
| 3:I:654:ARG:HG3 | 3:I:722:GLN:HB3 | 2.03 | 0.40 |
| 5:U:3:BMA:H62 | 5:U:4:BMA:H2 | 1.58 | 0.40 |
| 1:A:363:TYR:HD2 | 1:A:381:GLY:HA2 | 1.86 | 0.40 |
| 1:A:342:PHE:CZ | 1:A:423:PRO:HG3 | 2.56 | 0.40 |
| 1:C:391:THR:HG22 | 1:C:392:HIS:N | 2.36 | 0.40 |
| 1:C:392:HIS:C | 1:C:394:SER:H | 2.25 | 0.40 |
| 1:C:583:LEU:HD12 | 1:C:583:LEU:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1229:PRO:HA | 2:D:1232:ARG:NH1 | 2.36 | 0.40 |
| 2:D:776:SER:HB2 | 2:D:780:TRP:HZ2 | 1.86 | 0.40 |
| 1:E:100:LEU:HD12 | 1:E:101:VAL:H | 1.86 | 0.40 |
| 1:E:583:LEU:N | 1:E:583:LEU:HD12 | 2.36 | 0.40 |
| 2:H:1370:TYR:CE2 | 2:H:1372:GLY:HA3 | 2.56 | 0.40 |
| 2:H:1609:TRP:HD1 | 2:H:1610:PRO:O | 2.04 | 0.40 |
| 3:I:298:LYS:HB2 | 3:I:301:GLU:HG3 | 2.02 | 0.40 |
| 3:I:402:VAL:HG11 | 3:I:414:ILE:HG23 | 2.04 | 0.40 |
| 3:I:428:PHE:CE1 | 3:I:439:VAL:HG13 | 2.56 | 0.40 |
| 3:I:540:LYS:HB2 | 3:I:540:LYS:NZ | 2.35 | 0.40 |
| 3:K:328:THR:N | 3:K:368:ASN:HD21 | 2.20 | 0.40 |
| 3:K:494:TYR:O | 3:K:556:LYS:HA | 2.21 | 0.40 |
| 3:L:244:MET:HG2 | 3:L:245:ASN:N | 2.35 | 0.40 |
| 3:I:461:LYS:CG | 4:M:28:VAL:HG12 | 2.51 | 0.40 |
| 2:B:1446:ASN:HB2 | 4:Q:4:LEU:HD12 | 2.03 | 0.40 |
| 2:B:1609:TRP:HD1 | 2:B:1610:PRO:O | 2.04 | 0.40 |
| 1:C:400:ILE:N | 1:C:400:ILE:HD12 | 2.36 | 0.40 |
| 1:C:480:LYS:HG2 | 1:C:481:ALA:N | 2.37 | 0.40 |
| 1:C:199:GLU:HB2 | 1:C:587:ASN:OD1 | 2.22 | 0.40 |
| 1:C:24:ALA:HB3 | 1:C:60:HIS:HB3 | 2.03 | 0.40 |
| 2:D:1527:LEU:HD22 | 2:D:1574:LEU:HB3 | 2.04 | 0.40 |
| 1:E:642:GLN:O | 1:E:644:ALA:N | 2.54 | 0.40 |
| 2:F:1143:LEU:O | 2:F:1147:ILE:HG13 | 2.22 | 0.40 |
| 2:F:1632:GLU:HA | 2:F:1635:VAL:HG22 | 2.04 | 0.40 |
| 1:G:220:PHE:CZ | 1:G:330:PRO:HB3 | 2.56 | 0.40 |
| 3:J:292:TYR:HA | 3:J:293:PRO:HD3 | 1.95 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 632/645 (98%) | 576 (91%) | 52 (8%) | 4 (1%) | 25 | 63 |
| 1 | C | 632/645 (98%) | 576 (91%) | 52 (8%) | 4 (1%) | 25 | 63 |
| 1 | E | 632/645 (98%) | 575 (91%) | 53 (8%) | 4 (1%) | 25 | 63 |
| 1 | G | 632/645 (98%) | 575 (91%) | 53 (8%) | 4 (1%) | 25 | 63 |
| 2 | B | 893/915 (98%) | 785 (88%) | 80 (9%) | 28 (3%) | 4 | 32 |
| 2 | D | 893/915 (98%) | 784 (88%) | 82 (9%) | 27 (3%) | 4 | 33 |
| 2 | F | 894/915 (98%) | 786 (88%) | 78 (9%) | 30 (3%) | 3 | 31 |
| 2 | H | 890/915 (97%) | 782 (88%) | 75 (8%) | 33 (4%) | 3 | 29 |
| 3 | I | 505/507 (100%) | 446 (88%) | 51 (10%) | 8 (2%) | 9 | 44 |
| 3 | J | 505/507 (100%) | 446 (88%) | 51 (10%) | 8 (2%) | 9 | 44 |
| 3 | K | 505/507 (100%) | 445 (88%) | 52 (10%) | 8 (2%) | 9 | 44 |
| 3 | L | 505/507 (100%) | 446 (88%) | 51 (10%) | 8 (2%) | 9 | 44 |
| 4 | M | 82/92 (89%) | 77 (94%) | 4 (5%) | 1 (1%) | 13 | 49 |
| 4 | N | 82/92 (89%) | 77 (94%) | 4 (5%) | 1 (1%) | 13 | 49 |
| 4 | P | 82/92 (89%) | 77 (94%) | 4 (5%) | 1 (1%) | 13 | 49 |
| 4 | Q | 82/92 (89%) | 77 (94%) | 4 (5%) | 1 (1%) | 13 | 49 |
| All | All | 8446/8636 (98%) | 7530 (89%) | 746 (9%) | 170 (2%) | 7 | 40 |

All (170) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 933 | GLU |
| 2 | B | 967 | GLN |
| 2 | B | 1269 | GLU |
| 2 | B | 1281 | ARG |
| 2 | B | 1291 | TRP |
| 2 | B | 1292 | GLU |
| 2 | B | 1294 | ALA |
| 2 | B | 1337 | ASN |
| 2 | B | 1338 | LYS |
| 2 | B | 1359 | LYS |
| 2 | B | 1377 | THR |
| 2 | B | 1503 | ASP |
| 2 | D | 933 | GLU |
| 2 | D | 967 | GLN |
| 2 | D | 1281 | ARG |
| 2 | D | 1291 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1292 | GLU |
| 2 | D | 1294 | ALA |
| 2 | D | 1337 | ASN |
| 2 | D | 1338 | LYS |
| 2 | D | 1359 | LYS |
| 2 | D | 1377 | THR |
| 2 | D | 1503 | ASP |
| 2 | F | 933 | GLU |
| 2 | F | 967 | GLN |
| 2 | F | 1269 | GLU |
| 2 | F | 1281 | ARG |
| 2 | F | 1291 | TRP |
| 2 | F | 1292 | GLU |
| 2 | F | 1337 | ASN |
| 2 | F | 1338 | LYS |
| 2 | F | 1361 | THR |
| 2 | F | 1377 | THR |
| 2 | F | 1417 | SER |
| 2 | F | 1446 | ASN |
| 2 | H | 933 | GLU |
| 2 | H | 968 | MET |
| 2 | H | 1281 | ARG |
| 2 | H | 1291 | TRP |
| 2 | H | 1292 | GLU |
| 2 | H | 1337 | ASN |
| 2 | H | 1338 | LYS |
| 2 | H | 1361 | THR |
| 2 | H | 1377 | THR |
| 2 | H | 1417 | SER |
| 2 | H | 1446 | ASN |
| 2 | H | 1493 | GLU |
| 3 | I | 236 | ILE |
| 3 | I | 407 | PRO |
| 3 | I | 701 | LYS |
| 3 | I | 706 | GLN |
| 3 | J | 236 | ILE |
| 3 | J | 407 | PRO |
| 3 | J | 701 | LYS |
| 3 | J | 706 | GLN |
| 3 | K | 236 | ILE |
| 3 | K | 407 | PRO |
| 3 | K | 701 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | K | 706 | GLN |
| 3 | L | 236 | ILE |
| 3 | L | 407 | PRO |
| 3 | L | 701 | LYS |
| 3 | L | 706 | GLN |
| 2 | B | 911 | PRO |
| 2 | B | 1360 | ASN |
| 2 | B | 1361 | THR |
| 2 | B | 1476 | GLU |
| 2 | B | 1571 | ALA |
| 2 | D | 911 | PRO |
| 2 | D | 1360 | ASN |
| 2 | D | 1361 | THR |
| 2 | D | 1476 | GLU |
| 2 | D | 1480 | LEU |
| 2 | D | 1571 | ALA |
| 2 | F | 911 | PRO |
| 2 | F | 1267 | HIS |
| 2 | F | 1294 | ALA |
| 2 | F | 1476 | GLU |
| 2 | F | 1498 | ILE |
| 2 | F | 1571 | ALA |
| 2 | H | 1266 | ASP |
| 2 | H | 1269 | GLU |
| 2 | H | 1294 | ALA |
| 2 | H | 1476 | GLU |
| 2 | H | 1496 | CYS |
| 2 | H | 1498 | ILE |
| 2 | H | 1571 | ALA |
| 1 | A | 442 | GLU |
| 1 | A | 643 | PRO |
| 2 | B | 1387 | THR |
| 2 | B | 1502 | ASP |
| 2 | B | 1573 | LYS |
| 1 | C | 442 | GLU |
| 1 | C | 643 | PRO |
| 2 | D | 1387 | THR |
| 2 | D | 1502 | ASP |
| 2 | D | 1573 | LYS |
| 1 | E | 442 | GLU |
| 1 | E | 643 | PRO |
| 2 | F | 1387 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | F | 1573 | LYS |
| 1 | G | 442 | GLU |
| 2 | H | 911 | PRO |
| 2 | H | 1387 | THR |
| 2 | H | 1573 | LYS |
| 3 | I | 707 | LYS |
| 3 | J | 516 | VAL |
| 3 | J | 707 | LYS |
| 3 | K | 516 | VAL |
| 3 | K | 707 | LYS |
| 3 | L | 707 | LYS |
| 1 | A | 505 | PRO |
| 2 | B | 1196 | ASN |
| 2 | B | 1265 | PRO |
| 2 | B | 1480 | LEU |
| 1 | C | 505 | PRO |
| 2 | D | 1196 | ASN |
| 2 | D | 1265 | PRO |
| 2 | D | 1269 | GLU |
| 1 | E | 505 | PRO |
| 2 | F | 1196 | ASN |
| 2 | F | 1265 | PRO |
| 2 | F | 1268 | GLN |
| 2 | F | 1331 | LYS |
| 2 | F | 1637 | PHE |
| 1 | G | 505 | PRO |
| 2 | H | 967 | GLN |
| 2 | H | 1267 | HIS |
| 2 | H | 1486 | ASP |
| 2 | H | 1495 | ASN |
| 2 | H | 1502 | ASP |
| 3 | I | 516 | VAL |
| 3 | L | 516 | VAL |
| 4 | M | 7 | SER |
| 4 | N | 7 | SER |
| 4 | P | 7 | SER |
| 4 | Q | 7 | SER |
| 2 | B | 834 | GLN |
| 2 | B | 1201 | PRO |
| 2 | B | 1267 | HIS |
| 2 | B | 1536 | PHE |
| 2 | D | 834 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1201 | PRO |
| 2 | D | 1536 | PHE |
| 2 | F | 834 | GLN |
| 2 | F | 1201 | PRO |
| 2 | F | 1270 | LEU |
| 2 | F | 1536 | PHE |
| 1 | G | 643 | PRO |
| 2 | H | 834 | GLN |
| 2 | H | 1196 | ASN |
| 2 | H | 1201 | PRO |
| 2 | H | 1264 | ALA |
| 2 | H | 1536 | PHE |
| 3 | I | 268 | LEU |
| 3 | J | 268 | LEU |
| 3 | K | 268 | LEU |
| 3 | L | 268 | LEU |
| 3 | I | 482 | GLY |
| 3 | J | 482 | GLY |
| 3 | K | 482 | GLY |
| 3 | L | 482 | GLY |
| 2 | B | 1517 | PRO |
| 2 | D | 1517 | PRO |
| 2 | F | 1517 | PRO |
| 2 | H | 1517 | PRO |
| 1 | A | 208 | PRO |
| 1 | C | 208 | PRO |
| 1 | E | 208 | PRO |
| 1 | G | 208 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 558/567 (98%) | 549 (98%) | 9 (2%) | 62 | 79 |
| 1 | C | 558/567 (98%) | 549 (98%) | 9 (2%) | 62 | 79 |
| 1 | E | 558/567 (98%) | 549 (98%) | 9 (2%) | 62 | 79 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | G | 558/567 (98%) | 549 (98%) | 9 (2%) | 62 | 79 |
| 2 | B | 793/810 (98%) | 769 (97%) | 24 (3%) | 41 | 64 |
| 2 | D | 790/810 (98%) | 766 (97%) | 24 (3%) | 41 | 64 |
| 2 | F | 793/810 (98%) | 769 (97%) | 24 (3%) | 41 | 64 |
| 2 | H | 793/810 (98%) | 766 (97%) | 27 (3%) | 37 | 62 |
| 3 | I | 442/446 (99%) | 429 (97%) | 13 (3%) | 42 | 65 |
| 3 | J | 442/446 (99%) | 429 (97%) | 13 (3%) | 42 | 65 |
| 3 | K | 442/446 (99%) | 429 (97%) | 13 (3%) | 42 | 65 |
| 3 | L | 442/446 (99%) | 429 (97%) | 13 (3%) | 42 | 65 |
| 4 | M | 76/84 (90%) | 73 (96%) | 3 (4%) | 32 | 59 |
| 4 | N | 76/84 (90%) | 73 (96%) | 3 (4%) | 32 | 59 |
| 4 | P | 76/84 (90%) | 73 (96%) | 3 (4%) | 32 | 59 |
| 4 | Q | 76/84 (90%) | 73 (96%) | 3 (4%) | 32 | 59 |
| All | All | 7473/7628 (98%) | 7274 (97%) | 199 (3%) | 44 | 67 |

All (199) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 10 | ASN |
| 1 | A | 81 | ASN |
| 1 | A | 144 | ASN |
| 1 | A | 155 | GLN |
| 1 | A | 289 | VAL |
| 1 | A | 398 | LEU |
| 1 | A | 404 | THR |
| 1 | A | 440 | ARG |
| 1 | A | 551 | ARG |
| 2 | B | 757 | LYS |
| 2 | B | 770 | ASN |
| 2 | B | 833 | ARG |
| 2 | B | 834 | GLN |
| 2 | B | 841 | ARG |
| 2 | B | 937 | LYS |
| 2 | B | 945 | LEU |
| 2 | B | 953 | GLU |
| 2 | B | 1018 | GLU |
| 2 | B | 1196 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1292 | GLU |
| 2 | B | 1334 | LEU |
| 2 | B | 1335 | THR |
| 2 | B | 1342 | LYS |
| 2 | B | 1361 | THR |
| 2 | B | 1416 | PHE |
| 2 | B | 1433 | GLU |
| 2 | B | 1445 | PHE |
| 2 | B | 1462 | ASN |
| 2 | B | 1520 | ASP |
| 2 | B | 1535 | ASP |
| 2 | B | 1536 | PHE |
| 2 | B | 1569 | ARG |
| 2 | B | 1637 | PHE |
| 1 | C | 10 | ASN |
| 1 | C | 81 | ASN |
| 1 | C | 144 | ASN |
| 1 | C | 155 | GLN |
| 1 | C | 289 | VAL |
| 1 | C | 398 | LEU |
| 1 | C | 404 | THR |
| 1 | C | 440 | ARG |
| 1 | C | 551 | ARG |
| 2 | D | 757 | LYS |
| 2 | D | 770 | ASN |
| 2 | D | 833 | ARG |
| 2 | D | 834 | GLN |
| 2 | D | 841 | ARG |
| 2 | D | 937 | LYS |
| 2 | D | 945 | LEU |
| 2 | D | 953 | GLU |
| 2 | D | 1018 | GLU |
| 2 | D | 1196 | ASN |
| 2 | D | 1292 | GLU |
| 2 | D | 1334 | LEU |
| 2 | D | 1335 | THR |
| 2 | D | 1342 | LYS |
| 2 | D | 1361 | THR |
| 2 | D | 1416 | PHE |
| 2 | D | 1433 | GLU |
| 2 | D | 1445 | PHE |
| 2 | D | 1462 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1520 | ASP |
| 2 | D | 1535 | ASP |
| 2 | D | 1536 | PHE |
| 2 | D | 1569 | ARG |
| 2 | D | 1637 | PHE |
| 1 | E | 10 | ASN |
| 1 | E | 81 | ASN |
| 1 | E | 144 | ASN |
| 1 | E | 155 | GLN |
| 1 | E | 289 | VAL |
| 1 | E | 398 | LEU |
| 1 | E | 404 | THR |
| 1 | E | 440 | ARG |
| 1 | E | 551 | ARG |
| 2 | F | 757 | LYS |
| 2 | F | 770 | ASN |
| 2 | F | 833 | ARG |
| 2 | F | 834 | GLN |
| 2 | F | 841 | ARG |
| 2 | F | 937 | LYS |
| 2 | F | 945 | LEU |
| 2 | F | 953 | GLU |
| 2 | F | 1018 | GLU |
| 2 | F | 1196 | ASN |
| 2 | F | 1268 | GLN |
| 2 | F | 1292 | GLU |
| 2 | F | 1334 | LEU |
| 2 | F | 1335 | THR |
| 2 | F | 1342 | LYS |
| 2 | F | 1397 | LYS |
| 2 | F | 1433 | GLU |
| 2 | F | 1462 | ASN |
| 2 | F | 1520 | ASP |
| 2 | F | 1535 | ASP |
| 2 | F | 1536 | PHE |
| 2 | F | 1569 | ARG |
| 2 | F | 1572 | LEU |
| 2 | F | 1640 | PRO |
| 1 | G | 10 | ASN |
| 1 | G | 81 | ASN |
| 1 | G | 144 | ASN |
| 1 | G | 155 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | G | 289 | VAL |
| 1 | G | 398 | LEU |
| 1 | G | 404 | THR |
| 1 | G | 440 | ARG |
| 1 | G | 551 | ARG |
| 2 | H | 757 | LYS |
| 2 | H | 770 | ASN |
| 2 | H | 833 | ARG |
| 2 | H | 834 | GLN |
| 2 | H | 841 | ARG |
| 2 | H | 937 | LYS |
| 2 | H | 945 | LEU |
| 2 | H | 953 | GLU |
| 2 | H | 968 | MET |
| 2 | H | 969 | THR |
| 2 | H | 1018 | GLU |
| 2 | H | 1196 | ASN |
| 2 | H | 1267 | HIS |
| 2 | H | 1292 | GLU |
| 2 | H | 1334 | LEU |
| 2 | H | 1335 | THR |
| 2 | H | 1342 | LYS |
| 2 | H | 1397 | LYS |
| 2 | H | 1433 | GLU |
| 2 | H | 1462 | ASN |
| 2 | H | 1498 | ILE |
| 2 | H | 1499 | GLN |
| 2 | H | 1520 | ASP |
| 2 | H | 1535 | ASP |
| 2 | H | 1536 | PHE |
| 2 | H | 1569 | ARG |
| 2 | H | 1572 | LEU |
| 3 | I | 237 | VAL |
| 3 | I | 255 | SER |
| 3 | I | 322 | HIS |
| 3 | I | 329 | ASN |
| 3 | I | 368 | ASN |
| 3 | I | 381 | ARG |
| 3 | I | 423 | ASN |
| 3 | I | 446 | GLU |
| 3 | I | 539 | LYS |
| 3 | I | 540 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 654 | ARG |
| 3 | I | 702 | ASN |
| 3 | I | 703 | GLN |
| 3 | J | 237 | VAL |
| 3 | J | 255 | SER |
| 3 | J | 322 | HIS |
| 3 | J | 329 | ASN |
| 3 | J | 368 | ASN |
| 3 | J | 381 | ARG |
| 3 | J | 423 | ASN |
| 3 | J | 446 | GLU |
| 3 | J | 539 | LYS |
| 3 | J | 540 | LYS |
| 3 | J | 654 | ARG |
| 3 | J | 702 | ASN |
| 3 | J | 703 | GLN |
| 3 | K | 237 | VAL |
| 3 | K | 255 | SER |
| 3 | K | 322 | HIS |
| 3 | K | 329 | ASN |
| 3 | K | 368 | ASN |
| 3 | K | 381 | ARG |
| 3 | K | 423 | ASN |
| 3 | K | 446 | GLU |
| 3 | K | 539 | LYS |
| 3 | K | 540 | LYS |
| 3 | K | 654 | ARG |
| 3 | K | 702 | ASN |
| 3 | K | 703 | GLN |
| 3 | L | 237 | VAL |
| 3 | L | 255 | SER |
| 3 | L | 322 | HIS |
| 3 | L | 329 | ASN |
| 3 | L | 368 | ASN |
| 3 | L | 381 | ARG |
| 3 | L | 423 | ASN |
| 3 | L | 446 | GLU |
| 3 | L | 539 | LYS |
| 3 | L | 540 | LYS |
| 3 | L | 654 | ARG |
| 3 | L | 702 | ASN |
| 3 | L | 703 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M | 11 | GLN |
| 4 | M | 69 | GLN |
| 4 | M | 71 | GLN |
| 4 | N | 11 | GLN |
| 4 | N | 69 | GLN |
| 4 | N | 71 | GLN |
| 4 | P | 11 | GLN |
| 4 | P | 69 | GLN |
| 4 | P | 71 | GLN |
| 4 | Q | 11 | GLN |
| 4 | Q | 69 | GLN |
| 4 | Q | 71 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (256) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 60 | HIS |
| 1 | A | 87 | GLN |
| 1 | A | 104 | GLN |
| 1 | A | 144 | ASN |
| 1 | A | 155 | GLN |
| 1 | A | 161 | GLN |
| 1 | A | 162 | ASN |
| 1 | A | 163 | GLN |
| 1 | A | 370 | GLN |
| 1 | A | 380 | GLN |
| 1 | A | 390 | ASN |
| 1 | A | 414 | GLN |
| 1 | A | 490 | GLN |
| 1 | A | 558 | GLN |
| 1 | A | 567 | HIS |
| 1 | A | 634 | GLN |
| 1 | A | 639 | GLN |
| 2 | B | 738 | ASN |
| 2 | B | 752 | ASN |
| 2 | B | 762 | ASN |
| 2 | B | 770 | ASN |
| 2 | B | 820 | ASN |
| 2 | B | 834 | GLN |
| 2 | B | 860 | HIS |
| 2 | B | 886 | GLN |
| 2 | B | 896 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 897 | HIS |
| 2 | B | 1011 | GLN |
| 2 | B | 1069 | ASN |
| 2 | B | 1076 | GLN |
| 2 | B | 1114 | ASN |
| 2 | B | 1130 | GLN |
| 2 | B | 1141 | ASN |
| 2 | B | 1160 | ASN |
| 2 | B | 1196 | ASN |
| 2 | B | 1204 | GLN |
| 2 | B | 1267 | HIS |
| 2 | B | 1277 | GLN |
| 2 | B | 1333 | GLN |
| 2 | B | 1337 | ASN |
| 2 | B | 1401 | ASN |
| 2 | B | 1431 | HIS |
| 2 | B | 1451 | GLN |
| 2 | B | 1462 | ASN |
| 2 | B | 1559 | GLN |
| 2 | B | 1579 | HIS |
| 2 | B | 1608 | HIS |
| 2 | B | 1620 | ASN |
| 1 | C | 10 | ASN |
| 1 | C | 60 | HIS |
| 1 | C | 87 | GLN |
| 1 | C | 104 | GLN |
| 1 | C | 132 | HIS |
| 1 | C | 144 | ASN |
| 1 | C | 155 | GLN |
| 1 | C | 161 | GLN |
| 1 | C | 162 | ASN |
| 1 | C | 163 | GLN |
| 1 | C | 356 | ASN |
| 1 | C | 370 | GLN |
| 1 | C | 380 | GLN |
| 1 | C | 390 | ASN |
| 1 | C | 414 | GLN |
| 1 | C | 450 | ASN |
| 1 | C | 490 | GLN |
| 1 | C | 558 | GLN |
| 1 | C | 567 | HIS |
| 1 | C | 634 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 639 | GLN |
| 2 | D | 738 | ASN |
| 2 | D | 752 | ASN |
| 2 | D | 762 | ASN |
| 2 | D | 770 | ASN |
| 2 | D | 820 | ASN |
| 2 | D | 834 | GLN |
| 2 | D | 860 | HIS |
| 2 | D | 897 | HIS |
| 2 | D | 1011 | GLN |
| 2 | D | 1069 | ASN |
| 2 | D | 1076 | GLN |
| 2 | D | 1114 | ASN |
| 2 | D | 1130 | GLN |
| 2 | D | 1141 | ASN |
| 2 | D | 1160 | ASN |
| 2 | D | 1196 | ASN |
| 2 | D | 1204 | GLN |
| 2 | D | 1267 | HIS |
| 2 | D | 1277 | GLN |
| 2 | D | 1333 | GLN |
| 2 | D | 1337 | ASN |
| 2 | D | 1401 | ASN |
| 2 | D | 1431 | HIS |
| 2 | D | 1451 | GLN |
| 2 | D | 1462 | ASN |
| 2 | D | 1559 | GLN |
| 2 | D | 1579 | HIS |
| 2 | D | 1608 | HIS |
| 2 | D | 1620 | ASN |
| 1 | E | 60 | HIS |
| 1 | E | 87 | GLN |
| 1 | E | 104 | GLN |
| 1 | E | 132 | HIS |
| 1 | E | 144 | ASN |
| 1 | E | 155 | GLN |
| 1 | E | 161 | GLN |
| 1 | E | 162 | ASN |
| 1 | E | 163 | GLN |
| 1 | E | 356 | ASN |
| 1 | E | 370 | GLN |
| 1 | E | 380 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | E | 390 | ASN |
| 1 | E | 414 | GLN |
| 1 | E | 450 | ASN |
| 1 | E | 490 | GLN |
| 1 | E | 558 | GLN |
| 1 | E | 567 | HIS |
| 1 | E | 639 | GLN |
| 2 | F | 738 | ASN |
| 2 | F | 752 | ASN |
| 2 | F | 762 | ASN |
| 2 | F | 770 | ASN |
| 2 | F | 820 | ASN |
| 2 | F | 834 | GLN |
| 2 | F | 860 | HIS |
| 2 | F | 897 | HIS |
| 2 | F | 1011 | GLN |
| 2 | F | 1069 | ASN |
| 2 | F | 1076 | GLN |
| 2 | F | 1114 | ASN |
| 2 | F | 1130 | GLN |
| 2 | F | 1141 | ASN |
| 2 | F | 1160 | ASN |
| 2 | F | 1196 | ASN |
| 2 | F | 1204 | GLN |
| 2 | F | 1267 | HIS |
| 2 | F | 1277 | GLN |
| 2 | F | 1333 | GLN |
| 2 | F | 1337 | ASN |
| 2 | F | 1401 | ASN |
| 2 | F | 1431 | HIS |
| 2 | F | 1451 | GLN |
| 2 | F | 1462 | ASN |
| 2 | F | 1559 | GLN |
| 2 | F | 1579 | HIS |
| 2 | F | 1608 | HIS |
| 2 | F | 1620 | ASN |
| 2 | F | 1641 | ASN |
| 1 | G | 60 | HIS |
| 1 | G | 87 | GLN |
| 1 | G | 104 | GLN |
| 1 | G | 132 | HIS |
| 1 | G | 144 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | G | 155 | GLN |
| 1 | G | 161 | GLN |
| 1 | G | 162 | ASN |
| 1 | G | 163 | GLN |
| 1 | G | 356 | ASN |
| 1 | G | 370 | GLN |
| 1 | G | 380 | GLN |
| 1 | G | 390 | ASN |
| 1 | G | 414 | GLN |
| 1 | G | 490 | GLN |
| 1 | G | 558 | GLN |
| 1 | G | 587 | ASN |
| 1 | G | 634 | GLN |
| 1 | G | 639 | GLN |
| 2 | H | 738 | ASN |
| 2 | H | 752 | ASN |
| 2 | H | 762 | ASN |
| 2 | H | 770 | ASN |
| 2 | H | 820 | ASN |
| 2 | H | 834 | GLN |
| 2 | H | 860 | HIS |
| 2 | H | 896 | HIS |
| 2 | H | 897 | HIS |
| 2 | H | 1277 | GLN |
| 2 | H | 1333 | GLN |
| 2 | H | 1337 | ASN |
| 2 | H | 1401 | ASN |
| 2 | H | 1431 | HIS |
| 2 | H | 1451 | GLN |
| 2 | H | 1462 | ASN |
| 2 | H | 1559 | GLN |
| 2 | H | 1579 | HIS |
| 2 | H | 1608 | HIS |
| 2 | H | 1620 | ASN |
| 3 | I | 270 | ASN |
| 3 | I | 329 | ASN |
| 3 | I | 368 | ASN |
| 3 | I | 392 | ASN |
| 3 | I | 411 | GLN |
| 3 | I | 413 | ASN |
| 3 | I | 423 | ASN |
| 3 | I | 466 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 531 | HIS |
| 3 | I | 533 | ASN |
| 3 | I | 591 | GLN |
| 3 | I | 703 | GLN |
| 3 | J | 270 | ASN |
| 3 | J | 329 | ASN |
| 3 | J | 368 | ASN |
| 3 | J | 392 | ASN |
| 3 | J | 411 | GLN |
| 3 | J | 413 | ASN |
| 3 | J | 423 | ASN |
| 3 | J | 435 | ASN |
| 3 | J | 466 | HIS |
| 3 | J | 531 | HIS |
| 3 | J | 533 | ASN |
| 3 | J | 591 | GLN |
| 3 | J | 703 | GLN |
| 3 | K | 270 | ASN |
| 3 | K | 329 | ASN |
| 3 | K | 368 | ASN |
| 3 | K | 392 | ASN |
| 3 | K | 411 | GLN |
| 3 | K | 413 | ASN |
| 3 | K | 423 | ASN |
| 3 | K | 435 | ASN |
| 3 | K | 466 | HIS |
| 3 | K | 531 | HIS |
| 3 | K | 533 | ASN |
| 3 | K | 591 | GLN |
| 3 | K | 703 | GLN |
| 3 | L | 270 | ASN |
| 3 | L | 329 | ASN |
| 3 | L | 368 | ASN |
| 3 | L | 392 | ASN |
| 3 | L | 411 | GLN |
| 3 | L | 413 | ASN |
| 3 | L | 423 | ASN |
| 3 | L | 466 | HIS |
| 3 | L | 531 | HIS |
| 3 | L | 533 | ASN |
| 3 | L | 591 | GLN |
| 3 | L | 703 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M | 11 | GLN |
| 4 | M | 27 | ASN |
| 4 | M | 49 | GLN |
| 4 | M | 69 | GLN |
| 4 | M | 71 | GLN |
| 4 | N | 11 | GLN |
| 4 | N | 27 | ASN |
| 4 | N | 49 | GLN |
| 4 | N | 69 | GLN |
| 4 | N | 71 | GLN |
| 4 | P | 11 | GLN |
| 4 | P | 27 | ASN |
| 4 | P | 49 | GLN |
| 4 | P | 69 | GLN |
| 4 | P | 71 | GLN |
| 4 | Q | 11 | GLN |
| 4 | Q | 27 | ASN |
| 4 | Q | 49 | GLN |
| 4 | Q | 69 | GLN |
| 4 | Q | 71 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

52 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | NAG | O | 1 | 1,5 | 14,14,15 | 0.46 | 0 | 17,19,21 | 0.79 | 0 |
| 5 | NAG | O | 2 | 5 | 14,14,15 | 0.65 | 0 | 17,19,21 | 1.80 | 4 (23%) |
| 5 | BMA | O | 3 | 5 | 11,11,12 | 0.57 | 0 | 15,15,17 | 1.40 | 2 (13%) |
| 5 | BMA | O | 4 | 5 | 11,11,12 | 0.67 | 0 | 15,15,17 | 1.38 | 2 (13%) |
| 5 | NAG | R | 1 | 2,5 | 14,14,15 | 0.55 | 0 | 17,19,21 | 1.11 | 2 (11%) |
| 5 | NAG | R | 2 | 5 | 14,14,15 | 0.54 | 0 | 17,19,21 | 2.19 | 3 (17%) |
| 5 | BMA | R | 3 | 5 | 11,11,12 | 0.95 | 0 | 15,15,17 | 1.97 | 6 (40%) |
| 5 | BMA | R | 4 | 5 | 11,11,12 | 0.73 | 0 | 15,15,17 | 0.81 | 0 |
| 6 | NAG | S | 1 | 1,6 | 14,14,15 | 0.62 | 0 | 17,19,21 | 1.17 | 2 (11%) |
| 6 | NAG | S | 2 | 6 | 14,14,15 | 0.67 | 0 | 17,19,21 | 1.13 | 2 (11%) |
| 6 | BMA | S | 3 | 6 | 11,11,12 | 0.68 | 0 | 15,15,17 | 1.14 | 1 (6%) |
| 6 | BMA | S | 4 | 6 | 11,11,12 | 0.77 | 0 | 15,15,17 | 1.54 | 3 (20%) |
| 6 | BMA | S | 5 | 6 | 11,11,12 | 0.67 | 0 | 15,15,17 | 1.76 | 4 (26%) |
| 5 | NAG | T | 1 | 2,5 | 14,14,15 | 0.50 | 0 | 17,19,21 | 0.83 | 0 |
| 5 | NAG | T | 2 | 5 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.05 | 2 (11%) |
| 5 | BMA | T | 3 | 5 | 11,11,12 | 0.64 | 0 | 15,15,17 | 1.37 | 2 (13%) |
| 5 | BMA | T | 4 | 5 | 11,11,12 | 0.67 | 0 | 15,15,17 | 1.30 | 2 (13%) |
| 5 | NAG | U | 1 | 1,5 | 14,14,15 | 0.56 | 0 | 17,19,21 | 0.87 | 1 (5%) |
| 5 | NAG | U | 2 | 5 | 14,14,15 | 0.60 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 5 | BMA | U | 3 | 5 | 11,11,12 | 0.70 | 0 | 15,15,17 | 1.07 | 1 (6%) |
| 5 | BMA | U | 4 | 5 | 11,11,12 | 0.94 | 1 (9%) | 15,15,17 | 1.70 | 3 (20%) |
| 7 | NAG | V | 1 | 2,7 | 14,14,15 | 0.39 | 0 | 17,19,21 | 1.28 | 3 (17%) |
| 7 | NAG | V | 2 | 7 | 14,14,15 | 0.44 | 0 | 17,19,21 | 1.66 | 4 (23%) |
| 7 | BMA | V | 3 | 7 | 11,11,12 | 0.60 | 0 | 15,15,17 | 1.60 | 4 (26%) |
| 7 | BMA | V | 4 | 7 | 11,11,12 | 1.00 | 1 (9%) | 15,15,17 | 1.68 | 4 (26%) |
| 7 | BMA | V | 5 | 7 | 11,11,12 | 0.67 | 0 | 15,15,17 | 1.86 | 4 (26%) |
| 7 | BMA | V | 6 | 7 | 11,11,12 | 0.71 | 0 | 15,15,17 | 1.05 | 1 (6%) |
| 6 | NAG | W | 1 | 1,6 | 14,14,15 | 0.45 | 0 | 17,19,21 | 1.17 | 1 (5%) |
| 6 | NAG | W | 2 | 6 | 14,14,15 | 0.50 | 0 | 17,19,21 | 2.17 | 4 (23%) |
| 6 | BMA | W | 3 | 6 | 11,11,12 | 0.52 | 0 | 15,15,17 | 2.97 | 6 (40%) |
| 6 | BMA | W | 4 | 6 | 11,11,12 | 0.57 | 0 | 15,15,17 | 4.54 | 6 (40%) |
| 6 | BMA | W | 5 | 6 | 11,11,12 | 0.65 | 0 | 15,15,17 | 1.41 | 2 (13%) |
| 8 | NAG | X | 1 | 8,2 | 14,14,15 | 0.59 | 0 | 17,19,21 | 0.80 | 0 |
| 8 | NAG | X | 2 | 8 | 14,14,15 | 0.49 | 0 | 17,19,21 | 0.79 | 0 |
| 8 | MAN | X | 3 | 8 | 11,11,12 | 0.78 | 0 | 15,15,17 | 1.39 | 2 (13%) |
| 8 | MAN | X | 4 | 8 | 11,11,12 | 0.77 | 0 | 15,15,17 | 1.06 | 2 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 9 | NAG | Y | 1 | 9,3 | 14,14,15 | 0.57 | 0 | 17,19,21 | 1.00 | 2 (11%) |
| 9 | NAG | Y | 2 | 9 | 14,14,15 | 0.63 | 0 | 17,19,21 | 1.03 | 1 (5%) |
| 9 | MAN | Y | 3 | 9 | 11,11,12 | 0.65 | 0 | 15,15,17 | 1.05 | 1 (6%) |
| 10 | NAG | Z | 1 | 10,3 | 14,14,15 | 0.55 | 0 | 17,19,21 | 1.12 | 2 (11%) |
| 10 | NAG | Z | 2 | 10 | 14,14,15 | 0.55 | 0 | 17,19,21 | 0.93 | 1 (5%) |
| 9 | NAG | a | 1 | 9,3 | 14,14,15 | 0.52 | 0 | 17,19,21 | 1.01 | 1 (5%) |
| 9 | NAG | a | 2 | 9 | 14,14,15 | 0.61 | 0 | 17,19,21 | 1.05 | 1 (5%) |
| 9 | MAN | a | 3 | 9 | 11,11,12 | 0.65 | 0 | 15,15,17 | 0.99 | 1 (6%) |
| 11 | NAG | b | 1 | 11,3 | 14,14,15 | 0.63 | 0 | 17,19,21 | 1.04 | 2 (11%) |
| 11 | NAG | b | 2 | 11 | 14,14,15 | 0.71 | 0 | 17,19,21 | 1.39 | 3 (17%) |
| 11 | MAN | b | 3 | 11 | 11,11,12 | 0.57 | 0 | 15,15,17 | 1.91 | 5 (33%) |
| 11 | MAN | b | 4 | 11 | 11,11,12 | 0.61 | 0 | 15,15,17 | 1.15 | 3 (20%) |
| 11 | MAN | b | 5 | 11 | 11,11,12 | 0.76 | 0 | 15,15,17 | 1.64 | 3 (20%) |
| 12 | NAG | c | 1 | 3,12 | 14,14,15 | 0.49 | 0 | 17,19,21 | 0.89 | 0 |
| 12 | NAG | c | 2 | 12 | 14,14,15 | 0.61 | 0 | 17,19,21 | 1.06 | 1 (5%) |
| 12 | BMA | c | 3 | 12 | 11,11,12 | 0.65 | 0 | 15,15,17 | 0.90 | 1 (6%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5 | NAG | O | 1 | 1,5 | 1/1/5/7 | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | O | 2 | 5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | BMA | O | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 5 | BMA | O | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | R | 1 | 2,5 | - | 3/6/23/26 | 0/1/1/1 |
| 5 | NAG | R | 2 | 5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | BMA | R | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 5 | BMA | R | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | S | 1 | 1,6 | - | 3/6/23/26 | 0/1/1/1 |
| 6 | NAG | S | 2 | 6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | BMA | S | 3 | 6 | - | 2/2/19/22 | 0/1/1/1 |
| 6 | BMA | S | 4 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | BMA | S | 5 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | T | 1 | 2,5 | - | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5 | NAG | T | 2 | 5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | BMA | T | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 5 | BMA | T | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | U | 1 | 1,5 | - | 3/6/23/26 | 0/1/1/1 |
| 5 | NAG | U | 2 | 5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | BMA | U | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 5 | BMA | U | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | NAG | V | 1 | 2,7 | 1/1/5/7 | 3/6/23/26 | 0/1/1/1 |
| 7 | NAG | V | 2 | 7 | - | 4/6/23/26 | 0/1/1/1 |
| 7 | BMA | V | 3 | 7 | - | 2/2/19/22 | 0/1/1/1 |
| 7 | BMA | V | 4 | 7 | - | 2/2/19/22 | 0/1/1/1 |
| 7 | BMA | V | 5 | 7 | - | 1/2/19/22 | 0/1/1/1 |
| 7 | BMA | V | 6 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | W | 1 | 1,6 | - | 3/6/23/26 | 0/1/1/1 |
| 6 | NAG | W | 2 | 6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | BMA | W | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | BMA | W | 4 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | BMA | W | 5 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 8 | NAG | X | 1 | 8,2 | - | 3/6/23/26 | 0/1/1/1 |
| 8 | NAG | X | 2 | 8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | MAN | X | 3 | 8 | 1/1/4/5 | 2/2/19/22 | 0/1/1/1 |
| 8 | MAN | X | 4 | 8 | 1/1/4/5 | 2/2/19/22 | 0/1/1/1 |
| 9 | NAG | Y | 1 | 9,3 | - | 3/6/23/26 | 0/1/1/1 |
| 9 | NAG | Y | 2 | 9 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | MAN | Y | 3 | 9 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 10 | NAG | Z | 1 | 10,3 | 1/1/5/7 | 3/6/23/26 | 0/1/1/1 |
| 10 | NAG | Z | 2 | 10 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | a | 1 | 9,3 | - | 3/6/23/26 | 0/1/1/1 |
| 9 | NAG | a | 2 | 9 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | MAN | a | 3 | 9 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 11 | NAG | b | 1 | 11,3 | 1/1/5/7 | 4/6/23/26 | 0/1/1/1 |
| 11 | NAG | b | 2 | 11 | - | 4/6/23/26 | 0/1/1/1 |
| 11 | MAN | b | 3 | 11 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 11 | MAN | b | 4 | 11 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 11 | MAN | b | 5 | 11 | 1/1/4/5 | 2/2/19/22 | 0/1/1/1 |
| 12 | NAG | c | 1 | 3,12 | - | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 12 | NAG | c | 2 | 12 | - | 2/6/23/26 | 0/1/1/1 |
| 12 | BMA | c | 3 | 12 | - | 0/2/19/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5 | U | 4 | BMA | O5-C1 | -2.34 | 1.40 | 1.43 |
| 7 | V | 4 | BMA | O5-C1 | -2.22 | 1.40 | 1.43 |

All (115) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 6 | W | 4 | BMA | C1-C2-C3 | -10.68 | 96.54 | 109.67 |
| 6 | W | 4 | BMA | C3-C4-C5 | -7.10 | 97.58 | 110.24 |
| 5 | R | 2 | NAG | C1-O5-C5 | 7.08 | 121.79 | 112.19 |
| 6 | W | 4 | BMA | C1-O5-C5 | -6.98 | 102.74 | 112.19 |
| 6 | W | 4 | BMA | O5-C5-C6 | 6.86 | 117.96 | 107.20 |
| 6 | W | 3 | BMA | O5-C5-C6 | 6.61 | 117.57 | 107.20 |
| 6 | W | 4 | BMA | O3-C3-C4 | 6.14 | 124.55 | 110.35 |
| 6 | W | 2 | NAG | C1-O5-C5 | 5.96 | 120.26 | 112.19 |
| 6 | W | 3 | BMA | C1-C2-C3 | -5.51 | 102.89 | 109.67 |
| 5 | O | 2 | NAG | C4-C3-C2 | 4.96 | 118.29 | 111.02 |
| 5 | U | 4 | BMA | C1-O5-C5 | -4.45 | 106.16 | 112.19 |
| 7 | V | 5 | BMA | C1-C2-C3 | -4.45 | 104.20 | 109.67 |
| 5 | R | 3 | BMA | C1-C2-C3 | 4.44 | 115.13 | 109.67 |
| 6 | W | 3 | BMA | C6-C5-C4 | -4.37 | 102.77 | 113.00 |
| 6 | S | 5 | BMA | C1-C2-C3 | -4.23 | 104.46 | 109.67 |
| 11 | b | 3 | MAN | O5-C5-C6 | 4.23 | 113.83 | 107.20 |
| 6 | W | 3 | BMA | C1-O5-C5 | -4.03 | 106.73 | 112.19 |
| 8 | X | 3 | MAN | C1-C2-C3 | 3.90 | 114.46 | 109.67 |
| 7 | V | 4 | BMA | C1-C2-C3 | 3.88 | 114.44 | 109.67 |
| 5 | R | 2 | NAG | O5-C1-C2 | 3.79 | 117.27 | 111.29 |
| 5 | R | 3 | BMA | C1-O5-C5 | -3.74 | 107.13 | 112.19 |
| 5 | T | 3 | BMA | C1-O5-C5 | -3.73 | 107.14 | 112.19 |
| 11 | b | 3 | MAN | C1-O5-C5 | -3.72 | 107.16 | 112.19 |
| 11 | b | 5 | MAN | C3-C4-C5 | 3.72 | 116.87 | 110.24 |
| 11 | b | 2 | NAG | C4-C3-C2 | 3.67 | 116.40 | 111.02 |
| 5 | O | 3 | BMA | O5-C5-C6 | 3.63 | 112.90 | 107.20 |
| 7 | V | 3 | BMA | O5-C1-C2 | -3.63 | 105.17 | 110.77 |
| 7 | V | 2 | NAG | C1-O5-C5 | 3.52 | 116.97 | 112.19 |
| 6 | W | 2 | NAG | C4-C3-C2 | -3.48 | 105.92 | 111.02 |
| 7 | V | 5 | BMA | O5-C1-C2 | -3.39 | 105.53 | 110.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7 | V | 2 | NAG | C4-C3-C2 | -3.30 | 106.18 | 111.02 |
| 5 | O | 2 | NAG | C1-O5-C5 | 3.28 | 116.63 | 112.19 |
| 6 | S | 4 | BMA | O3-C3-C4 | -3.27 | 102.78 | 110.35 |
| 6 | W | 5 | BMA | C1-C2-C3 | -3.25 | 105.68 | 109.67 |
| 6 | W | 2 | NAG | O4-C4-C5 | 3.20 | 117.25 | 109.30 |
| 6 | W | 3 | BMA | C3-C4-C5 | 3.15 | 115.85 | 110.24 |
| 5 | O | 4 | BMA | O5-C1-C2 | -3.13 | 105.94 | 110.77 |
| 5 | O | 3 | BMA | C1-O5-C5 | -3.10 | 107.99 | 112.19 |
| 6 | W | 5 | BMA | O5-C1-C2 | -3.07 | 106.03 | 110.77 |
| 6 | S | 4 | BMA | C3-C4-C5 | 3.06 | 115.70 | 110.24 |
| 5 | U | 4 | BMA | O5-C1-C2 | -3.02 | 106.11 | 110.77 |
| 5 | T | 3 | BMA | O5-C5-C6 | 3.02 | 111.93 | 107.20 |
| 5 | O | 4 | BMA | C1-C2-C3 | -2.98 | 106.00 | 109.67 |
| 6 | S | 5 | BMA | O5-C1-C2 | -2.98 | 106.17 | 110.77 |
| 6 | S | 1 | NAG | C3-C4-C5 | 2.97 | 115.54 | 110.24 |
| 5 | T | 4 | BMA | O5-C1-C2 | -2.97 | 106.19 | 110.77 |
| 11 | b | 5 | MAN | O5-C1-C2 | -2.96 | 106.21 | 110.77 |
| 5 | R | 1 | NAG | C1-O5-C5 | 2.93 | 116.17 | 112.19 |
| 9 | Y | 3 | MAN | C1-O5-C5 | -2.91 | 108.24 | 112.19 |
| 7 | V | 4 | BMA | C2-C3-C4 | 2.90 | 115.91 | 110.89 |
| 5 | U | 4 | BMA | C1-C2-C3 | -2.88 | 106.13 | 109.67 |
| 7 | V | 2 | NAG | O4-C4-C3 | 2.82 | 116.87 | 110.35 |
| 6 | W | 1 | NAG | C4-C3-C2 | 2.82 | 115.15 | 111.02 |
| 11 | b | 2 | NAG | C3-C4-C5 | 2.78 | 115.19 | 110.24 |
| 5 | T | 4 | BMA | C1-C2-C3 | -2.77 | 106.25 | 109.67 |
| 11 | b | 3 | MAN | C1-C2-C3 | -2.77 | 106.26 | 109.67 |
| 11 | b | 3 | MAN | O3-C3-C2 | 2.75 | 115.25 | 109.99 |
| 11 | b | 1 | NAG | C3-C4-C5 | 2.70 | 115.05 | 110.24 |
| 6 | S | 5 | BMA | C1-O5-C5 | -2.69 | 108.54 | 112.19 |
| 12 | c | 2 | NAG | C4-C3-C2 | 2.64 | 114.89 | 111.02 |
| 9 | a | 1 | NAG | C1-O5-C5 | 2.61 | 115.73 | 112.19 |
| 7 | V | 5 | BMA | C3-C4-C5 | 2.61 | 114.89 | 110.24 |
| 7 | V | 2 | NAG | O5-C5-C6 | 2.60 | 111.27 | 107.20 |
| 5 | O | 2 | NAG | C3-C4-C5 | 2.60 | 114.87 | 110.24 |
| 10 | Z | 1 | NAG | C3-C4-C5 | 2.58 | 114.84 | 110.24 |
| 9 | a | 2 | NAG | C4-C3-C2 | 2.58 | 114.79 | 111.02 |
| 6 | S | 3 | BMA | C1-O5-C5 | -2.56 | 108.72 | 112.19 |
| 9 | a | 3 | MAN | C1-O5-C5 | -2.56 | 108.73 | 112.19 |
| 9 | Y | 2 | NAG | C4-C3-C2 | 2.55 | 114.76 | 111.02 |
| 7 | V | 4 | BMA | C1-O5-C5 | -2.54 | 108.75 | 112.19 |
| 6 | W | 3 | BMA | O6-C6-C5 | 2.50 | 119.86 | 111.29 |
| 6 | W | 2 | NAG | O5-C1-C2 | 2.48 | 115.21 | 111.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7 | V | 1 | NAG | O5-C1-C2 | -2.48 | 107.37 | 111.29 |
| 5 | U | 2 | NAG | C1-O5-C5 | 2.46 | 115.53 | 112.19 |
| 10 | Z | 2 | NAG | C1-O5-C5 | 2.46 | 115.53 | 112.19 |
| 7 | V | 5 | BMA | C1-O5-C5 | -2.45 | 108.87 | 112.19 |
| 6 | S | 4 | BMA | C1-O5-C5 | -2.44 | 108.88 | 112.19 |
| 11 | b | 4 | MAN | O5-C5-C6 | 2.44 | 111.02 | 107.20 |
| 10 | Z | 1 | NAG | C4-C3-C2 | 2.43 | 114.57 | 111.02 |
| 5 | U | 2 | NAG | O5-C1-C2 | 2.42 | 115.11 | 111.29 |
| 5 | U | 3 | BMA | C1-O5-C5 | -2.42 | 108.92 | 112.19 |
| 6 | S | 5 | BMA | C3-C4-C5 | 2.39 | 114.50 | 110.24 |
| 5 | R | 3 | BMA | O5-C5-C6 | 2.38 | 110.93 | 107.20 |
| 7 | V | 3 | BMA | C2-C3-C4 | -2.36 | 106.81 | 110.89 |
| 5 | R | 3 | BMA | C2-C3-C4 | 2.36 | 114.97 | 110.89 |
| 8 | X | 4 | MAN | C1-O5-C5 | -2.34 | 109.03 | 112.19 |
| 6 | S | 2 | NAG | C4-C3-C2 | 2.31 | 114.41 | 111.02 |
| 7 | V | 3 | BMA | C1-C2-C3 | -2.30 | 106.84 | 109.67 |
| 6 | S | 1 | NAG | C1-O5-C5 | 2.29 | 115.30 | 112.19 |
| 7 | V | 1 | NAG | O4-C4-C5 | 2.29 | 114.99 | 109.30 |
| 5 | T | 2 | NAG | C1-O5-C5 | 2.29 | 115.29 | 112.19 |
| 5 | R | 3 | BMA | O5-C5-C4 | -2.28 | 105.29 | 110.83 |
| 5 | O | 2 | NAG | O4-C4-C3 | -2.27 | 105.10 | 110.35 |
| 7 | V | 6 | BMA | O5-C1-C2 | -2.26 | 107.29 | 110.77 |
| 11 | b | 5 | MAN | C6-C5-C4 | -2.22 | 107.81 | 113.00 |
| 7 | V | 1 | NAG | C4-C3-C2 | -2.21 | 107.77 | 111.02 |
| 6 | W | 4 | BMA | O3-C3-C2 | 2.20 | 114.21 | 109.99 |
| 9 | Y | 1 | NAG | C3-C4-C5 | 2.17 | 114.11 | 110.24 |
| 8 | X | 4 | MAN | O5-C1-C2 | -2.17 | 107.43 | 110.77 |
| 8 | X | 3 | MAN | O5-C5-C6 | 2.16 | 110.58 | 107.20 |
| 12 | c | 3 | BMA | C1-O5-C5 | -2.16 | 109.27 | 112.19 |
| 9 | Y | 1 | NAG | C1-O5-C5 | 2.15 | 115.11 | 112.19 |
| 7 | V | 3 | BMA | C6-C5-C4 | -2.12 | 108.03 | 113.00 |
| 7 | V | 4 | BMA | C3-C4-C5 | 2.12 | 114.02 | 110.24 |
| 5 | R | 1 | NAG | C3-C4-C5 | 2.11 | 113.99 | 110.24 |
| 11 | b | 3 | MAN | C2-C3-C4 | -2.10 | 107.26 | 110.89 |
| 6 | S | 2 | NAG | O5-C1-C2 | 2.09 | 114.58 | 111.29 |
| 11 | b | 4 | MAN | C3-C4-C5 | 2.07 | 113.94 | 110.24 |
| 5 | R | 2 | NAG | C6-C5-C4 | -2.07 | 108.15 | 113.00 |
| 5 | R | 3 | BMA | C6-C5-C4 | 2.05 | 117.80 | 113.00 |
| 11 | b | 2 | NAG | O4-C4-C3 | -2.04 | 105.62 | 110.35 |
| 11 | b | 4 | MAN | C1-O5-C5 | 2.04 | 114.96 | 112.19 |
| 5 | T | 2 | NAG | C4-C3-C2 | 2.03 | 114.00 | 111.02 |
| 11 | b | 1 | NAG | C4-C3-C2 | 2.02 | 113.98 | 111.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 5 | U | 1 | NAG | C3-C4-C5 | 2.00 | 113.81 | 110.24 |

All (11) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11 | b | 3 | MAN | C1 |
| 8 | X | 3 | MAN | C1 |
| 7 | V | 1 | NAG | C1 |
| 11 | b | 4 | MAN | C1 |
| 8 | X | 4 | MAN | C1 |
| 5 | O | 1 | NAG | C1 |
| 11 | b | 1 | NAG | C1 |
| 9 | a | 3 | MAN | C1 |
| 9 | Y | 3 | MAN | C1 |
| 10 | Z | 1 | NAG | C1 |
| 11 | b | 5 | MAN | C1 |

All (94) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 8 | X | 1 | NAG | C3-C2-N2-C7 |
| 8 | X | 1 | NAG | C8-C7-N2-C2 |
| 8 | X | 1 | NAG | O7-C7-N2-C2 |
| 7 | V | 1 | NAG | C8-C7-N2-C2 |
| 7 | V | 1 | NAG | O7-C7-N2-C2 |
| 6 | W | 1 | NAG | C8-C7-N2-C2 |
| 6 | W | 1 | NAG | O7-C7-N2-C2 |
| 5 | T | 1 | NAG | C8-C7-N2-C2 |
| 5 | T | 1 | NAG | O7-C7-N2-C2 |
| 5 | R | 1 | NAG | C8-C7-N2-C2 |
| 5 | R | 1 | NAG | O7-C7-N2-C2 |
| 5 | U | 1 | NAG | C8-C7-N2-C2 |
| 5 | U | 1 | NAG | O7-C7-N2-C2 |
| 12 | c | 1 | NAG | O7-C7-N2-C2 |
| 6 | S | 1 | NAG | C1-C2-N2-C7 |
| 6 | S | 1 | NAG | C8-C7-N2-C2 |
| 6 | S | 1 | NAG | O7-C7-N2-C2 |
| 5 | O | 2 | NAG | C8-C7-N2-C2 |
| 5 | O | 2 | NAG | O7-C7-N2-C2 |
| 12 | c | 2 | NAG | C8-C7-N2-C2 |
| 9 | Y | 2 | NAG | C8-C7-N2-C2 |
| 12 | c | 1 | NAG | C8-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 12 | c | 2 | NAG | O7-C7-N2-C2 |
| 9 | a | 2 | NAG | C8-C7-N2-C2 |
| 5 | U | 3 | BMA | O5-C5-C6-O6 |
| 9 | Y | 1 | NAG | C8-C7-N2-C2 |
| 9 | Y | 1 | NAG | O7-C7-N2-C2 |
| 9 | Y | 2 | NAG | O7-C7-N2-C2 |
| 10 | Z | 1 | NAG | C8-C7-N2-C2 |
| 10 | Z | 1 | NAG | O7-C7-N2-C2 |
| 9 | a | 2 | NAG | O7-C7-N2-C2 |
| 7 | V | 4 | BMA | O5-C5-C6-O6 |
| 5 | O | 2 | NAG | O5-C5-C6-O6 |
| 7 | V | 2 | NAG | C4-C5-C6-O6 |
| 7 | V | 3 | BMA | O5-C5-C6-O6 |
| 11 | b | 2 | NAG | O5-C5-C6-O6 |
| 6 | S | 2 | NAG | C8-C7-N2-C2 |
| 6 | S | 2 | NAG | O7-C7-N2-C2 |
| 5 | O | 1 | NAG | C8-C7-N2-C2 |
| 11 | b | 1 | NAG | C8-C7-N2-C2 |
| 7 | V | 1 | NAG | C1-C2-N2-C7 |
| 6 | W | 1 | NAG | C1-C2-N2-C7 |
| 5 | T | 1 | NAG | C1-C2-N2-C7 |
| 5 | R | 1 | NAG | C1-C2-N2-C7 |
| 5 | U | 1 | NAG | C1-C2-N2-C7 |
| 6 | S | 3 | BMA | C4-C5-C6-O6 |
| 11 | b | 2 | NAG | C4-C5-C6-O6 |
| 11 | b | 5 | MAN | C4-C5-C6-O6 |
| 5 | U | 3 | BMA | C4-C5-C6-O6 |
| 6 | W | 2 | NAG | C8-C7-N2-C2 |
| 6 | W | 2 | NAG | O7-C7-N2-C2 |
| 5 | U | 2 | NAG | C8-C7-N2-C2 |
| 5 | U | 2 | NAG | O7-C7-N2-C2 |
| 8 | X | 2 | NAG | C8-C7-N2-C2 |
| 8 | X | 2 | NAG | O7-C7-N2-C2 |
| 5 | O | 1 | NAG | O7-C7-N2-C2 |
| 7 | V | 2 | NAG | C8-C7-N2-C2 |
| 7 | V | 2 | NAG | O7-C7-N2-C2 |
| 11 | b | 1 | NAG | O7-C7-N2-C2 |
| 9 | a | 1 | NAG | C8-C7-N2-C2 |
| 5 | T | 2 | NAG | C8-C7-N2-C2 |
| 5 | T | 2 | NAG | O7-C7-N2-C2 |
| 5 | R | 2 | NAG | C8-C7-N2-C2 |
| 5 | R | 2 | NAG | O7-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 11 | b | 2 | NAG | C8-C7-N2-C2 |
| 11 | b | 2 | NAG | O7-C7-N2-C2 |
| 10 | Z | 2 | NAG | C8-C7-N2-C2 |
| 10 | Z | 2 | NAG | O7-C7-N2-C2 |
| 5 | O | 2 | NAG | C4-C5-C6-O6 |
| 5 | O | 3 | BMA | C4-C5-C6-O6 |
| 9 | Y | 1 | NAG | C1-C2-N2-C7 |
| 10 | Z | 1 | NAG | C1-C2-N2-C7 |
| 12 | c | 1 | NAG | C1-C2-N2-C7 |
| 9 | a | 1 | NAG | O7-C7-N2-C2 |
| 7 | V | 3 | BMA | C4-C5-C6-O6 |
| 7 | V | 2 | NAG | O5-C5-C6-O6 |
| 6 | S | 3 | BMA | O5-C5-C6-O6 |
| 7 | V | 4 | BMA | C4-C5-C6-O6 |
| 11 | b | 5 | MAN | O5-C5-C6-O6 |
| 8 | X | 3 | MAN | O5-C5-C6-O6 |
| 11 | b | 1 | NAG | C1-C2-N2-C7 |
| 9 | a | 1 | NAG | C1-C2-N2-C7 |
| 5 | T | 3 | BMA | C4-C5-C6-O6 |
| 8 | X | 3 | MAN | C4-C5-C6-O6 |
| 5 | O | 3 | BMA | O5-C5-C6-O6 |
| 8 | X | 4 | MAN | C4-C5-C6-O6 |
| 5 | R | 3 | BMA | C4-C5-C6-O6 |
| 8 | X | 4 | MAN | O5-C5-C6-O6 |
| 6 | S | 2 | NAG | O5-C5-C6-O6 |
| 5 | R | 3 | BMA | O5-C5-C6-O6 |
| 5 | T | 3 | BMA | O5-C5-C6-O6 |
| 6 | S | 2 | NAG | C4-C5-C6-O6 |
| 11 | b | 1 | NAG | C4-C5-C6-O6 |
| 7 | V | 5 | BMA | C4-C5-C6-O6 |

There are no ring outliers.

23 monomers are involved in 18 short contacts:

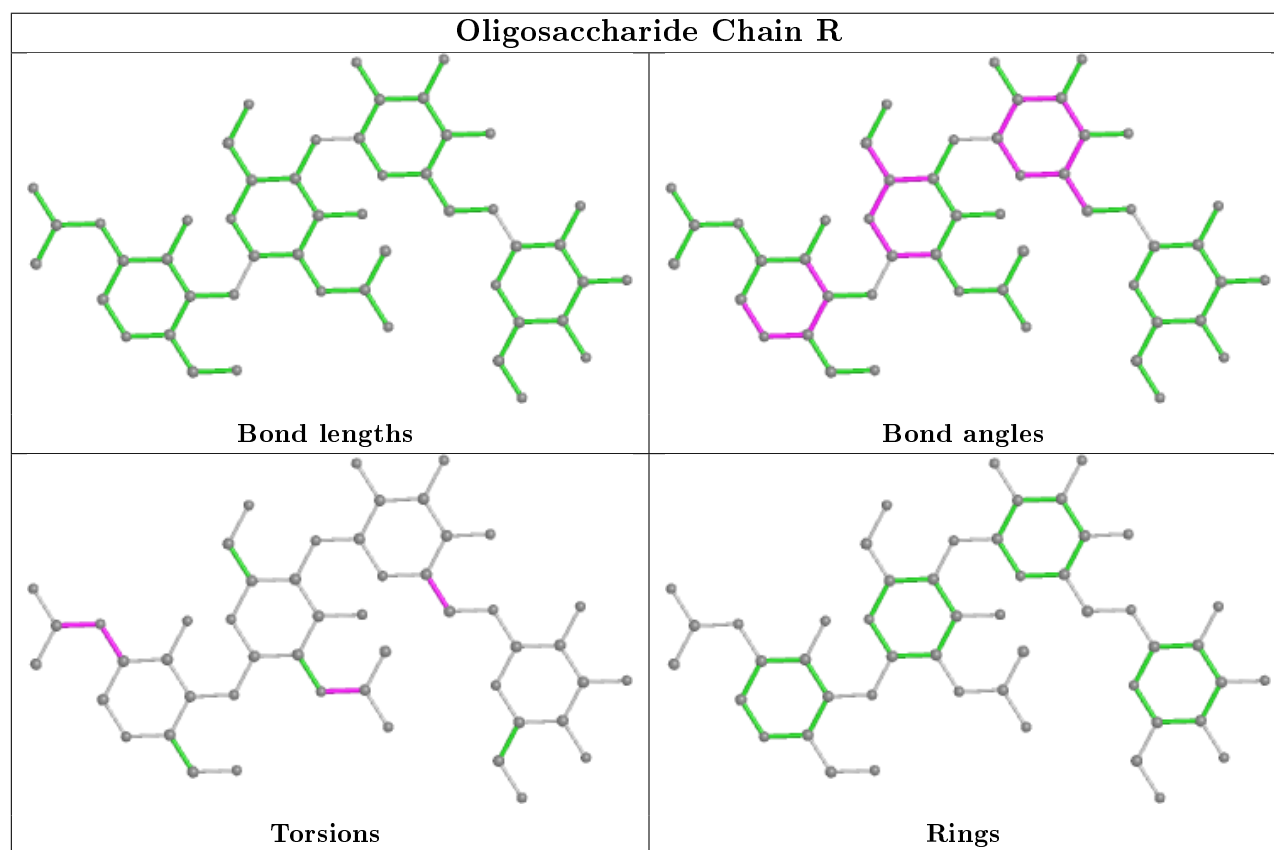
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7 | V | 4 | BMA | 2 | 0 |
| 5 | U | 3 | BMA | 1 | 0 |
| 6 | W | 2 | NAG | 3 | 0 |
| 5 | U | 2 | NAG | 1 | 0 |
| 8 | X | 3 | MAN | 1 | 0 |
| 9 | Y | 1 | NAG | 1 | 0 |
| 8 | X | 2 | NAG | 1 | 0 |

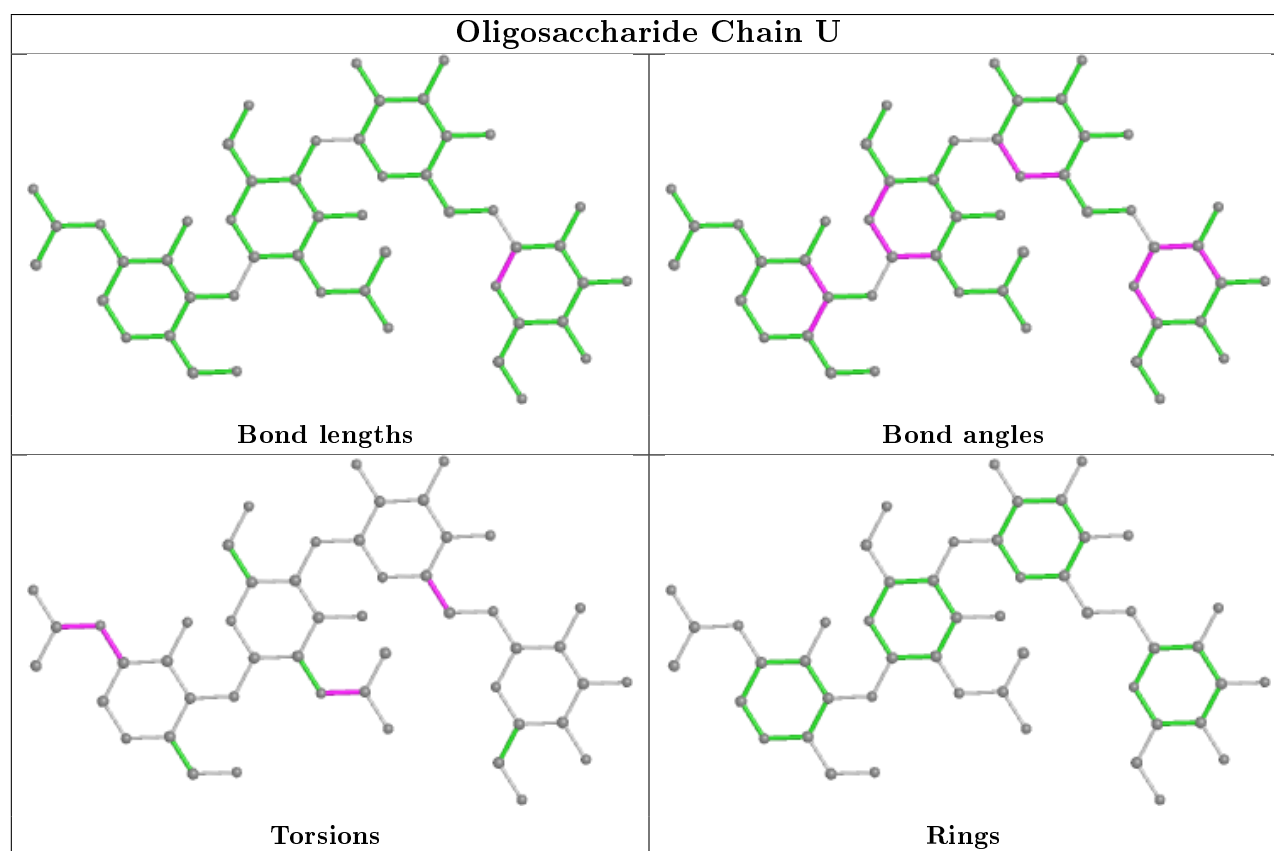
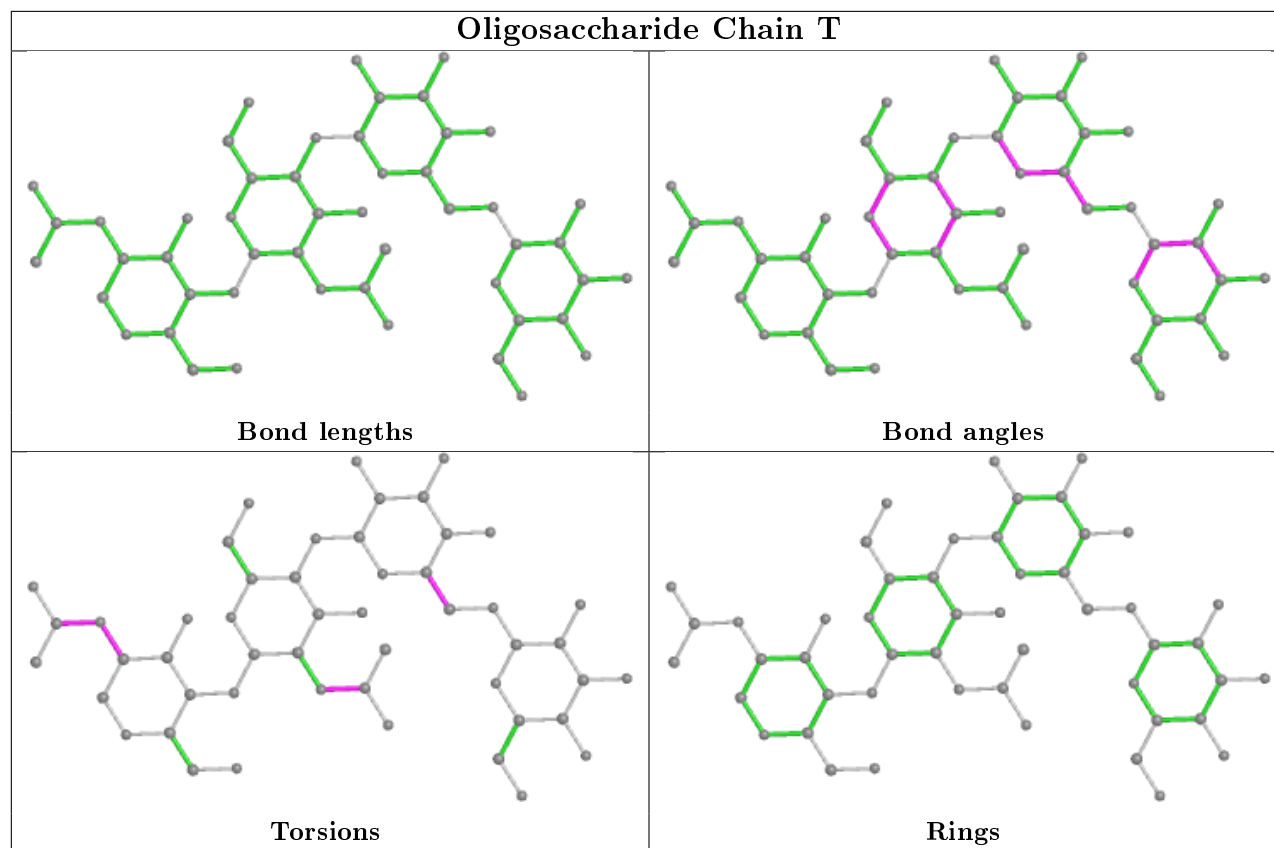
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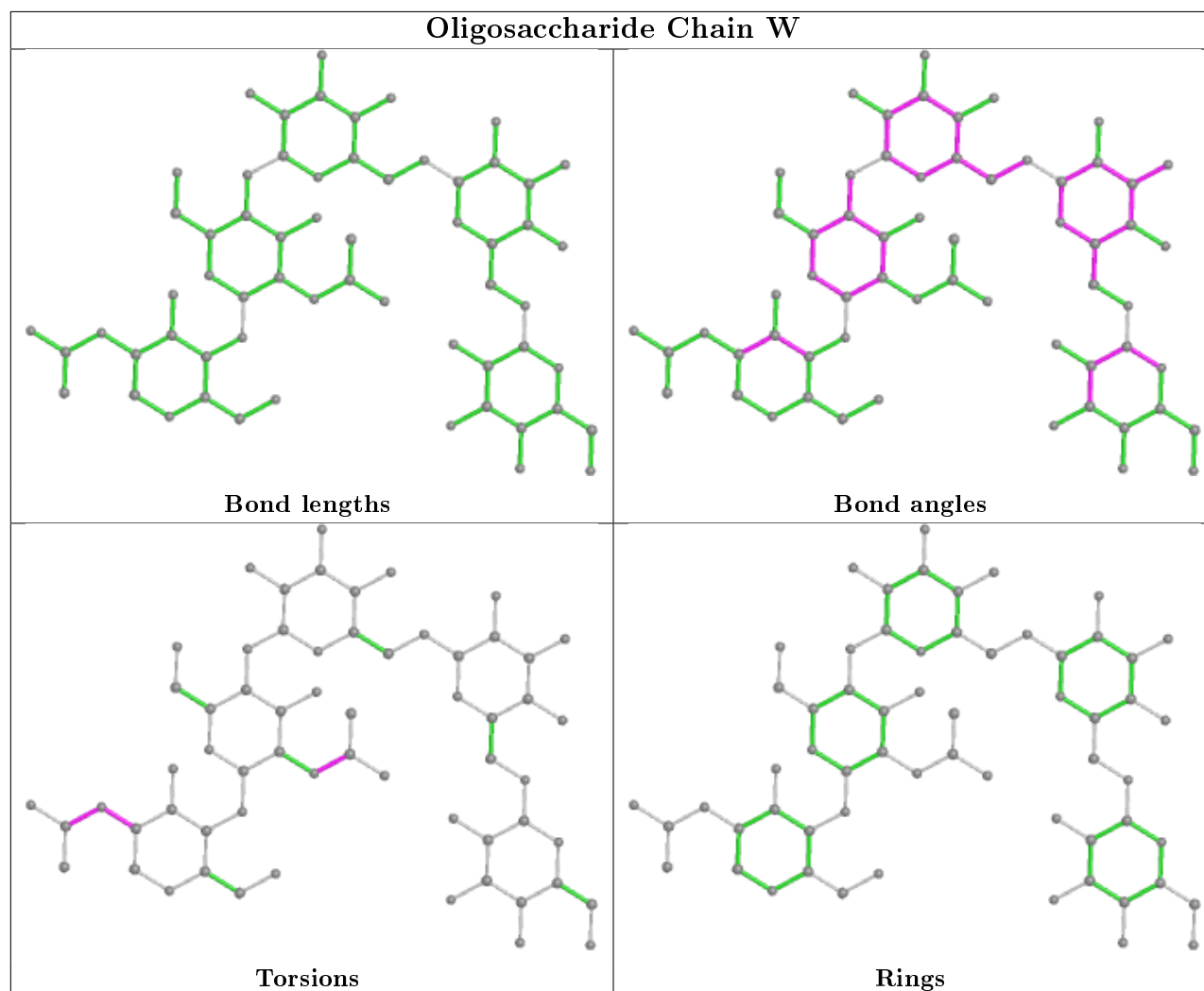
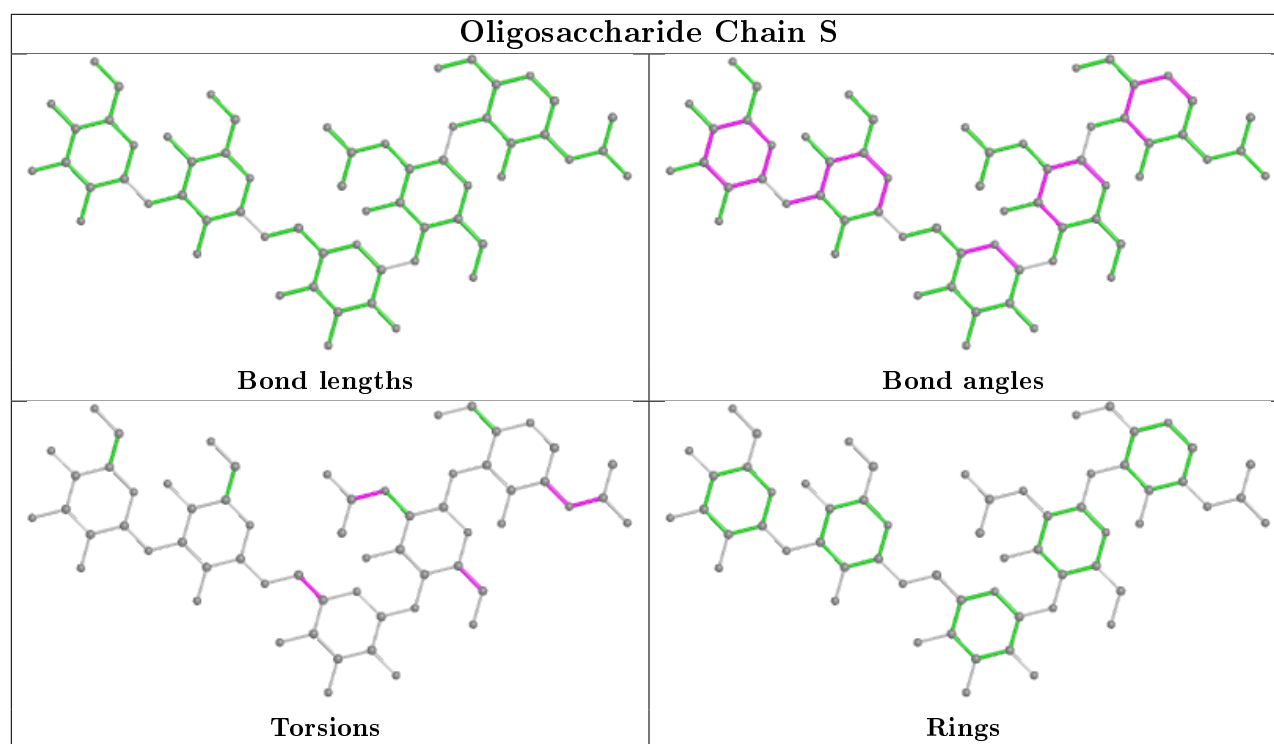
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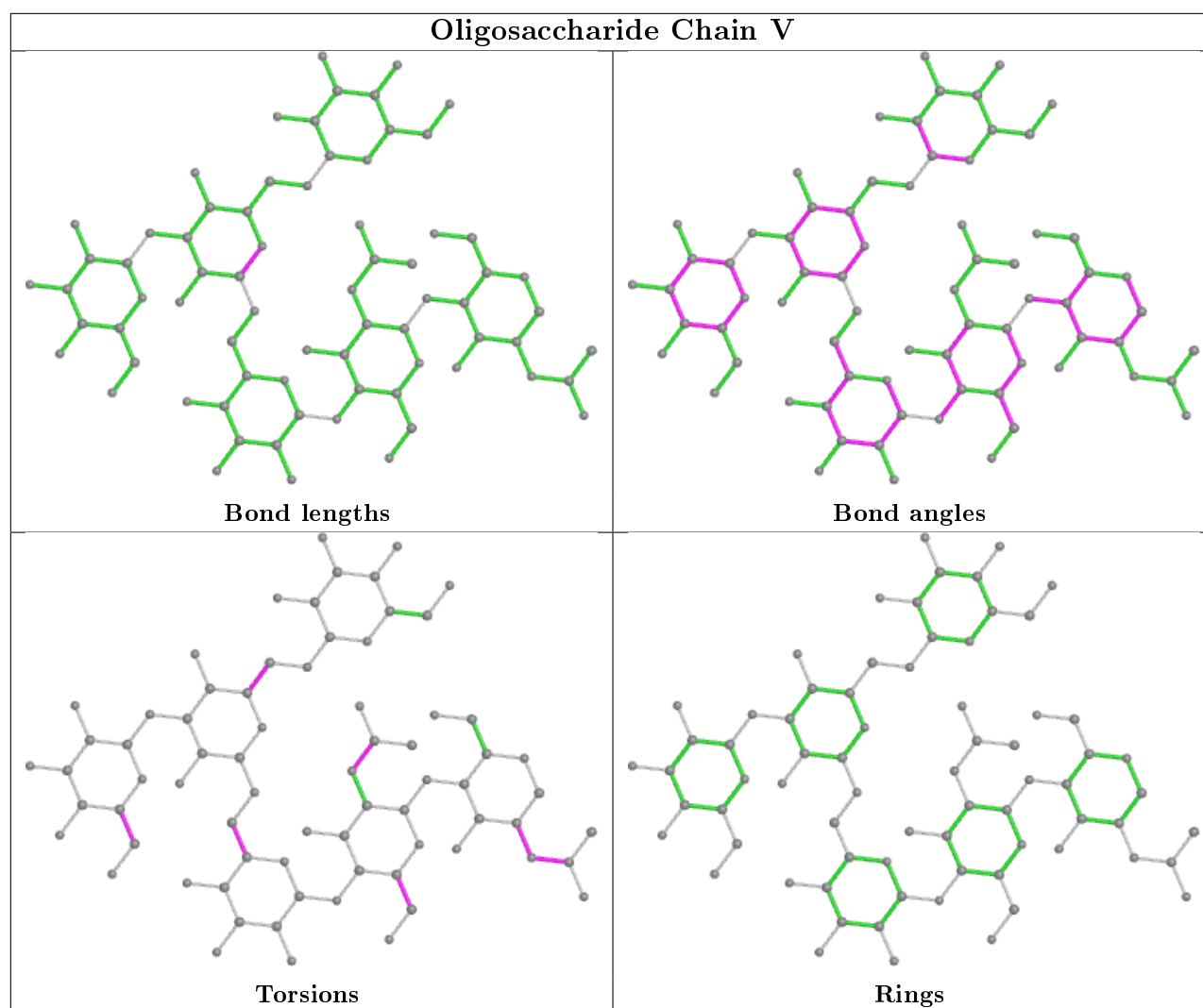
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6 | W | 1 | NAG | 1 | 0 |
| 8 | X | 4 | MAN | 1 | 0 |
| 6 | S | 2 | NAG | 1 | 0 |
| 5 | O | 1 | NAG | 1 | 0 |
| 5 | U | 4 | BMA | 1 | 0 |
| 5 | T | 2 | NAG | 1 | 0 |
| 6 | W | 3 | BMA | 2 | 0 |
| 9 | Y | 2 | NAG | 2 | 0 |
| 7 | V | 3 | BMA | 1 | 0 |
| 5 | T | 1 | NAG | 1 | 0 |
| 7 | V | 6 | BMA | 1 | 0 |
| 5 | R | 1 | NAG | 1 | 0 |
| 5 | U | 1 | NAG | 2 | 0 |
| 6 | W | 4 | BMA | 2 | 0 |
| 6 | S | 1 | NAG | 1 | 0 |
| 5 | O | 2 | NAG | 1 | 0 |

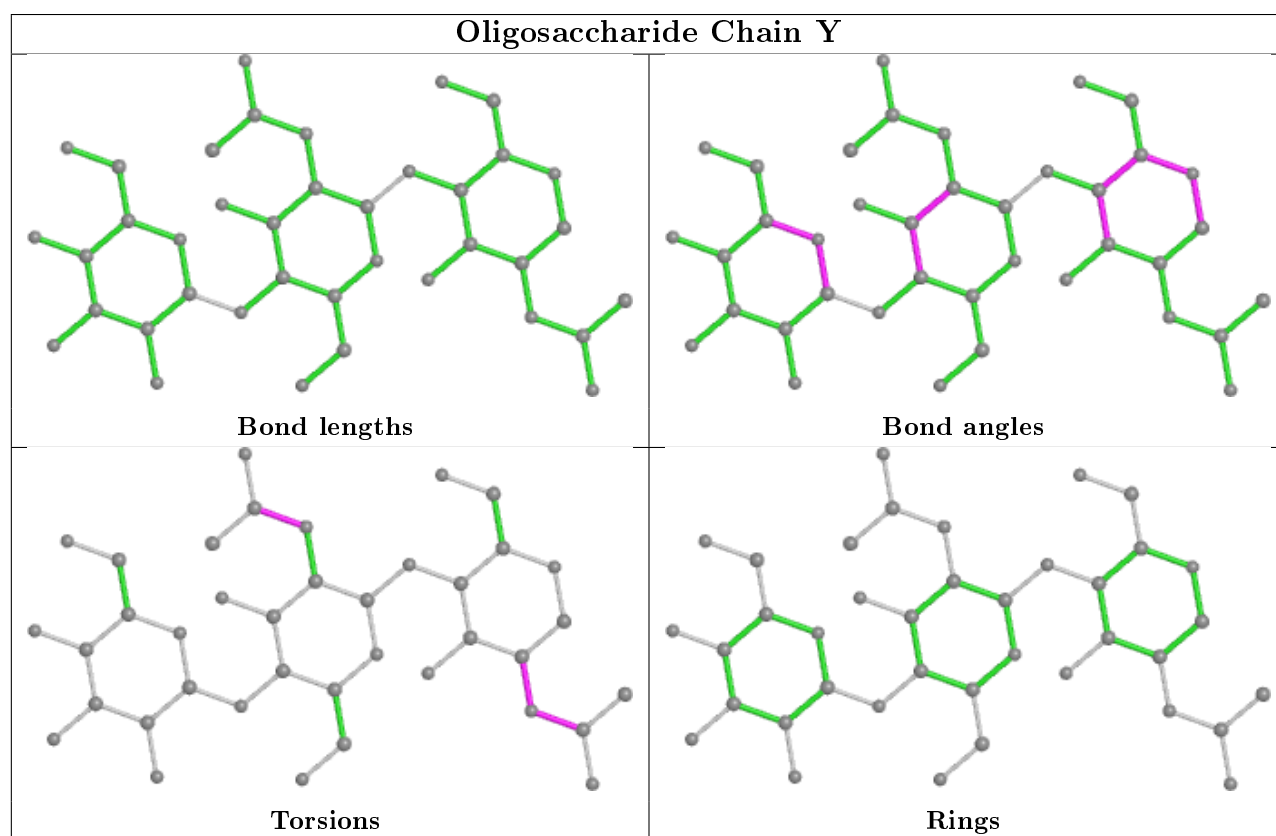
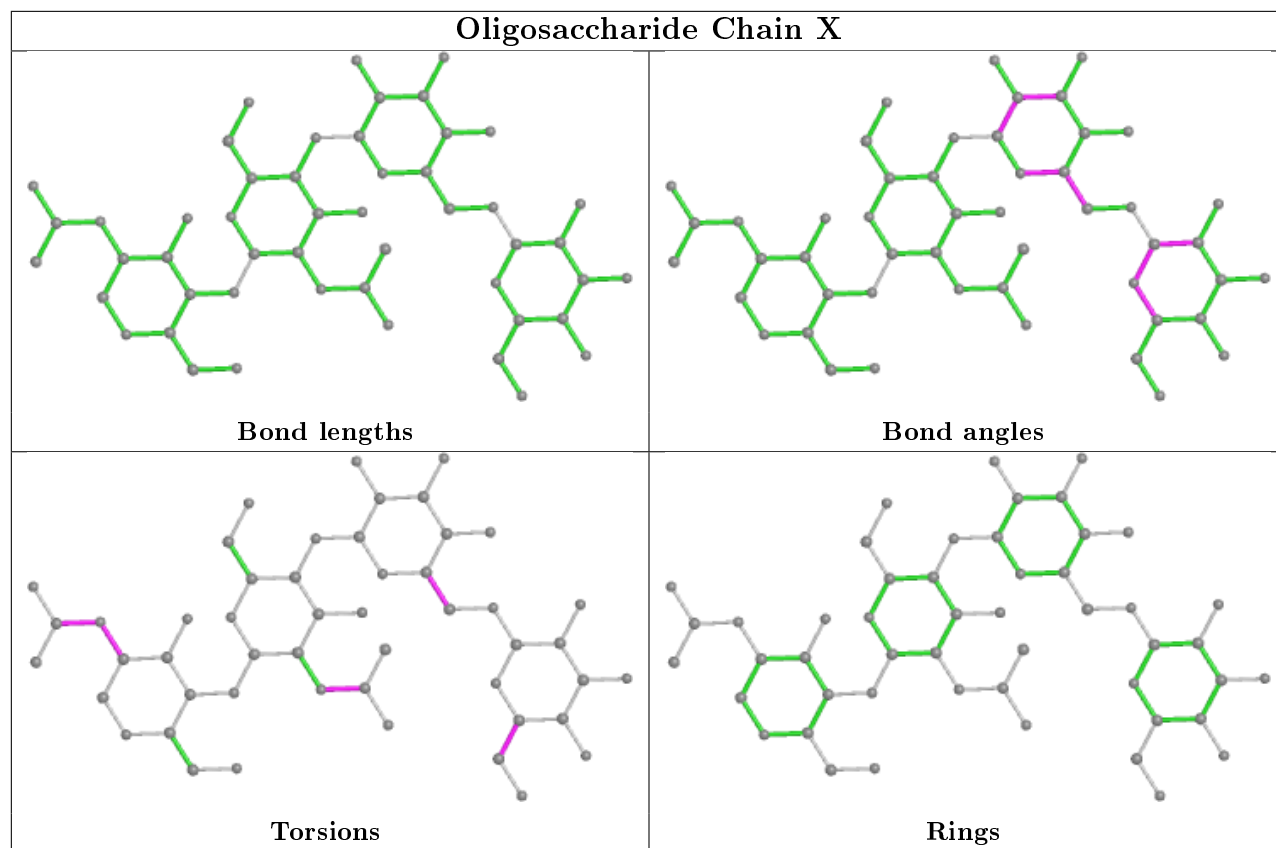
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

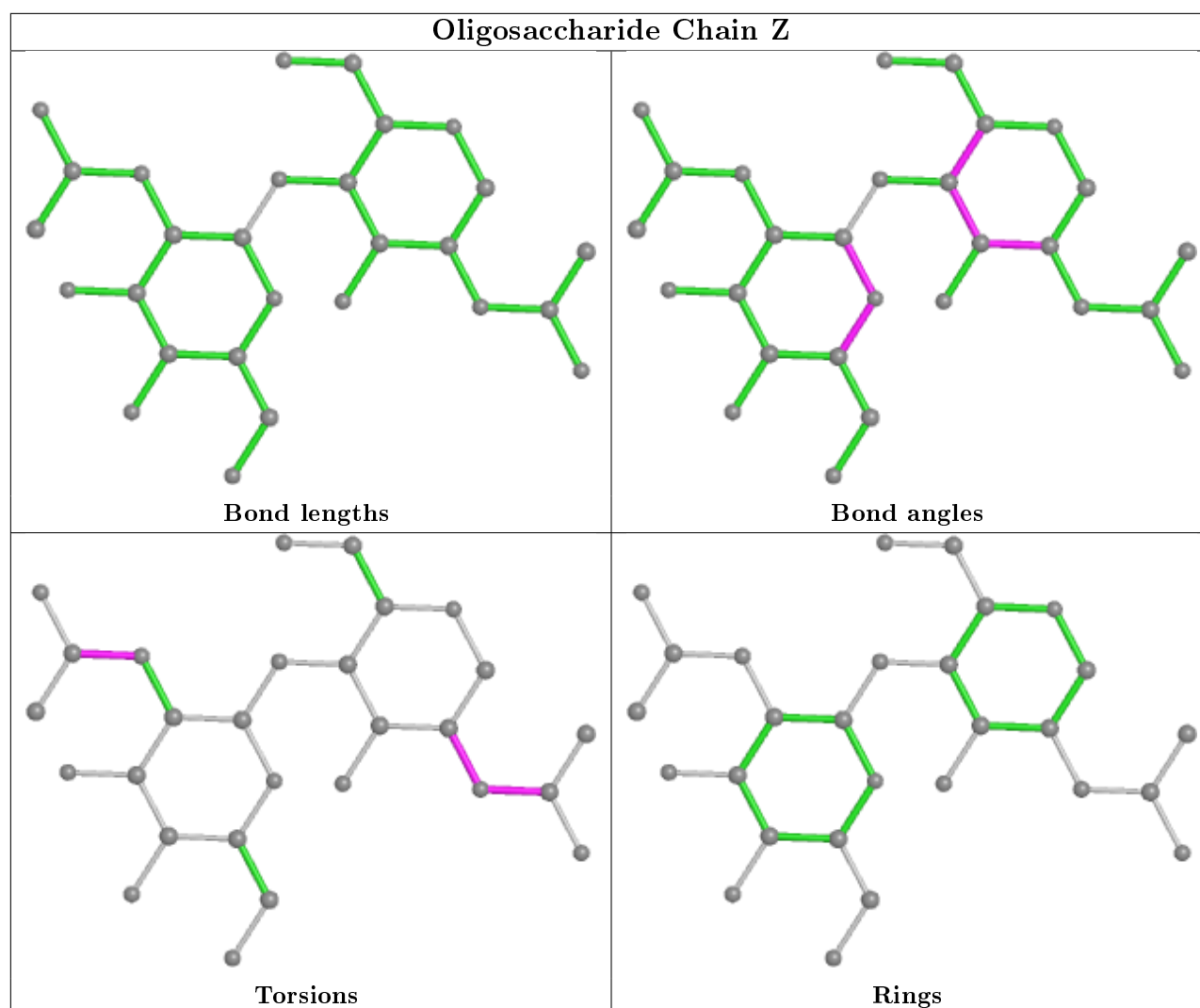












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 13 | BMA | B | 2646 | - | 11,11,12 | 0.74 | 0 | 15,15,17 | 1.42 | 3 (20%) |
| 16 | NAG | L | 1746 | 3 | 14,14,15 | 0.52 | 0 | 17,19,21 | 0.69 | 0 |
| 16 | NAG | K | 1749 | 3 | 14,14,15 | 0.52 | 0 | 17,19,21 | 1.79 | 2 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 13 | BMA | K | 1747 | - | 11,11,12 | 0.81 | 0 | 15,15,17 | 1.93 | 4 (26%) |
| 14 | MAN | G | 1651 | - | 11,11,12 | 0.83 | 1 (9%) | 15,15,17 | 1.71 | 4 (26%) |

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 |
|-----|------|-------|------|------|---------|-----------|---------|
| 13 | BMA | B | 2646 | - | - | 0/2/19/22 | 0/1/1/1 |
| 16 | NAG | K | 1749 | 3 | 1/1/5/7 | 3/6/23/26 | 0/1/1/1 |
| 16 | NAG | L | 1746 | 3 | 1/1/5/7 | 3/6/23/26 | 0/1/1/1 |
| 14 | MAN | G | 1651 | - | - | 0/2/19/22 | 0/1/1/1 |
| 13 | BMA | K | 1747 | - | - | 0/2/19/22 | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 14 | G | 1651 | MAN | O5-C1 | -2.03 | 1.40 | 1.43 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 13 | K | 1747 | BMA | C1-O5-C5 | -5.03 | 105.37 | 112.19 |
| 16 | K | 1749 | NAG | O5-C1-C2 | -4.75 | 103.78 | 111.29 |
| 14 | G | 1651 | MAN | C1-C2-C3 | -4.04 | 104.70 | 109.67 |
| 16 | K | 1749 | NAG | C1-C2-N2 | 3.83 | 117.04 | 110.49 |
| 13 | K | 1747 | BMA | C1-C2-C3 | -3.78 | 105.01 | 109.67 |
| 13 | B | 2646 | BMA | C1-C2-C3 | -3.38 | 105.52 | 109.67 |
| 14 | G | 1651 | MAN | O5-C1-C2 | 3.00 | 115.41 | 110.77 |
| 14 | G | 1651 | MAN | C1-O5-C5 | -3.00 | 108.12 | 112.19 |
| 13 | K | 1747 | BMA | O5-C1-C2 | 2.67 | 114.90 | 110.77 |
| 14 | G | 1651 | MAN | C3-C4-C5 | 2.65 | 114.96 | 110.24 |
| 13 | B | 2646 | BMA | O5-C1-C2 | 2.63 | 114.83 | 110.77 |
| 13 | B | 2646 | BMA | C1-O5-C5 | -2.15 | 109.28 | 112.19 |
| 13 | K | 1747 | BMA | C3-C4-C5 | 2.13 | 114.03 | 110.24 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 16 | K | 1749 | NAG | C1 |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 16 | L | 1746 | NAG | C1 |

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 16 | K | 1749 | NAG | C8-C7-N2-C2 |
| 16 | K | 1749 | NAG | O7-C7-N2-C2 |
| 16 | L | 1746 | NAG | C8-C7-N2-C2 |
| 16 | L | 1746 | NAG | O7-C7-N2-C2 |
| 16 | K | 1749 | NAG | C1-C2-N2-C7 |
| 16 | L | 1746 | NAG | C1-C2-N2-C7 |

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 16 | K | 1749 | NAG | 3 | 0 |
| 14 | G | 1651 | MAN | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2 | H | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | H | 1500:LYS | C | 1501:SER | N | 3.64 |
| 1 | H | 988:CYS | C | 989:GLY | N | 2.97 |

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | A | 638/645 (98%) | 0.24 | 11 (1%) 70 60 | 87, 142, 190, 237 | 0 |
| 1 | C | 638/645 (98%) | 0.27 | 10 (1%) 72 62 | 80, 127, 176, 228 | 0 |
| 1 | E | 638/645 (98%) | 0.28 | 12 (1%) 66 57 | 84, 142, 196, 245 | 0 |
| 1 | G | 638/645 (98%) | 0.53 | 56 (8%) 10 7 | 93, 180, 241, 267 | 0 |
| 2 | B | 901/915 (98%) | 0.17 | 12 (1%) 77 68 | 91, 167, 229, 260 | 0 |
| 2 | D | 901/915 (98%) | 0.23 | 13 (1%) 75 66 | 81, 155, 216, 266 | 0 |
| 2 | F | 900/915 (98%) | 0.40 | 49 (5%) 25 21 | 96, 179, 284, 329 | 0 |
| 2 | H | 605/915 (66%) | 0.38 | 28 (4%) 32 26 | 98, 162, 231, 294 | 0 |
| 3 | I | 507/507 (100%) | 0.17 | 4 (0%) 86 79 | 93, 142, 197, 240 | 0 |
| 3 | J | 507/507 (100%) | 0.15 | 10 (1%) 65 55 | 127, 170, 220, 261 | 0 |
| 3 | K | 507/507 (100%) | 0.20 | 21 (4%) 37 29 | 132, 183, 230, 284 | 0 |
| 3 | L | 507/507 (100%) | 0.15 | 4 (0%) 86 79 | 101, 144, 194, 239 | 0 |
| 4 | M | 84/92 (91%) | 0.34 | 2 (2%) 59 48 | 87, 110, 186, 221 | 0 |
| 4 | N | 84/92 (91%) | 0.33 | 3 (3%) 42 33 | 97, 116, 189, 227 | 0 |
| 4 | P | 84/92 (91%) | 0.23 | 2 (2%) 59 48 | 100, 124, 176, 211 | 0 |
| 4 | Q | 84/92 (91%) | 0.20 | 1 (1%) 79 70 | 100, 119, 186, 200 | 0 |
| All | All | 8223/8636 (95%) | 0.27 | 238 (2%) 51 40 | 80, 155, 228, 329 | 0 |

All (238) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 421 | ALA | 8.9 |
| 1 | G | 529 | VAL | 7.9 |
| 1 | G | 509 | LEU | 7.7 |
| 1 | G | 437 | SER | 7.0 |
| 1 | C | 645 | ALA | 6.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | G | 609 | SER | 5.5 |
| 1 | G | 373 | ASP | 5.4 |
| 1 | A | 645 | ALA | 5.2 |
| 4 | M | 85 | TYR | 4.9 |
| 1 | G | 400 | ILE | 4.8 |
| 1 | G | 511 | ALA | 4.7 |
| 1 | G | 608 | GLY | 4.7 |
| 2 | F | 1501 | SER | 4.7 |
| 2 | F | 1120 | ALA | 4.6 |
| 1 | G | 436 | LEU | 4.5 |
| 1 | G | 626 | SER | 4.5 |
| 2 | F | 1078 | LEU | 4.5 |
| 3 | J | 235 | LYS | 4.5 |
| 4 | N | 85 | TYR | 4.4 |
| 1 | G | 528 | SER | 4.4 |
| 2 | H | 1593 | LYS | 4.3 |
| 1 | G | 374 | THR | 4.3 |
| 2 | F | 1122 | THR | 4.3 |
| 1 | G | 510 | VAL | 4.3 |
| 2 | F | 1049 | LYS | 4.1 |
| 1 | G | 399 | SER | 4.1 |
| 1 | G | 71 | ASN | 4.0 |
| 1 | G | 339 | PRO | 4.0 |
| 2 | H | 1501 | SER | 3.9 |
| 2 | F | 1077 | VAL | 3.9 |
| 2 | H | 1547 | ILE | 3.9 |
| 2 | F | 1593 | LYS | 3.8 |
| 2 | H | 1268 | GLN | 3.8 |
| 1 | G | 514 | THR | 3.7 |
| 1 | C | 48 | SER | 3.7 |
| 1 | G | 452 | ASN | 3.6 |
| 2 | F | 1166 | THR | 3.6 |
| 2 | F | 925 | LEU | 3.6 |
| 2 | D | 1603 | ASP | 3.6 |
| 1 | C | 376 | GLN | 3.5 |
| 2 | H | 935 | VAL | 3.5 |
| 2 | F | 1169 | ILE | 3.5 |
| 2 | H | 1316 | GLY | 3.5 |
| 1 | G | 645 | ALA | 3.5 |
| 1 | G | 7 | ILE | 3.5 |
| 1 | G | 20 | MET | 3.5 |
| 1 | G | 610 | GLY | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | E | 71 | ASN | 3.5 |
| 3 | I | 366 | LEU | 3.4 |
| 4 | P | 2 | THR | 3.4 |
| 2 | D | 925 | LEU | 3.4 |
| 2 | F | 1038 | ARG | 3.3 |
| 3 | L | 267 | CYS | 3.3 |
| 1 | G | 470 | TYR | 3.3 |
| 2 | B | 1201 | PRO | 3.3 |
| 1 | C | 19 | THR | 3.3 |
| 1 | A | 20 | MET | 3.3 |
| 2 | F | 1329 | LYS | 3.2 |
| 1 | A | 22 | LEU | 3.2 |
| 2 | F | 1143 | LEU | 3.2 |
| 1 | E | 509 | LEU | 3.2 |
| 2 | H | 967 | GLN | 3.2 |
| 2 | H | 921 | ALA | 3.2 |
| 1 | A | 19 | THR | 3.2 |
| 2 | F | 1070 | LEU | 3.1 |
| 1 | G | 72 | ARG | 3.1 |
| 2 | F | 1168 | ALA | 3.1 |
| 1 | G | 471 | LEU | 3.1 |
| 3 | K | 608 | VAL | 3.1 |
| 1 | A | 48 | SER | 3.1 |
| 1 | G | 398 | LEU | 3.1 |
| 2 | H | 1308 | PHE | 3.1 |
| 1 | G | 438 | VAL | 3.0 |
| 3 | K | 479 | PRO | 3.0 |
| 3 | K | 284 | TYR | 3.0 |
| 1 | G | 494 | VAL | 3.0 |
| 1 | G | 453 | PHE | 3.0 |
| 3 | K | 324 | LEU | 3.0 |
| 1 | G | 636 | ALA | 3.0 |
| 2 | F | 1047 | PHE | 3.0 |
| 1 | G | 333 | ILE | 3.0 |
| 1 | E | 636 | ALA | 3.0 |
| 1 | E | 83 | PHE | 3.0 |
| 2 | F | 932 | ARG | 3.0 |
| 2 | H | 1317 | GLN | 2.9 |
| 1 | A | 12 | LEU | 2.9 |
| 2 | F | 1054 | THR | 2.9 |
| 2 | H | 925 | LEU | 2.9 |
| 1 | G | 435 | HIS | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | F | 1121 | LEU | 2.9 |
| 2 | H | 964 | PRO | 2.9 |
| 2 | F | 1082 | VAL | 2.9 |
| 2 | D | 1269 | GLU | 2.8 |
| 2 | F | 1119 | MET | 2.8 |
| 3 | K | 286 | LEU | 2.8 |
| 1 | C | 374 | THR | 2.8 |
| 2 | B | 1606 | VAL | 2.8 |
| 1 | G | 352 | VAL | 2.8 |
| 2 | B | 1205 | LEU | 2.8 |
| 3 | K | 527 | VAL | 2.8 |
| 2 | H | 932 | ARG | 2.8 |
| 1 | G | 507 | PHE | 2.7 |
| 3 | K | 699 | VAL | 2.7 |
| 2 | F | 1198 | TRP | 2.7 |
| 2 | F | 1116 | GLU | 2.7 |
| 2 | F | 1001 | ILE | 2.7 |
| 2 | B | 1574 | LEU | 2.7 |
| 4 | N | 84 | LYS | 2.7 |
| 1 | E | 436 | LEU | 2.7 |
| 1 | G | 99 | VAL | 2.7 |
| 1 | G | 369 | VAL | 2.6 |
| 2 | H | 1328 | ALA | 2.6 |
| 3 | J | 284 | TYR | 2.6 |
| 2 | F | 1147 | ILE | 2.6 |
| 2 | B | 925 | LEU | 2.6 |
| 2 | D | 1332 | ASP | 2.6 |
| 1 | E | 528 | SER | 2.6 |
| 2 | F | 1096 | PHE | 2.6 |
| 1 | G | 200 | PHE | 2.6 |
| 2 | F | 1547 | ILE | 2.6 |
| 1 | C | 290 | GLN | 2.6 |
| 3 | J | 510 | HIS | 2.6 |
| 3 | J | 267 | CYS | 2.6 |
| 2 | D | 1158 | TYR | 2.6 |
| 1 | G | 102 | SER | 2.6 |
| 3 | J | 738 | PHE | 2.6 |
| 2 | B | 1203 | LYS | 2.6 |
| 3 | K | 686 | PHE | 2.5 |
| 2 | F | 1136 | CYS | 2.5 |
| 2 | B | 962 | GLY | 2.5 |
| 2 | D | 1314 | GLY | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | F | 1073 | ILE | 2.5 |
| 3 | K | 503 | PHE | 2.5 |
| 1 | G | 643 | PRO | 2.5 |
| 2 | F | 1094 | GLY | 2.5 |
| 2 | H | 1323 | VAL | 2.5 |
| 1 | G | 335 | PHE | 2.5 |
| 1 | G | 376 | GLN | 2.5 |
| 1 | E | 68 | ILE | 2.4 |
| 3 | K | 705 | ARG | 2.4 |
| 1 | G | 439 | LEU | 2.4 |
| 2 | B | 912 | GLU | 2.4 |
| 1 | C | 20 | MET | 2.4 |
| 2 | F | 1594 | PRO | 2.4 |
| 2 | H | 1546 | THR | 2.4 |
| 2 | F | 960 | LEU | 2.4 |
| 1 | G | 386 | LYS | 2.4 |
| 3 | K | 528 | VAL | 2.4 |
| 2 | F | 1062 | LYS | 2.4 |
| 2 | D | 1483 | LEU | 2.4 |
| 1 | E | 101 | VAL | 2.4 |
| 3 | K | 544 | ILE | 2.4 |
| 2 | D | 1534 | ASN | 2.4 |
| 2 | H | 1594 | PRO | 2.4 |
| 3 | K | 512 | ILE | 2.4 |
| 3 | K | 398 | LEU | 2.3 |
| 3 | J | 610 | GLU | 2.3 |
| 2 | F | 967 | GLN | 2.3 |
| 2 | H | 920 | VAL | 2.3 |
| 2 | F | 1079 | CYS | 2.3 |
| 2 | F | 1460 | TYR | 2.3 |
| 1 | A | 7 | ILE | 2.3 |
| 2 | F | 1294 | ALA | 2.3 |
| 2 | H | 965 | VAL | 2.3 |
| 3 | J | 471 | GLN | 2.3 |
| 2 | F | 1298 | ARG | 2.3 |
| 1 | G | 346 | MET | 2.3 |
| 2 | F | 836 | GLN | 2.3 |
| 2 | F | 1123 | ALA | 2.3 |
| 3 | K | 514 | VAL | 2.3 |
| 2 | B | 1464 | GLU | 2.3 |
| 3 | K | 668 | ASN | 2.3 |
| 2 | F | 1295 | SER | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | F | 1194 | ASP | 2.3 |
| 2 | H | 1598 | TYR | 2.2 |
| 1 | G | 635 | ARG | 2.2 |
| 2 | H | 1559 | GLN | 2.2 |
| 2 | H | 924 | THR | 2.2 |
| 1 | G | 526 | ALA | 2.2 |
| 3 | L | 286 | LEU | 2.2 |
| 2 | H | 1320 | LEU | 2.2 |
| 3 | I | 364 | ASP | 2.2 |
| 2 | F | 964 | PRO | 2.2 |
| 1 | A | 509 | LEU | 2.2 |
| 1 | G | 26 | ASP | 2.2 |
| 2 | H | 922 | VAL | 2.2 |
| 4 | Q | 85 | TYR | 2.2 |
| 3 | L | 693 | SER | 2.2 |
| 3 | J | 573 | PRO | 2.2 |
| 3 | K | 496 | VAL | 2.2 |
| 3 | L | 503 | PHE | 2.2 |
| 1 | A | 479 | LEU | 2.2 |
| 2 | B | 1391 | PRO | 2.2 |
| 2 | H | 1562 | PHE | 2.2 |
| 4 | N | 12 | ASN | 2.2 |
| 4 | M | 84 | LYS | 2.1 |
| 1 | C | 190 | ASN | 2.1 |
| 2 | F | 1056 | LEU | 2.1 |
| 2 | H | 1310 | VAL | 2.1 |
| 3 | I | 267 | CYS | 2.1 |
| 1 | A | 101 | VAL | 2.1 |
| 1 | E | 350 | LEU | 2.1 |
| 1 | G | 450 | ASN | 2.1 |
| 1 | E | 609 | SER | 2.1 |
| 1 | G | 340 | LYS | 2.1 |
| 2 | F | 1208 | VAL | 2.1 |
| 2 | H | 958 | ILE | 2.1 |
| 2 | F | 1596 | LEU | 2.1 |
| 1 | G | 19 | THR | 2.1 |
| 3 | J | 237 | VAL | 2.1 |
| 1 | G | 492 | LEU | 2.1 |
| 3 | K | 607 | PHE | 2.1 |
| 1 | G | 9 | PRO | 2.1 |
| 3 | K | 574 | CYS | 2.1 |
| 2 | F | 1135 | ILE | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 956 | THR | 2.0 |
| 2 | F | 1046 | ALA | 2.0 |
| 4 | P | 85 | TYR | 2.0 |
| 3 | J | 699 | VAL | 2.0 |
| 1 | E | 257 | GLU | 2.0 |
| 3 | I | 503 | PHE | 2.0 |
| 2 | D | 1606 | VAL | 2.0 |
| 1 | G | 370 | GLN | 2.0 |
| 2 | B | 1493 | GLU | 2.0 |
| 2 | H | 1499 | GLN | 2.0 |
| 1 | C | 368 | ALA | 2.0 |
| 1 | G | 46 | VAL | 2.0 |
| 3 | K | 248 | LEU | 2.0 |
| 2 | D | 1510 | ARG | 2.0 |
| 1 | E | 84 | VAL | 2.0 |
| 2 | D | 1082 | VAL | 2.0 |
| 2 | D | 1085 | LEU | 2.0 |
| 3 | K | 697 | VAL | 2.0 |
| 1 | A | 548 | SER | 2.0 |
| 2 | F | 1502 | ASP | 2.0 |
| 1 | C | 509 | LEU | 2.0 |
| 1 | G | 434 | LEU | 2.0 |
| 2 | D | 932 | ARG | 2.0 |

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

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

6.3 Carbohydrates [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 5 | BMA | R | 4 | 11/12 | 0.29 | 0.30 | 237,239,240,241 | 0 |
| 5 | BMA | R | 3 | 11/12 | 0.56 | 0.23 | 218,220,222,223 | 0 |
| 6 | BMA | S | 4 | 11/12 | 0.58 | 0.21 | 235,237,239,240 | 0 |
| 6 | BMA | W | 5 | 11/12 | 0.62 | 0.41 | 229,231,232,232 | 0 |
| 7 | BMA | V | 6 | 11/12 | 0.66 | 0.39 | 214,215,217,217 | 0 |

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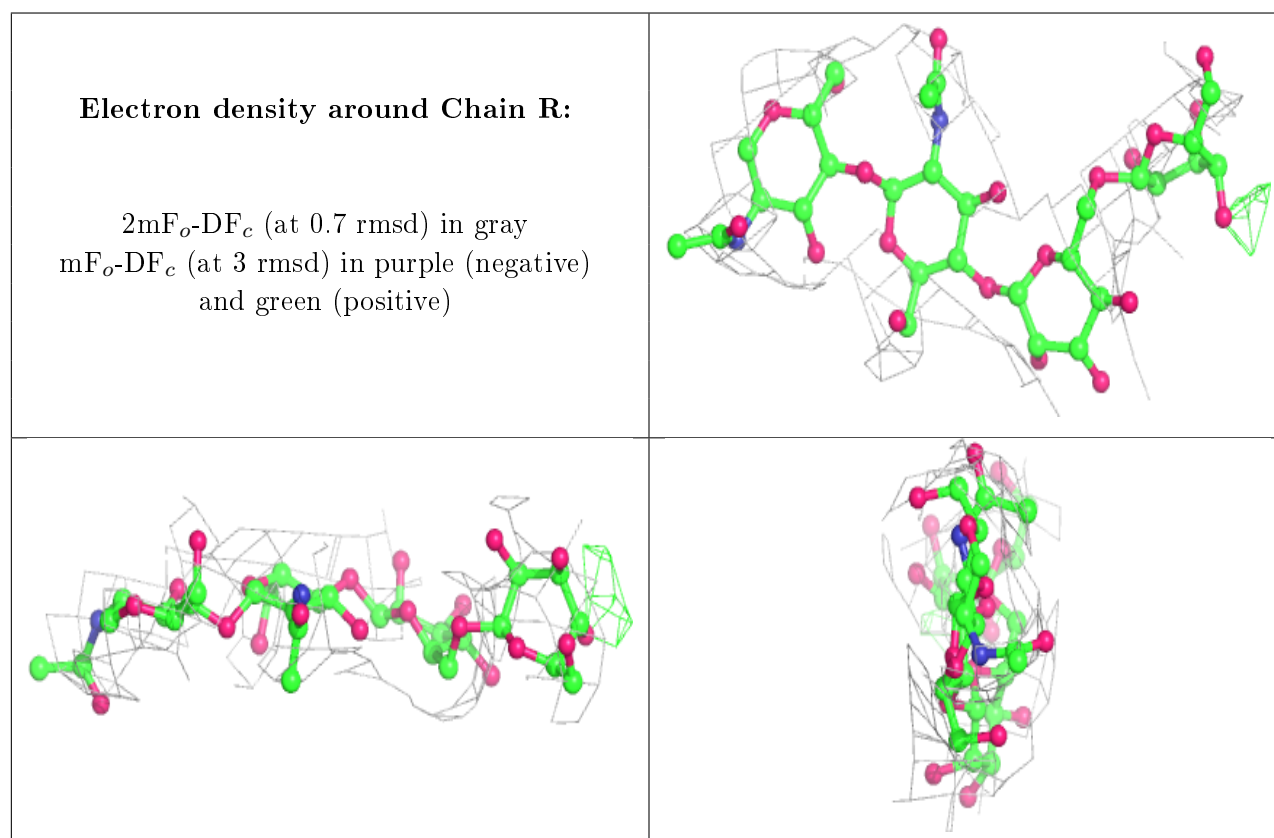
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8 | MAN | X | 4 | 11/12 | 0.67 | 0.37 | 234,236,237,238 | 0 |
| 10 | NAG | Z | 2 | 14/15 | 0.70 | 0.37 | 222,223,224,224 | 0 |
| 6 | BMA | S | 3 | 11/12 | 0.72 | 0.19 | 219,220,222,223 | 0 |
| 9 | MAN | Y | 3 | 11/12 | 0.73 | 0.28 | 205,207,208,209 | 0 |
| 9 | MAN | a | 3 | 11/12 | 0.73 | 0.21 | 206,210,211,212 | 0 |
| 6 | BMA | W | 3 | 11/12 | 0.74 | 0.32 | 247,249,250,251 | 0 |
| 11 | MAN | b | 3 | 11/12 | 0.75 | 0.16 | 249,252,253,254 | 0 |
| 7 | BMA | V | 4 | 11/12 | 0.75 | 0.17 | 248,249,249,250 | 0 |
| 12 | BMA | c | 3 | 11/12 | 0.75 | 0.21 | 197,201,202,202 | 0 |
| 7 | BMA | V | 5 | 11/12 | 0.76 | 0.23 | 221,222,224,224 | 0 |
| 6 | BMA | W | 4 | 11/12 | 0.76 | 0.18 | 226,228,229,230 | 0 |
| 6 | BMA | S | 5 | 11/12 | 0.76 | 0.23 | 231,233,235,235 | 0 |
| 5 | BMA | T | 3 | 11/12 | 0.77 | 0.19 | 220,221,223,223 | 0 |
| 6 | NAG | S | 1 | 14/15 | 0.79 | 0.28 | 163,191,192,193 | 0 |
| 6 | NAG | S | 2 | 14/15 | 0.80 | 0.21 | 200,202,203,203 | 0 |
| 5 | BMA | U | 4 | 11/12 | 0.81 | 0.17 | 209,212,214,215 | 0 |
| 10 | NAG | Z | 1 | 14/15 | 0.81 | 0.33 | 198,225,227,227 | 0 |
| 7 | BMA | V | 3 | 11/12 | 0.83 | 0.18 | 232,233,234,234 | 0 |
| 11 | MAN | b | 4 | 11/12 | 0.84 | 0.22 | 230,232,235,235 | 0 |
| 5 | BMA | O | 3 | 11/12 | 0.84 | 0.17 | 212,214,215,216 | 0 |
| 5 | NAG | O | 2 | 14/15 | 0.84 | 0.19 | 199,200,201,203 | 0 |
| 8 | MAN | X | 3 | 11/12 | 0.84 | 0.19 | 229,230,231,232 | 0 |
| 5 | NAG | U | 1 | 14/15 | 0.84 | 0.17 | 174,204,206,206 | 0 |
| 6 | NAG | W | 1 | 14/15 | 0.84 | 0.14 | 198,201,208,215 | 0 |
| 11 | NAG | b | 2 | 14/15 | 0.85 | 0.16 | 196,199,201,202 | 0 |
| 9 | NAG | a | 2 | 14/15 | 0.85 | 0.18 | 177,179,180,180 | 0 |
| 11 | MAN | b | 5 | 11/12 | 0.85 | 0.25 | 229,230,232,232 | 0 |
| 5 | BMA | T | 4 | 11/12 | 0.85 | 0.13 | 229,232,233,234 | 0 |
| 11 | NAG | b | 1 | 14/15 | 0.85 | 0.19 | 174,204,206,207 | 0 |
| 8 | NAG | X | 2 | 14/15 | 0.86 | 0.17 | 221,222,224,225 | 0 |
| 5 | NAG | O | 1 | 14/15 | 0.86 | 0.24 | 156,185,187,188 | 0 |
| 5 | BMA | U | 3 | 11/12 | 0.86 | 0.19 | 229,230,231,232 | 0 |
| 12 | NAG | c | 2 | 14/15 | 0.86 | 0.26 | 185,187,189,189 | 0 |
| 5 | BMA | O | 4 | 11/12 | 0.87 | 0.24 | 226,227,228,228 | 0 |
| 7 | NAG | V | 1 | 14/15 | 0.87 | 0.24 | 169,193,194,194 | 0 |
| 5 | NAG | R | 1 | 14/15 | 0.88 | 0.23 | 163,194,194,195 | 0 |
| 12 | NAG | c | 1 | 14/15 | 0.89 | 0.27 | 122,147,148,148 | 0 |
| 5 | NAG | T | 1 | 14/15 | 0.89 | 0.23 | 147,176,178,179 | 0 |
| 9 | NAG | a | 1 | 14/15 | 0.89 | 0.21 | 158,188,189,189 | 0 |
| 5 | NAG | U | 2 | 14/15 | 0.89 | 0.17 | 223,225,227,227 | 0 |
| 7 | NAG | V | 2 | 14/15 | 0.90 | 0.14 | 200,202,204,204 | 0 |
| 6 | NAG | W | 2 | 14/15 | 0.90 | 0.12 | 213,216,216,217 | 0 |

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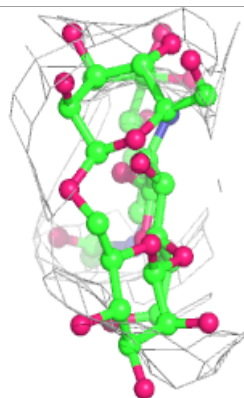
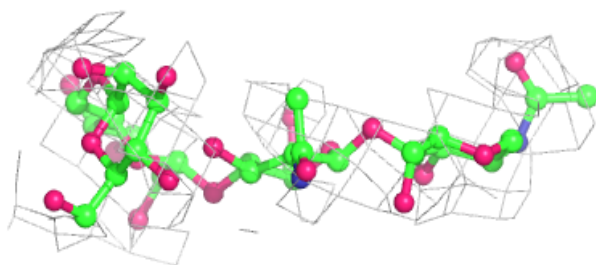
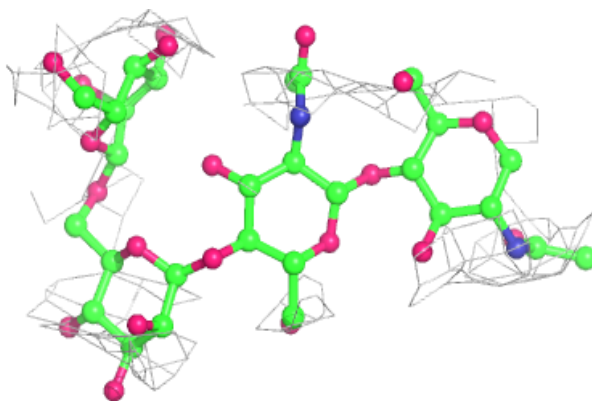
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5 | NAG | T | 2 | 14/15 | 0.91 | 0.17 | 200,201,202,203 | 0 |
| 5 | NAG | R | 2 | 14/15 | 0.91 | 0.14 | 193,196,196,197 | 0 |
| 8 | NAG | X | 1 | 14/15 | 0.92 | 0.17 | 183,213,214,215 | 0 |
| 9 | NAG | Y | 2 | 14/15 | 0.93 | 0.21 | 178,180,181,182 | 0 |
| 9 | NAG | Y | 1 | 14/15 | 0.93 | 0.26 | 122,149,151,152 | 0 |

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

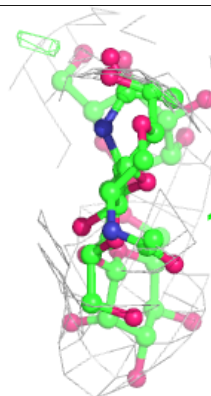
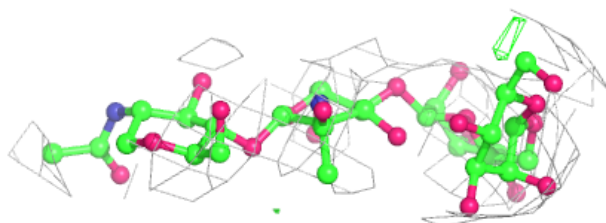
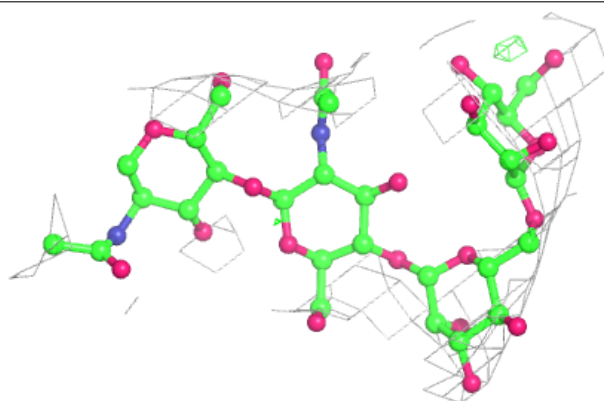


Electron density around Chain T:

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

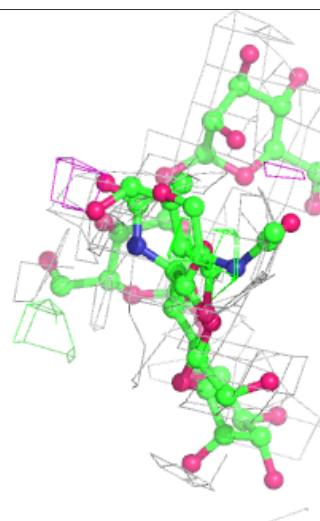
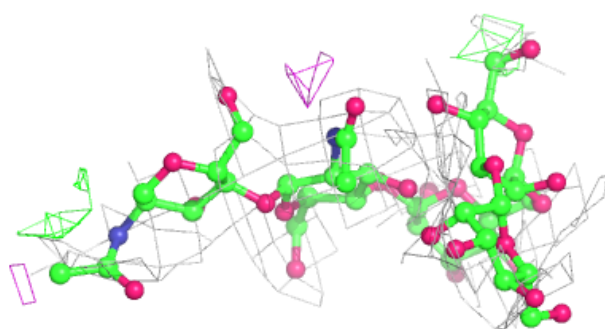
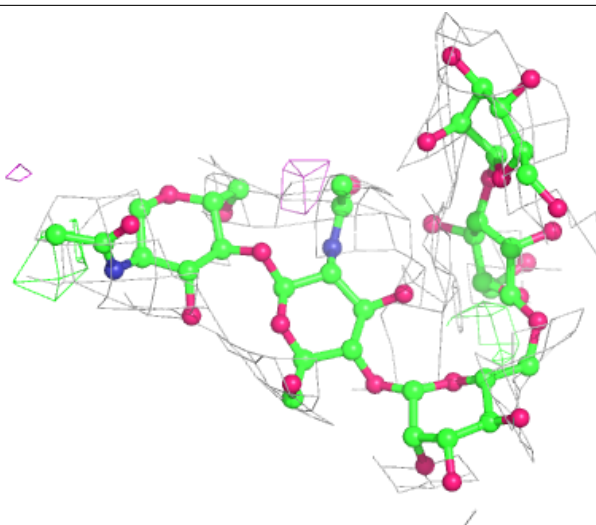
**Electron density around Chain U:**

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



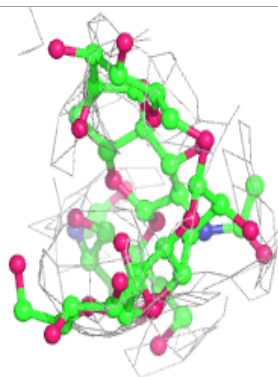
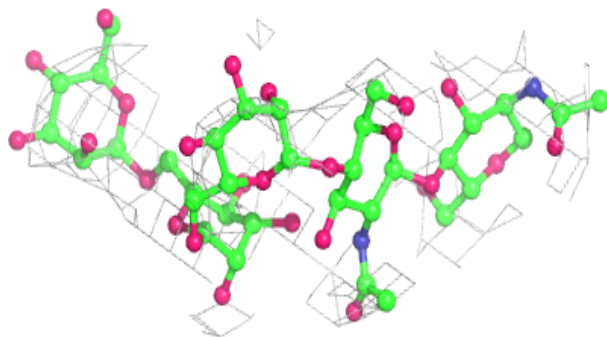
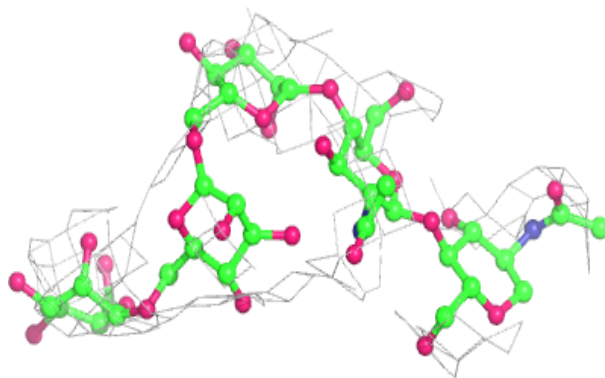
Electron density around Chain S:

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



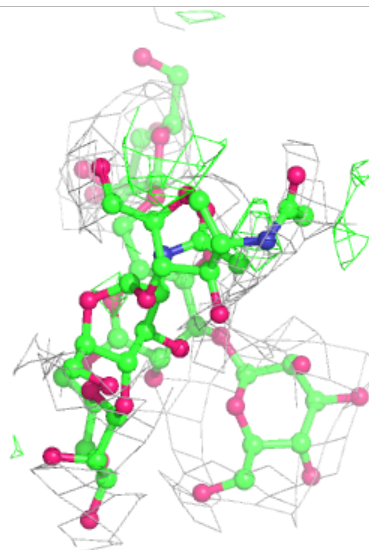
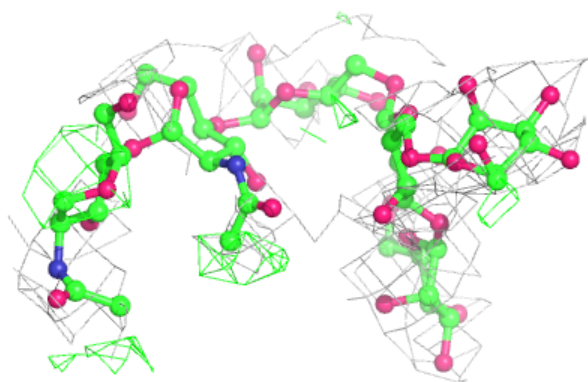
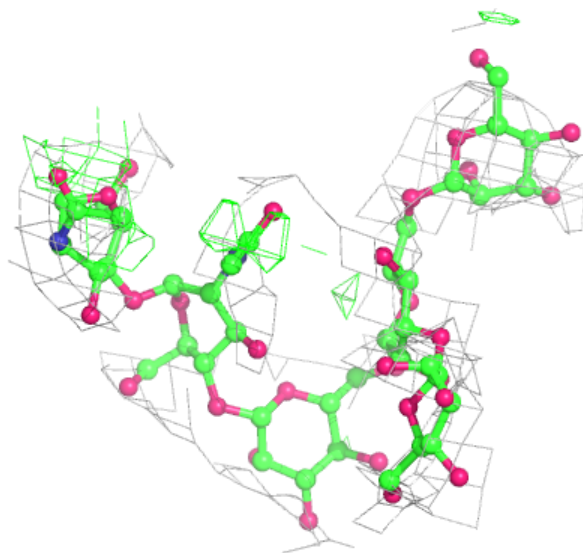
Electron density around Chain W:

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



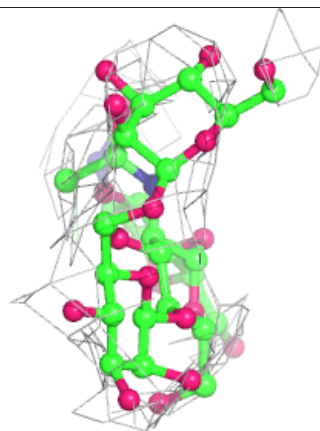
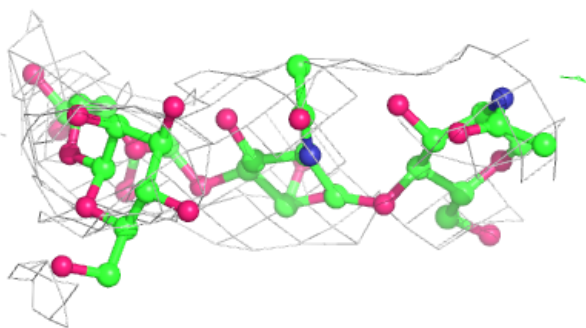
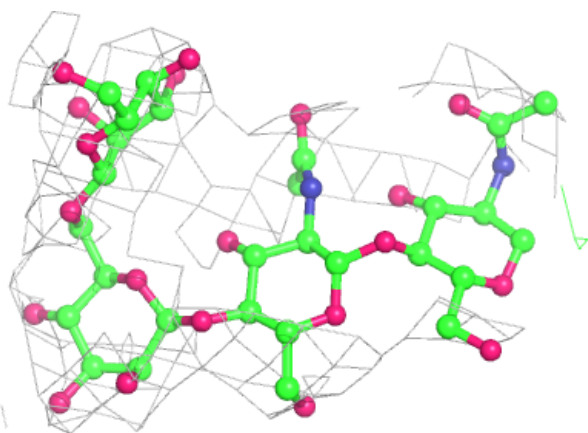
Electron density around Chain V:

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

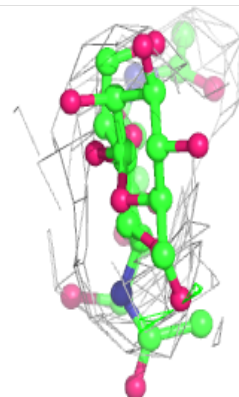
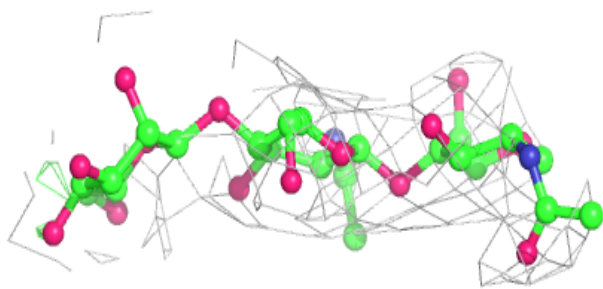
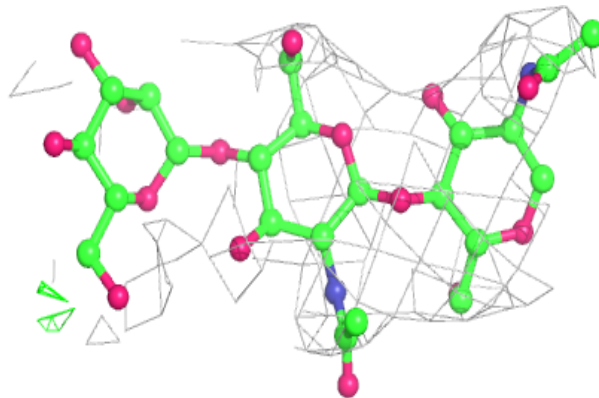


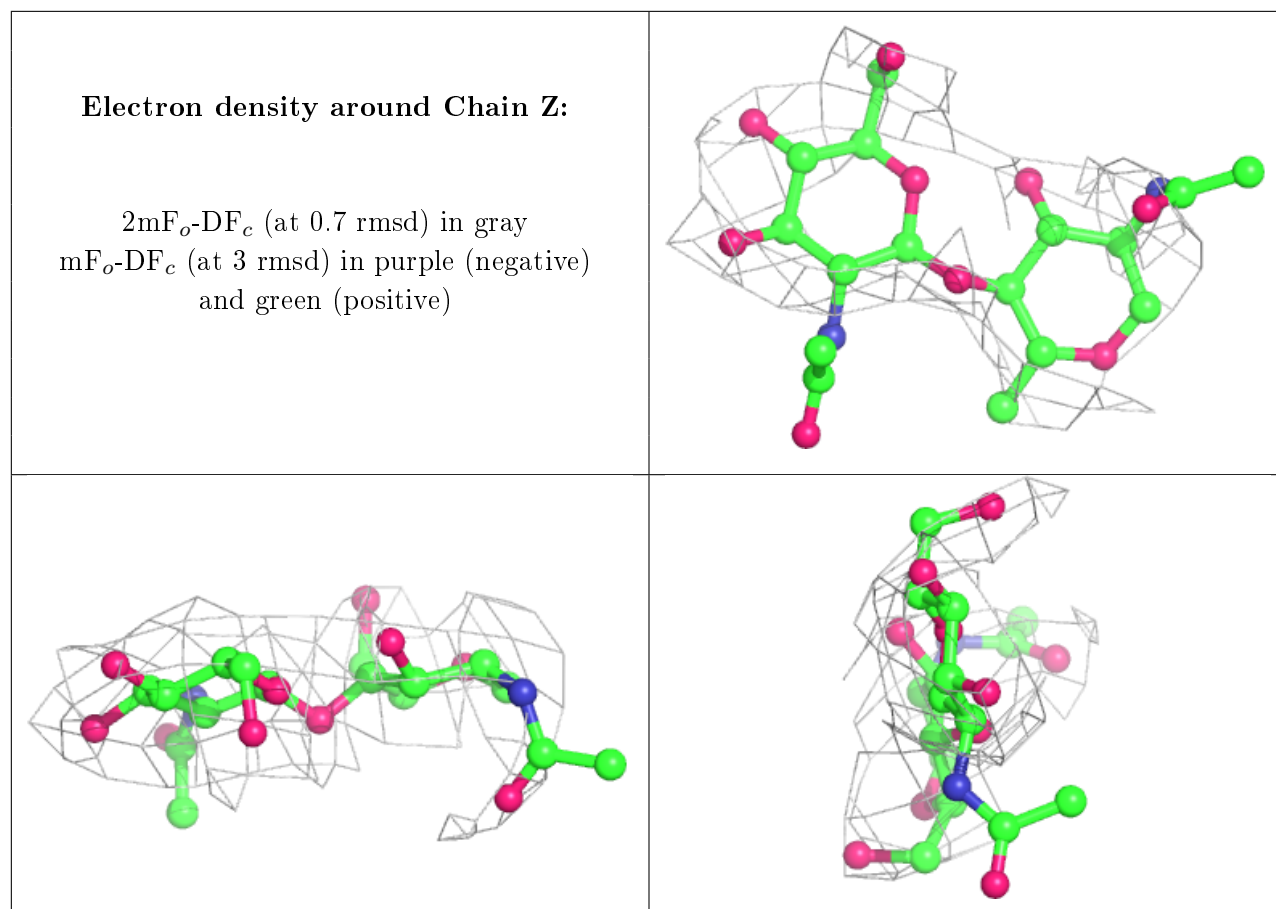
Electron density around Chain X:

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

**Electron density around Chain Y:**

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





6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 14 | MAN | G | 1651 | 11/12 | 0.55 | 0.25 | 222,225,227,228 | 0 |
| 13 | BMA | B | 2646 | 11/12 | 0.65 | 0.29 | 198,200,200,201 | 0 |
| 15 | MG | I | 1742 | 1/1 | 0.71 | 0.20 | 120,120,120,120 | 0 |
| 16 | NAG | K | 1749 | 14/15 | 0.78 | 0.24 | 184,214,216,217 | 0 |
| 13 | BMA | K | 1747 | 11/12 | 0.79 | 0.35 | 194,195,196,196 | 0 |
| 15 | MG | J | 1742 | 1/1 | 0.80 | 0.14 | 148,148,148,148 | 0 |
| 15 | MG | K | 1742 | 1/1 | 0.87 | 0.14 | 138,138,138,138 | 0 |
| 16 | NAG | L | 1746 | 14/15 | 0.88 | 0.26 | 176,204,205,205 | 0 |
| 15 | MG | L | 1742 | 1/1 | 0.93 | 0.24 | 127,127,127,127 | 0 |

6.5 Other polymers

There are no such residues in this entry.